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Supplementary material for

DFT study of the spin state energetics of polypyrazolylborato complexes of some first-row transition metals

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Table S1. Average bond length (Å) of $[M^x(Tp)_2]^q$ complexes.

M^{n+}	Spin state	State	LDA	OPBE	EXP. Bond lenght	exp. spin state
Cr^{3+}	HS	$^4A_{2g}$	2.05	2.15	-	HS
	LS	$^2A_{2g}$	1.96	2.04		
Mn^{4+}	HS	$^4A_{2g}$	1.93	1.98	1.97	HS
	LS	^2E_g	1.92	1.96		
Mn^{3+}	HS	^5E_g	2.04	2.11	1.99	IS
	IS	$^3A_{2g}$	1.94	1.99		
	LS	^1E_g	1.93	1.98		
Mn^{2+}	HS	$^6A_{1g}$	2.18	2.29	2.26	HS
	IS	^4E_g	2.04	2.15		
	LS	^2E_g	1.94	2.00		
Fe^{3+}	HS	$^6A_{1g}$	2.07	2.13	1.95	LS
	IS	^4E_g	1.98	2.05		
	LS	^2E_g	1.90	1.95		
Fe^{2+}	HS	$^5A_{1g}$	2.10	2.21	1.97	LS
	IS	^3E_g	1.99	2.08		
	LS	$^1A_{1g}$	1.90	1.96		
Co^{3+}	HS	$^5A_{1g}$	2.02	2.09	1.93	LS
	IS	^3E_g	1.95	2.02		
	LS	$^1A_{1g}$	1.88	1.93		
Co^{2+}	HS	^4E_g	2.05	2.15	2.13	HS
	LS	^2E_g	1.96	2.04		

Table S2. Spin state energies (kcal mol^{-1}) relative to the high spin electronic state, at OPBE level of theory, for substituted $[M^{x}(Tp^{4\text{-}R})_2]^{q}$ complexes.[1]

					OPBE		
M^{n+}	d^n	Symm.	Spin state	Electronic state	$H(Bz)_3$	4-NH2	4-NO2
Cr^{3+}	d^3	D_{3d}	HS	$^4A_{2g}$	0	0	0
			LS	$^2A_{2g}$	43.57	28.75	30.21
Mn^{4+}	d^3	D_{3d}	HS	$^4A_{2g}$	0	0	0
			LS	^2E_g	21.03	3.2	7.5
Mn^{3+}	d^4	D_{3d}	HS	^5E_g	0	0	0
			IS	$^3A_{2g}$	-5.75	-6.7	-3.44
			LS	^1E_g	20.01	13.69	22.48
Mn^{2+}	d^5	D_{3d}	HS	$^6A_{1g}$	0	0	0
			IS	^4E_g	41.3	40.92	41.03
			LS	^2E_g	29.93	29.41	29.08
Fe^{3+}	d^5	D_{3d}	HS	$^6A_{1g}$	0	0	0
			IS	^4E_g	23.43	12.62	8.93
			LS	^2E_g	-6.82	-4.24	-6.23
Fe^{2+}	d^6	D_{3d}	HS	$^5A_{1g}$	0	0	0
			IS	^3E_g	35.47	23.85	23.31
			LS	$^1A_{1g}$	-5.78	-4.99	-6.8
Co^{3+}	d^6	D_{3d}	HS	$^5A_{1g}$	0	0	0
			IS	^3E_g	1.01	6.31	-0.22
			LS	$^1A_{1g}$	-31.96	-16.68	-32.2
Co^{2+}	d^7	D_{3d}	HS	^4E_g	0	0	0
			LS	^2E_g	2	1.13	1.44

[1] JT active systems were calculated with equally populated Eg orbitals in D3d symmetry.

Table S3. Calculations of energy gap between two sets of e_g orbitals, calculated at OPBE level of theory, energies are given in kcal/mol.

	Co^{2+}			Co^{3+}			Fe^{2+}			Fe^{3+}			Mn^{2+}		
	$[Co(Tp)_2]$	**5-NH2**	**5-NO2**	**$[Co(Tp)_2]^+$**	**5-NH2**	**5-NO2**	**$[Fe(Tp)_2]$**	**5-NH2**	**5-NO2**	**$[Fe(Tp)_2]^+$**	**5-NH2**	**5-NO2**	**$[Mn(Tp)_2]$**	**5-NH2**	**5-NO2**
$e_g(d_{yz};d_{xz})$	-2.788	-1.837	-4.462	-6.787	-5.427	-7.581	-2.428	-1.504	-4.138	-6.523	-5.14	-7.508	-2.157	-1.327	-3.906
$e_g(d_{x^2-y^2};d_{xy})$	-4.403	-3.245	-6.35	-8.466	-6.696	-9.615	-3.93	-2.899	-5.903	-8.214	-6.502	-9.747	-3.51	-2.596	-5.506
$a_{1g}(d_{z^2})$	-4.725	-3.729	-6.652	-9.413	-7.893	-9.871	-4.168	-3.259	-6.09	-8.926	-7.422	-9.782	-3.641	-2.825	-5.558
Energy gap	1.62	1.41	1.89	1.68	1.27	2.03	1.50	1.40	1.77	1.69	1.36	2.24	1.35	1.27	1.60

Table S4. Free energy and solvation contributions to the ΔE_{LH} ($=E_{low\text{-}spin} - E_{high\text{-}spin}$) for $[Co^{II}(Tb)_2]$ in C_{2h} symmetry. Energies are calculated at OPBE level of theory, and are given in kcal/mol.

Electronic state	^2Ag	^2Bg	^4Ag	^4Bg	
E_{cosmo}[2]	**-8220.25**	-8217.69	-8219.82	**-8220.07**	-0.18
G	**-7992.50**	-7989.14	-7993.58	**-7993.93**	1.43

[2] Dichloroethane

Coordinates of metal complexes

$[Cr(Tb)_2]^+$ $^4A_{2g}$ D_{3d} LDA

Cr	0.00000000	0.00000000	0.00000000
N	1.38083458	-0.79722510	-1.19694284
N	1.22909671	-0.70961928	-2.53262220
N	0.00000000	1.59445021	-1.19694284
N	0.00000000	1.41923909	-2.53262220
N	-1.38083458	-0.79722510	-1.19694284
N	-1.22909671	-0.70961928	-2.53262220
C	2.52052256	-1.45522420	-0.96210509
C	3.11570145	-1.79885127	-2.16912241
C	2.26232746	-1.30615550	-3.14039603
C	0.00000000	2.91044841	-0.96210509
C	0.00000000	3.59770254	-2.16912241
C	0.00000000	2.61231100	-3.14039603
C	-2.52052256	-1.45522420	-0.96210509
C	-3.11570145	-1.79885127	-2.16912241
C	-2.26232746	-1.30615550	-3.14039603
H	4.04847477	-2.33738808	-2.32002524
H	2.31966329	-1.33925818	-4.22663235
H	0.00000000	4.67477616	-2.32002524
H	0.00000000	3.28295426	0.06165656
H	0.00000000	2.67851637	-4.22663235
H	2.84312172	-1.64147713	0.06165656
H	0.00000000	0.00000000	-4.29077286
H	-4.04847477	-2.33738808	-2.32002524
H	-2.31966329	-1.33925818	-4.22663235
H	-2.84312172	-1.64147713	0.06165656
B	0.00000000	0.00000000	-3.09028453
N	0.00000000	-1.59445021	1.19694284
N	0.00000000	-1.41923909	2.53262220
N	1.38083458	0.79722510	1.19694284
N	1.22909671	0.70961928	2.53262220
N	-1.38083458	0.79722510	1.19694284
N	-1.22909671	0.70961928	2.53262220
C	0.00000000	-2.91044841	0.96210509
C	0.00000000	-3.59770254	2.16912241
C	0.00000000	-2.61231100	3.14039603
C	2.52052256	1.45522420	0.96210509
C	3.11570145	1.79885127	2.16912241
C	2.26232746	1.30615550	3.14039603
C	-2.52052256	1.45522420	0.96210509
C	-3.11570145	1.79885127	2.16912241
C	-2.26232746	1.30615550	3.14039603
H	0.00000000	-4.67477616	2.32002524
H	0.00000000	-2.67851637	4.22663235
H	4.04847477	2.33738808	2.32002524
H	2.84312172	1.64147713	-0.06165656
H	2.31966329	1.33925818	4.22663235
H	0.00000000	-3.28295426	-0.06165656
H	0.00000000	0.00000000	4.29077286
H	-4.04847477	2.33738808	2.32002524
H	-2.31966329	1.33925818	4.22663235
H	-2.84312172	1.64147713	-0.06165656
B	0.00000000	0.00000000	3.09028453

$[Cr(Tb)_2]^+$ $^4A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	1.41369861	-0.81619928	-1.24790526
N	1.24408513	-0.71827292	-2.58188543
N	0.00000000	1.63239857	-1.24790526
N	0.00000000	1.43654531	-2.58188543
N	-1.41369861	-0.81619928	-1.24790526
N	-1.24408513	-0.71827292	-2.58188543
C	2.56164916	-1.47896892	-1.03796583
C	3.14375525	-1.81504833	-2.25893067
C	2.27180926	-1.31162931	-3.21366115
C	0.00000000	2.95793730	-1.03796583
C	0.00000000	3.63009613	-2.25893067
C	0.00000000	2.62325915	-3.21366115
C	-2.56164916	-1.47896892	-1.03796583
C	-3.14375525	-1.81504833	-2.25893067
C	-2.27180926	-1.31162931	-3.21366115
H	4.07061661	-2.35017194	-2.42660524
H	2.31272683	-1.33525337	-4.29562859
H	0.00000000	4.70034335	-2.42660524
H	0.00000000	3.35378834	-0.03087220
H	0.00000000	2.67050727	-4.29562859
H	2.90446606	-1.67689391	-0.03087220
H	0.00000000	0.00000000	-4.33610219
H	-4.07061661	-2.35017194	-2.42660524
H	-2.31272683	-1.33525337	-4.29562859
H	-2.90446606	-1.67689391	-0.03087220
B	0.00000000	0.00000000	-3.13747021
N	0.00000000	-1.63239857	1.24790526
N	0.00000000	-1.43654531	2.58188543
N	1.41369861	0.81619928	1.24790526
N	1.24408513	0.71827292	2.58188543
N	-1.41369861	0.81619928	1.24790526
N	-1.24408513	0.71827292	2.58188543
C	0.00000000	-2.95793730	1.03796583
C	0.00000000	-3.63009613	2.25893067
C	0.00000000	-2.62325915	3.21366115
C	2.56164916	1.47896892	1.03796583
C	3.14375525	1.81504833	2.25893067
C	2.27180926	1.31162931	3.21366115
C	-2.56164916	1.47896892	1.03796583
C	-3.14375525	1.81504833	2.25893067
C	-2.27180926	1.31162931	3.21366115
H	0.00000000	-4.70034335	2.42660524
H	0.00000000	-2.67050727	4.29562859
H	4.07061661	2.35017194	2.42660524
H	2.90446606	1.67689391	0.03087220
H	2.31272683	1.33525337	4.29562859
H	0.00000000	-3.35378834	0.03087220
H	0.00000000	0.00000000	4.33610219
H	-4.07061661	2.35017194	2.42660524
H	-2.31272683	1.33525337	4.29562859
H	-2.90446606	1.67689391	0.03087220
B	0.00000000	0.00000000	3.13747021

$[Cr(Tb)_2]^+$ $^2A_{2g}$ D_{3d} LDA

Cr	0.00000000	0.00000000	0.00000000
N	1.37526499	-0.79400929	-1.18692763
N	1.22827119	-0.70914249	-2.52442683
N	0.00000000	1.58801912	-1.18692763

N	0.00000000	1.41828499	-2.52442683
N	-1.37526499	-0.79400929	-1.18692763
N	-1.22827119	-0.70914249	-2.52442683
C	2.51542659	-1.45228251	-0.94834225
C	3.11385144	-1.79778286	-2.15265124
C	2.26319849	-1.30665822	-3.12786511
C	0.00000000	2.90456449	-0.94834225
C	0.00000000	3.59556625	-2.15265124
C	0.00000000	2.61331644	-3.12786511
C	-2.51542659	-1.45228251	-0.94834225
C	-3.11385144	-1.79778286	-2.15265124
C	-2.26319849	-1.30665822	-3.12786511
H	4.04707034	-2.33657685	-2.29999906
H	2.32413430	-1.34183951	-4.21386436
H	0.00000000	4.67315423	-2.29999906
H	0.00000000	3.27338992	0.07668149
H	0.00000000	2.68367955	-4.21386436
H	2.83483850	-1.63669496	0.07668149
H	0.00000000	0.00000000	-4.28432113
H	-4.04707034	-2.33657685	-2.29999906
H	-2.32413430	-1.34183951	-4.21386436
H	-2.83483850	-1.63669496	0.07668149
B	0.00000000	0.00000000	-3.08374919
N	0.00000000	-1.58801912	1.18692763
N	0.00000000	-1.41828499	2.52442683
N	1.37526499	0.79400929	1.18692763
N	1.22827119	0.70914249	2.52442683
N	-1.37526499	0.79400929	1.18692763
N	-1.22827119	0.70914249	2.52442683
C	0.00000000	-2.90456449	0.94834225
C	0.00000000	-3.59556625	2.15265124
C	0.00000000	-2.61331644	3.12786511
C	2.51542659	1.45228251	0.94834225
C	3.11385144	1.79778286	2.15265124
C	2.26319849	1.30665822	3.12786511
C	-2.51542659	1.45228251	0.94834225
C	-3.11385144	1.79778286	2.15265124
C	-2.26319849	1.30665822	3.12786511
H	0.00000000	-4.67315423	2.29999906
H	0.00000000	-2.68367955	4.21386436
H	4.04707034	2.33657685	2.29999906
H	2.83483850	1.63669496	-0.07668149
H	2.32413430	1.34183951	4.21386436
H	0.00000000	-3.27338992	-0.07668149
H	0.00000000	0.00000000	4.28432113
H	-4.04707034	2.33657685	2.29999906
H	-2.32413430	1.34183951	4.21386436
H	-2.83483850	1.63669496	-0.07668149
B	0.00000000	0.00000000	3.08374919

$[Cr(Tb)_2]^{+}$ $^2A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	-1.39980000	-0.80820000	-1.21320000
N	-1.24250000	-0.71740000	-2.55200000
N	1.39980000	-0.80820000	-1.21320000
N	1.24250000	-0.71740000	-2.55200000
N	0.00000000	1.61630000	-1.21320000
N	0.00000000	1.43480000	-2.55200000
C	-2.55180000	-1.47330000	-1.00020000
C	-3.14040000	-1.81310000	-2.21320000
C	-2.27070000	-1.31100000	-3.17630000
C	2.55180000	-1.47330000	-1.00020000
C	3.14040000	-1.81310000	-2.21320000
C	2.27070000	-1.31100000	-3.17630000
C	0.00000000	2.94660000	-1.00020000
C	0.00000000	3.62620000	-2.21320000
C	0.00000000	2.62190000	-3.17630000
H	-4.06790000	-2.34860000	-2.37730000
H	-2.31940000	-1.33910000	-4.25800000
H	4.06790000	-2.34860000	-2.37730000
H	2.88970000	-1.66840000	0.00900000
H	2.31940000	-1.33910000	-4.25800000
H	-2.88970000	-1.66840000	0.00900000
H	0.00000000	0.00000000	-4.30590000
H	0.00000000	4.69720000	-2.37730000
H	0.00000000	2.67820000	-4.25800000
H	0.00000000	3.33680000	0.00900000
B	0.00000000	0.00000000	-3.10610000
N	-1.39980000	0.80820000	1.21320000
N	-1.24250000	0.71740000	2.55200000
N	0.00000000	-1.61630000	1.21320000
N	0.00000000	-1.43480000	2.55200000
N	1.39980000	0.80820000	1.21320000
N	1.24250000	0.71740000	2.55200000
C	-2.55180000	1.47330000	1.00020000
C	-3.14040000	1.81310000	2.21320000
C	-2.27070000	1.31100000	3.17630000
C	0.00000000	-2.94660000	1.00020000
C	0.00000000	-3.62620000	2.21320000
C	0.00000000	-2.62190000	3.17630000
C	2.55180000	1.47330000	1.00020000
C	3.14040000	1.81310000	2.21320000
C	2.27070000	1.31100000	3.17630000
H	-4.06790000	2.34860000	2.37730000
H	-2.31940000	1.33910000	4.25800000
H	0.00000000	-4.69720000	2.37730000
H	0.00000000	-3.33680000	-0.00900000
H	0.00000000	-2.67820000	4.25800000
H	-2.88970000	1.66840000	-0.00900000
H	0.00000000	0.00000000	4.30590000
H	4.06790000	2.34860000	2.37730000
H	2.31940000	1.33910000	4.25800000
H	2.88970000	1.66840000	-0.00900000
B	0.00000000	0.00000000	3.10610000

$[Mn(Tb)_2]^{2+}$ $^4A_{2g}$ D_{3d} LDA

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.56150000	1.14020000
N	0.00000000	1.41230000	2.48230000
N	1.35230000	-0.78080000	1.14020000
N	1.22310000	-0.70620000	2.48230000
N	-1.35230000	-0.78080000	1.14020000
N	-1.22310000	-0.70620000	2.48230000
C	0.00000000	2.87620000	0.86670000
C	0.00000000	3.58400000	2.05460000
C	0.00000000	2.61970000	3.05430000
C	2.49090000	-1.43810000	0.86670000
C	3.10390000	-1.79200000	2.05460000

C	2.26880000	-1.30990000	3.05430000
C	-2.49090000	-1.43810000	0.86670000
C	-3.10390000	-1.79200000	2.05460000
C	-2.26880000	-1.30990000	3.05430000
H	0.00000000	4.66530000	2.18070000
H	0.00000000	2.71880000	4.13930000
H	4.04030000	-2.33270000	2.18070000
H	2.79710000	-1.61490000	-0.16390000
H	2.35460000	-1.35940000	4.13930000
H	0.00000000	3.22980000	-0.16390000
H	0.00000000	0.00000000	4.25500000
H	-4.04030000	-2.33270000	2.18070000
H	-2.35460000	-1.35940000	4.13930000
H	-2.79710000	-1.61490000	-0.16390000
B	0.00000000	0.00000000	3.05880000
N	-1.35230000	0.78080000	-1.14020000
N	-1.22310000	0.70620000	-2.48230000
N	1.35230000	0.78080000	-1.14020000
N	1.22310000	0.70620000	-2.48230000
N	0.00000000	-1.56150000	-1.14020000
N	0.00000000	-1.41230000	-2.48230000
C	-2.49090000	1.43810000	-0.86670000
C	-3.10390000	1.79200000	-2.05460000
C	-2.26880000	1.30990000	-3.05430000
C	2.49090000	1.43810000	-0.86670000
C	3.10390000	1.79200000	-2.05460000
C	2.26880000	1.30990000	-3.05430000
C	0.00000000	-2.87620000	-0.86670000
C	0.00000000	-3.58400000	-2.05460000
C	0.00000000	-2.61970000	-3.05430000
H	-4.04030000	2.33270000	-2.18070000
H	-2.35460000	1.35940000	-4.13930000
H	4.04030000	2.33270000	-2.18070000
H	2.79710000	1.61490000	0.16390000
H	2.35460000	1.35940000	-4.13930000
H	-2.79710000	1.61490000	0.16390000
H	0.00000000	0.00000000	-4.25500000
H	0.00000000	-4.66530000	-2.18070000
H	0.00000000	-2.71880000	-4.13930000
H	0.00000000	-3.22980000	0.16390000
B	0.00000000	0.00000000	-3.05880000

$[Mn(Tb)_2]^{2+}$ $^4A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.38230000	0.79810000	1.17480000
N	-1.23620000	0.71370000	2.51510000
N	1.38230000	0.79810000	1.17480000
N	1.23620000	0.71370000	2.51510000
N	0.00000000	-1.59610000	1.17480000
N	0.00000000	-1.42740000	2.51510000
C	-2.53030000	1.46090000	0.92400000
C	-3.13030000	1.80730000	2.12600000
C	-2.27720000	1.31480000	3.11020000
C	2.53030000	1.46090000	0.92400000
C	3.13030000	1.80730000	2.12600000
C	2.27720000	1.31480000	3.11020000
C	0.00000000	-2.92170000	0.92400000
C	0.00000000	-3.61460000	2.12600000
C	0.00000000	-2.62950000	3.11020000
H	-4.06100000	2.34460000	2.26730000
H	-2.34590000	1.35440000	4.19110000
H	4.06100000	2.34460000	2.26730000
H	2.85530000	1.64850000	-0.09040000
H	2.34590000	1.35440000	4.19110000
H	-2.85530000	1.64850000	-0.09040000
H	0.00000000	0.00000000	4.28600000
H	0.00000000	-4.68920000	2.26730000
H	0.00000000	-2.70880000	4.19110000
H	0.00000000	-3.29700000	-0.09040000
B	0.00000000	0.00000000	3.09190000
N	-1.38230000	-0.79810000	-1.17480000
N	-1.23620000	-0.71370000	-2.51510000
N	0.00000000	1.59610000	-1.17480000
N	0.00000000	1.42740000	-2.51510000
N	1.38230000	-0.79810000	-1.17480000
N	1.23620000	-0.71370000	-2.51510000
C	-2.53030000	-1.46090000	-0.92400000
C	-3.13030000	-1.80730000	-2.12600000
C	-2.27720000	-1.31480000	-3.11020000
C	0.00000000	2.92170000	-0.92400000
C	0.00000000	3.61460000	-2.12600000
C	0.00000000	2.62950000	-3.11020000
C	2.53030000	-1.46090000	-0.92400000
C	3.13030000	-1.80730000	-2.12600000
C	2.27720000	-1.31480000	-3.11020000
H	-4.06100000	-2.34460000	-2.26730000
H	-2.34590000	-1.35440000	-4.19110000
H	0.00000000	4.68920000	-2.26730000
H	0.00000000	3.29700000	0.09040000
H	0.00000000	2.70880000	-4.19110000
H	-2.85530000	-1.64850000	0.09040000
H	0.00000000	0.00000000	-4.28600000
H	4.06100000	-2.34460000	-2.26730000
H	2.34590000	-1.35440000	-4.19110000
H	2.85530000	-1.64850000	0.09040000
B	0.00000000	0.00000000	-3.09190000

$[Mn(Tb)_2]^{2+}$ ^2E_g D_{3d} LDA

Mn	0.00000000	0.00000000	0.00000000
N	1.34170000	0.77460000	-1.12800000
N	1.22150000	0.70530000	-2.47370000
N	-1.34170000	0.77460000	-1.12800000
N	-1.22150000	0.70530000	-2.47370000
N	0.00000000	-1.54920000	-1.12800000
N	0.00000000	-1.41050000	-2.47370000
C	2.48360000	1.43390000	-0.85710000
C	3.10120000	1.79050000	-2.03860000
C	2.26420000	1.30720000	-3.04450000
C	-2.48360000	1.43390000	-0.85710000
C	-3.10120000	1.79050000	-2.03860000
C	-2.26420000	1.30720000	-3.04450000
C	0.00000000	-2.86790000	-0.85710000
C	0.00000000	-3.58090000	-2.03860000
C	0.00000000	-2.61440000	-3.04450000
H	4.03750000	2.33110000	-2.16540000
H	2.35430000	1.35920000	-4.12920000
H	-4.03750000	2.33110000	-2.16540000
H	-2.78800000	1.60970000	0.17440000

H	-2.35430000	1.35920000	-4.12920000
H	2.78800000	1.60970000	0.17440000
H	0.00000000	0.00000000	-4.24670000
H	0.00000000	-4.66210000	-2.16540000
H	0.00000000	-2.71850000	-4.12920000
H	0.00000000	-3.21930000	0.17440000
B	0.00000000	0.00000000	-3.04970000
N	1.34170000	-0.77460000	1.12800000
N	1.22150000	-0.70530000	2.47370000
N	0.00000000	1.54920000	1.12800000
N	0.00000000	1.41050000	2.47370000
N	-1.34170000	-0.77460000	1.12800000
N	-1.22150000	-0.70530000	2.47370000
C	2.48360000	-1.43390000	0.85710000
C	3.10120000	-1.79050000	2.03860000
C	2.26420000	-1.30720000	3.04450000
C	0.00000000	2.86790000	0.85710000
C	0.00000000	3.58090000	2.03860000
C	0.00000000	2.61440000	3.04450000
C	-2.48360000	-1.43390000	0.85710000
C	-3.10120000	-1.79050000	2.03860000
C	-2.26420000	-1.30720000	3.04450000
H	4.03750000	-2.33110000	2.16540000
H	2.35430000	-1.35920000	4.12920000
H	0.00000000	4.66210000	2.16540000
H	0.00000000	3.21930000	-0.17440000
H	0.00000000	2.71850000	4.12920000
H	2.78800000	-1.60970000	-0.17440000
H	0.00000000	0.00000000	4.24670000
H	-4.03750000	-2.33110000	2.16540000
H	-2.35430000	-1.35920000	4.12920000
H	-2.78800000	-1.60970000	-0.17440000
B	0.00000000	0.00000000	3.04970000

$[Mn(Tb)_2]^{2+}$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.58350000	1.15920000
N	0.00000000	1.42740000	2.50410000
N	1.37130000	-0.79170000	1.15920000
N	1.23620000	-0.71370000	2.50410000
N	-1.37130000	-0.79170000	1.15920000
N	-1.23620000	-0.71370000	2.50410000
C	0.00000000	2.91160000	0.90860000
C	0.00000000	3.61330000	2.10330000
C	0.00000000	2.62780000	3.09590000
C	2.52160000	-1.45580000	0.90860000
C	3.12920000	-1.80660000	2.10330000
C	2.27580000	-1.31390000	3.09590000
C	-2.52160000	-1.45580000	0.90860000
C	-3.12920000	-1.80660000	2.10330000
C	-2.27580000	-1.31390000	3.09590000
H	0.00000000	4.68800000	2.24410000
H	0.00000000	2.71510000	4.17640000
H	4.05990000	-2.34400000	2.24410000
H	2.84340000	-1.64170000	-0.10720000
H	2.35130000	-1.35750000	4.17640000
H	0.00000000	3.28330000	-0.10720000
H	0.00000000	0.00000000	4.27290000
H	-4.05990000	-2.34400000	2.24410000
H	-2.35130000	-1.35750000	4.17640000
H	-2.84340000	-1.64170000	-0.10720000
B	0.00000000	0.00000000	3.07760000
N	-1.37130000	0.79170000	-1.15920000
N	-1.23620000	0.71370000	-2.50410000
N	1.37130000	0.79170000	-1.15920000
N	1.23620000	0.71370000	-2.50410000
N	0.00000000	-1.58350000	-1.15920000
N	0.00000000	-1.42740000	-2.50410000
C	-2.52160000	1.45580000	-0.90860000
C	-3.12920000	1.80660000	-2.10330000
C	-2.27580000	1.31390000	-3.09590000
C	2.52160000	1.45580000	-0.90860000
C	3.12920000	1.80660000	-2.10330000
C	2.27580000	1.31390000	-3.09590000
C	0.00000000	-2.91160000	-0.90860000
C	0.00000000	-3.61330000	-2.10330000
C	0.00000000	-2.62780000	-3.09590000
H	-4.05990000	2.34400000	-2.24410000
H	-2.35130000	1.35750000	-4.17640000
H	4.05990000	2.34400000	-2.24410000
H	2.84340000	1.64170000	0.10720000
H	2.35130000	1.35750000	-4.17640000
H	-2.84340000	1.64170000	0.10720000
H	0.00000000	0.00000000	-4.27290000
H	0.00000000	-4.68800000	-2.24410000
H	0.00000000	-2.71510000	-4.17640000
H	0.00000000	-3.28330000	0.10720000
B	0.00000000	0.00000000	-3.07760000

$[Mn(Tb)_2]^{+}$ ^5E_g D_{3d} LDA

Mn	0.00000000	0.00000000	0.00000000
N	1.40100000	-0.80890000	-1.23730000
N	1.23260000	-0.71170000	-2.56880000
N	0.00000000	1.61780000	-1.23730000
N	0.00000000	1.42330000	-2.56880000
N	-1.40100000	-0.80890000	-1.23730000
N	-1.23260000	-0.71170000	-2.56880000
C	2.54230000	-1.46780000	-1.01980000
C	3.12390000	-1.80360000	-2.23570000
C	2.25860000	-1.30400000	-3.19330000
C	0.00000000	2.93560000	-1.01980000
C	0.00000000	3.60720000	-2.23570000
C	0.00000000	2.60800000	-3.19330000
C	-2.54230000	-1.46780000	-1.01980000
C	-3.12390000	-1.80360000	-2.23570000
C	-2.25860000	-1.30400000	-3.19330000
H	4.05490000	-2.34110000	-2.40210000
H	2.30320000	-1.32980000	-4.28050000
H	0.00000000	4.68220000	-2.40210000
H	0.00000000	3.32140000	-0.00070000
H	0.00000000	2.65950000	-4.28050000
H	2.87640000	-1.66070000	-0.00070000
H	0.00000000	0.00000000	-4.31890000
H	-4.05490000	-2.34110000	-2.40210000
H	-2.30320000	-1.32980000	-4.28050000
H	-2.87640000	-1.66070000	-0.00070000
B	0.00000000	0.00000000	-3.11800000
N	0.00000000	-1.61780000	1.23730000

N	0.00000000	-1.42330000	2.56880000
N	1.40100000	0.80890000	1.23730000
N	1.23260000	0.71170000	2.56880000
N	-1.40100000	0.80890000	1.23730000
N	-1.23260000	0.71170000	2.56880000
C	0.00000000	-2.93560000	1.01980000
C	0.00000000	-3.60720000	2.23570000
C	0.00000000	-2.60800000	3.19330000
C	2.54230000	1.46780000	1.01980000
C	3.12390000	1.80360000	2.23570000
C	2.25860000	1.30400000	3.19330000
C	-2.54230000	1.46780000	1.01980000
C	-3.12390000	1.80360000	2.23570000
C	-2.25860000	1.30400000	3.19330000
H	0.00000000	-4.68220000	2.40210000
H	0.00000000	-2.65950000	4.28050000
H	4.05490000	2.34110000	2.40210000
H	2.87640000	1.66070000	0.00070000
H	2.30320000	1.32980000	4.28050000
H	0.00000000	-3.32140000	0.00070000
H	0.00000000	0.00000000	4.31890000
H	-4.05490000	2.34110000	2.40210000
H	-2.30320000	1.32980000	4.28050000
H	-2.87640000	1.66070000	0.00070000
B	0.00000000	0.00000000	3.11800000

$[Mn(Tb)_2]^+$ ^5E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.43870000	0.83070000	1.29910000
N	-1.24890000	0.72100000	2.62870000
N	1.43870000	0.83070000	1.29910000
N	1.24890000	0.72100000	2.62870000
N	0.00000000	-1.66130000	1.29910000
N	0.00000000	-1.44210000	2.62870000
C	-2.58890000	1.49470000	1.11060000
C	-3.15380000	1.82080000	2.34260000
C	-2.26780000	1.30930000	3.28030000
C	2.58890000	1.49470000	1.11060000
C	3.15380000	1.82080000	2.34260000
C	2.26780000	1.30930000	3.28030000
C	0.00000000	-2.98940000	1.11060000
C	0.00000000	-3.64160000	2.34260000
C	0.00000000	-2.61870000	3.28030000
H	-4.07810000	2.35450000	2.52870000
H	-2.29360000	1.32420000	4.36300000
H	4.07810000	2.35450000	2.52870000
H	2.94620000	1.70100000	0.11000000
H	2.29360000	1.32420000	4.36300000
H	-2.94620000	1.70100000	0.11000000
H	0.00000000	0.00000000	4.37310000
H	0.00000000	-4.70900000	2.52870000
H	0.00000000	-2.64850000	4.36300000
H	0.00000000	-3.40200000	0.11000000
B	0.00000000	0.00000000	3.17400000
N	-1.43870000	-0.83070000	-1.29910000
N	-1.24890000	-0.72100000	-2.62870000
N	0.00000000	1.66130000	-1.29910000
N	0.00000000	1.44210000	-2.62870000
N	1.43870000	-0.83070000	-1.29910000
N	1.24890000	-0.72100000	-2.62870000
C	-2.58890000	-1.49470000	-1.11060000
C	-3.15380000	-1.82080000	-2.34260000
C	-2.26780000	-1.30930000	-3.28030000
C	0.00000000	2.98940000	-1.11060000
C	0.00000000	3.64160000	-2.34260000
C	0.00000000	2.61870000	-3.28030000
C	2.58890000	-1.49470000	-1.11060000
C	3.15380000	-1.82080000	-2.34260000
C	2.26780000	-1.30930000	-3.28030000
H	-4.07810000	-2.35450000	-2.52870000
H	-2.29360000	-1.32420000	-4.36300000
H	0.00000000	4.70900000	-2.52870000
H	0.00000000	3.40200000	-0.11000000
H	0.00000000	2.64850000	-4.36300000
H	-2.94620000	-1.70100000	-0.11000000
H	0.00000000	0.00000000	-4.37310000
H	4.07810000	-2.35450000	-2.52870000
H	2.29360000	-1.32420000	-4.36300000
H	2.94620000	-1.70100000	-0.11000000
B	0.00000000	0.00000000	-3.17400000

$[Mn(Tb)_2]^+$ $^3A_{2g}$ D_{3d} LDA

Mn	0.00000000	0.00000000	0.00000000
N	-1.35170000	-0.78040000	-1.15190000
N	-1.22370000	-0.70650000	-2.49080000
N	1.35170000	-0.78040000	-1.15190000
N	1.22370000	-0.70650000	-2.49080000
N	0.00000000	1.56080000	-1.15190000
N	0.00000000	1.41300000	-2.49080000
C	-2.48910000	-1.43710000	-0.89340000
C	-3.10340000	-1.79170000	-2.08600000
C	-2.26460000	-1.30750000	-3.07680000
C	2.48910000	-1.43710000	-0.89340000
C	3.10340000	-1.79170000	-2.08600000
C	2.26460000	-1.30750000	-3.07680000
C	0.00000000	2.87410000	-0.89340000
C	0.00000000	3.58350000	-2.08600000
C	0.00000000	2.61500000	-3.07680000
H	-4.03840000	-2.33160000	-2.21720000
H	-2.33960000	-1.35080000	-4.16170000
H	4.03840000	-2.33160000	-2.21720000
H	2.79530000	-1.61390000	0.13700000
H	2.33960000	-1.35080000	-4.16170000
H	-2.79530000	-1.61390000	0.13700000
H	0.00000000	0.00000000	-4.25800000
H	0.00000000	4.66310000	-2.21720000
H	0.00000000	2.70160000	-4.16170000
H	0.00000000	3.22770000	0.13700000
B	0.00000000	0.00000000	-3.05730000
N	-1.35170000	0.78040000	1.15190000
N	-1.22370000	0.70650000	2.49080000
N	0.00000000	-1.56080000	1.15190000
N	0.00000000	-1.41300000	2.49080000
N	1.35170000	0.78040000	1.15190000
N	1.22370000	0.70650000	2.49080000
C	-2.48910000	1.43710000	0.89340000
C	-3.10340000	1.79170000	2.08600000
C	-2.26460000	1.30750000	3.07680000

C	0.00000000	-2.87410000	0.89340000
C	0.00000000	-3.58350000	2.08600000
C	0.00000000	-2.61500000	3.07680000
C	2.48910000	1.43710000	0.89340000
C	3.10340000	1.79170000	2.08600000
C	2.26460000	1.30750000	3.07680000
H	-4.03840000	2.33160000	2.21720000
H	-2.33960000	1.35080000	4.16170000
H	0.00000000	-4.66310000	2.21720000
H	0.00000000	-3.22770000	-0.13700000
H	0.00000000	-2.70160000	4.16170000
H	-2.79530000	1.61390000	-0.13700000
H	0.00000000	0.00000000	4.25800000
H	4.03840000	2.33160000	2.21720000
H	2.33960000	1.35080000	4.16170000
H	2.79530000	1.61390000	-0.13700000
B	0.00000000	0.00000000	3.05730000

$[Mn(Tb)_2]^+$ $^3A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.59930000	-1.18900000
N	0.00000000	1.43060000	-2.52660000
N	-1.38500000	-0.79960000	-1.18900000
N	-1.23900000	-0.71530000	-2.52660000
N	1.38500000	-0.79960000	-1.18900000
N	1.23900000	-0.71530000	-2.52660000
C	0.00000000	2.92290000	-0.95520000
C	0.00000000	3.61680000	-2.16230000
C	0.00000000	2.62710000	-3.13690000
C	-2.53130000	-1.46150000	-0.95520000
C	-3.13230000	-1.80840000	-2.16230000
C	-2.27510000	-1.31350000	-3.13690000
C	2.53130000	-1.46150000	-0.95520000
C	3.13230000	-1.80840000	-2.16230000
C	2.27510000	-1.31350000	-3.13690000
H	0.00000000	4.69000000	-2.31040000
H	0.00000000	2.69440000	-4.21780000
H	-4.06160000	-2.34500000	-2.31040000
H	-2.85860000	-1.65040000	0.05820000
H	-2.33340000	-1.34720000	-4.21780000
H	0.00000000	3.30090000	0.05820000
H	0.00000000	0.00000000	-4.28820000
H	4.06160000	-2.34500000	-2.31040000
H	2.33340000	-1.34720000	-4.21780000
H	2.85860000	-1.65040000	0.05820000
B	0.00000000	0.00000000	-3.08910000
N	1.38500000	0.79960000	1.18900000
N	1.23900000	0.71530000	2.52660000
N	-1.38500000	0.79960000	1.18900000
N	-1.23900000	0.71530000	2.52660000
N	0.00000000	-1.59930000	1.18900000
N	0.00000000	-1.43060000	2.52660000
C	2.53130000	1.46150000	0.95520000
C	3.13230000	1.80840000	2.16230000
C	2.27510000	1.31350000	3.13690000
C	-2.53130000	1.46150000	0.95520000
C	-3.13230000	1.80840000	2.16230000
C	-2.27510000	1.31350000	3.13690000
C	0.00000000	-2.92290000	0.95520000
C	0.00000000	-3.61680000	2.16230000
C	0.00000000	-2.62710000	3.13690000
H	4.06160000	2.34500000	2.31040000
H	2.33340000	1.34720000	4.21780000
H	-4.06160000	2.34500000	2.31040000
H	-2.85860000	1.65040000	-0.05820000
H	-2.33340000	1.34720000	4.21780000
H	2.85860000	1.65040000	-0.05820000
H	0.00000000	0.00000000	4.28820000
H	0.00000000	-4.69000000	2.31040000
H	0.00000000	-2.69440000	4.21780000
H	0.00000000	-3.30090000	-0.05820000
B	0.00000000	0.00000000	3.08910000

$[Mn(Tb)_2]^+$ ^1E_g D_{3d} LDA

Mn	0.000000	0.000000	0.000000
N	1.401000	-0.808900	-1.237300
N	1.232600	-0.711700	-2.568800
N	0.000000	1.617800	-1.237300
N	0.000000	1.423300	-2.568800
N	-1.401000	-0.808900	-1.237300
N	-1.232600	-0.711700	-2.568800
C	2.542300	-1.467800	-1.019800
C	3.123900	-1.803600	-2.235700
C	2.258600	-1.304000	-3.193300
C	0.000000	2.935600	-1.019800
C	0.000000	3.607200	-2.235700
C	0.000000	2.608000	-3.193300
C	-2.542300	-1.467800	-1.019800
C	-3.123900	-1.803600	-2.235700
C	-2.258600	-1.304000	-3.193300
H	4.054900	-2.341100	-2.402100
H	2.303200	-1.329800	-4.280500
H	0.000000	4.682200	-2.402100
H	0.000000	3.321400	-0.000700
H	0.000000	2.659500	-4.280500
H	2.876400	-1.660700	-0.000700
H	0.000000	0.000000	-4.318900
H	-4.054900	-2.341100	-2.402100
H	-2.303200	-1.329800	-4.280500
H	-2.876400	-1.660700	-0.000700
B	0.000000	0.000000	-3.118000
N	0.000000	-1.617800	1.237300
N	0.000000	-1.423300	2.568800
N	1.401000	0.808900	1.237300
N	1.232600	0.711700	2.568800
N	-1.401000	0.808900	1.237300
N	-1.232600	0.711700	2.568800
C	0.000000	-2.935600	1.019800
C	0.000000	-3.607200	2.235700
C	0.000000	-2.608000	3.193300
C	2.542300	1.467800	1.019800
C	3.123900	1.803600	2.235700
C	2.258600	1.304000	3.193300
C	-2.542300	1.467800	1.019800
C	-3.123900	1.803600	2.235700
C	-2.258600	1.304000	3.193300
H	0.000000	-4.682200	2.402100
H	0.000000	-2.659500	4.280500

H	4.054900	2.341100	2.402100
H	2.876400	1.660700	0.000700
H	2.303200	1.329800	4.280500
H	0.000000	-3.321400	0.000700
H	0.000000	0.000000	4.318900
H	-4.054900	2.341100	2.402100
H	-2.303200	1.329800	4.280500
H	-2.876400	1.660700	0.000700
B	0.000000	0.000000	3.118000

$[Mn(Tb)_2]^+$ ^1E_g D_{3d} OPBE

Mn	0.000000	0.000000	0.000000
N	0.000000	1.587906	-1.174794
N	0.000000	1.428849	-2.515130
N	-1.375167	-0.793953	-1.174794
N	-1.237419	-0.714424	-2.515130
N	1.375167	-0.793953	-1.174794
N	1.237419	-0.714424	-2.515130
C	0.000000	2.912883	-0.935687
C	0.000000	3.613318	-2.137739
C	0.000000	2.627995	-3.119152
C	-2.522630	-1.456441	-0.935687
C	-3.129225	-1.806659	-2.137739
C	-2.275911	-1.313998	-3.119152
C	2.522630	-1.456441	-0.935687
C	3.129225	-1.806659	-2.137739
C	2.275911	-1.313998	-3.119152
H	0.000000	4.687173	-2.280894
H	0.000000	2.702098	-4.199698
H	-4.059211	-2.343586	-2.280894
H	-2.845406	-1.642796	0.079523
H	-2.340086	-1.351049	-4.199698
H	0.000000	3.285591	0.079523
H	0.000000	0.000000	-4.280059
H	4.059211	-2.343586	-2.280894
H	2.340086	-1.351049	-4.199698
H	2.845406	-1.642796	0.079523
B	0.000000	0.000000	-3.080611
N	1.375167	0.793953	1.174794
N	1.237419	0.714424	2.515130
N	-1.375167	0.793953	1.174794
N	-1.237419	0.714424	2.515130
N	0.000000	-1.587906	1.174794
N	0.000000	-1.428849	2.515130
C	2.522630	1.456441	0.935687
C	3.129225	1.806659	2.137739
C	2.275911	1.313998	3.119152
C	-2.522630	1.456441	0.935687
C	-3.129225	1.806659	2.137739
C	-2.275911	1.313998	3.119152
C	0.000000	-2.912883	0.935687
C	0.000000	-3.613318	2.137739
C	0.000000	-2.627995	3.119152
H	4.059211	2.343586	2.280894
H	2.340086	1.351049	4.199698
H	-4.059211	2.343586	2.280894
H	-2.845406	1.642796	-0.079523
H	-2.340086	1.351049	4.199698
H	2.845406	1.642796	-0.079523
H	0.000000	0.000000	4.280059
H	0.000000	-4.687173	2.280894
H	0.000000	-2.702098	4.199698
H	0.000000	-3.285591	-0.079523
B	0.000000	0.000000	3.080611

$[Mn(Tb)_2]$ $^6A_{1g}$ D_{3d} LDA

Mn	0.00000000	0.00000000	0.00000000
N	1.46170000	-0.84390000	1.38000000
N	1.24380000	-0.71810000	2.69940000
N	-1.46170000	-0.84390000	1.38000000
N	-1.24380000	-0.71810000	2.69940000
N	0.00000000	1.68780000	1.38000000
N	0.00000000	1.43630000	2.69940000
C	2.60730000	-1.50530000	1.23510000
C	3.14590000	-1.81630000	2.48390000
C	2.24200000	-1.29440000	3.38880000
C	-2.60730000	-1.50530000	1.23510000
C	-3.14590000	-1.81630000	2.48390000
C	-2.24200000	-1.29440000	3.38880000
C	0.00000000	3.01070000	1.23510000
C	0.00000000	3.63260000	2.48390000
C	0.00000000	2.58880000	3.38880000
H	4.06870000	-2.34910000	2.70320000
H	2.23590000	-1.29090000	4.47690000
H	-4.06870000	-2.34910000	2.70320000
H	-2.98160000	-1.72140000	0.23450000
H	-2.23590000	-1.29090000	4.47690000
H	2.98160000	-1.72140000	0.23450000
H	0.00000000	0.00000000	4.42150000
H	0.00000000	4.69810000	2.70320000
H	0.00000000	2.58180000	4.47690000
H	0.00000000	3.44290000	0.23450000
B	0.00000000	0.00000000	3.21370000
N	1.46170000	0.84390000	-1.38000000
N	1.24380000	0.71810000	-2.69940000
N	0.00000000	-1.68780000	-1.38000000
N	0.00000000	-1.43630000	-2.69940000
N	-1.46170000	0.84390000	-1.38000000
N	-1.24380000	0.71810000	-2.69940000
C	2.60730000	1.50530000	-1.23510000
C	3.14590000	1.81630000	-2.48390000
C	2.24200000	1.29440000	-3.38880000
C	0.00000000	-3.01070000	-1.23510000
C	0.00000000	-3.63260000	-2.48390000
C	0.00000000	-2.58880000	-3.38880000
C	-2.60730000	1.50530000	-1.23510000
C	-3.14590000	1.81630000	-2.48390000
C	-2.24200000	1.29440000	-3.38880000
H	4.06870000	2.34910000	-2.70320000
H	2.23590000	1.29090000	-4.47690000
H	0.00000000	-4.69810000	-2.70320000
H	0.00000000	-3.44290000	-0.23450000
H	0.00000000	-2.58180000	-4.47690000
H	2.98160000	1.72140000	-0.23450000
H	0.00000000	0.00000000	-4.42150000
H	-4.06870000	2.34910000	-2.70320000
H	-2.23590000	1.29090000	-4.47690000
H	-2.98160000	1.72140000	-0.23450000

B	0.00000000	0.00000000	-3.21370000

[Mn(Tb)$_2$] $^6A_{1g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.50920000	0.87130000	1.48000000
N	-1.26420000	0.72990000	2.79690000
N	1.50920000	0.87130000	1.48000000
N	1.26420000	0.72990000	2.79690000
N	0.00000000	-1.74270000	1.48000000
N	0.00000000	-1.45970000	2.79690000
C	-2.66330000	1.53770000	1.37430000
C	-3.17900000	1.83540000	2.64120000
C	-2.25060000	1.29940000	3.51930000
C	2.66330000	1.53770000	1.37430000
C	3.17900000	1.83540000	2.64120000
C	2.25060000	1.29940000	3.51930000
C	0.00000000	-3.07530000	1.37430000
C	0.00000000	-3.67080000	2.64120000
C	0.00000000	-2.59870000	3.51930000
H	-4.09330000	2.36330000	2.88690000
H	-2.22290000	1.28340000	4.60190000
H	4.09330000	2.36330000	2.88690000
H	3.06510000	1.76960000	0.39460000
H	2.22290000	1.28340000	4.60190000
H	-3.06510000	1.76960000	0.39460000
H	0.00000000	0.00000000	4.50930000
H	0.00000000	-4.72660000	2.88690000
H	0.00000000	-2.56680000	4.60190000
H	0.00000000	-3.53920000	0.39460000
B	0.00000000	0.00000000	3.30340000
N	-1.50920000	-0.87130000	-1.48000000
N	-1.26420000	-0.72990000	-2.79690000
N	0.00000000	1.74270000	-1.48000000
N	0.00000000	1.45970000	-2.79690000
N	1.50920000	-0.87130000	-1.48000000
N	1.26420000	-0.72990000	-2.79690000
C	-2.66330000	-1.53770000	-1.37430000
C	-3.17900000	-1.83540000	-2.64120000
C	-2.25060000	-1.29940000	-3.51930000
C	0.00000000	3.07530000	-1.37430000
C	0.00000000	3.67080000	-2.64120000
C	0.00000000	2.59870000	-3.51930000
C	2.66330000	-1.53770000	-1.37430000
C	3.17900000	-1.83540000	-2.64120000
C	2.25060000	-1.29940000	-3.51930000
H	-4.09330000	-2.36330000	-2.88690000
H	-2.22290000	-1.28340000	-4.60190000
H	0.00000000	4.72660000	-2.88690000
H	0.00000000	3.53920000	-0.39460000
H	0.00000000	2.56680000	-4.60190000
H	-3.06510000	-1.76960000	-0.39460000
H	0.00000000	0.00000000	-4.50930000
H	4.09330000	-2.36330000	-2.88690000
H	2.22290000	-1.28340000	-4.60190000
H	3.06510000	-1.76960000	-0.39460000
B	0.00000000	0.00000000	-3.30340000

[Mn(Tb)$_2$] ^4E_g D_{3d} LDA

Mn	0.00000000	0.00000000	0.00000000
N	1.40560000	-0.81150000	-1.24180000
N	1.23450000	-0.71270000	-2.57270000
N	0.00000000	1.62310000	-1.24180000
N	0.00000000	1.42540000	-2.57270000
N	-1.40560000	-0.81150000	-1.24180000
N	-1.23450000	-0.71270000	-2.57270000
C	2.54640000	-1.47010000	-1.03690000
C	3.12680000	-1.80520000	-2.26080000
C	2.25870000	-1.30400000	-3.21130000
C	0.00000000	2.94030000	-1.03690000
C	0.00000000	3.61050000	-2.26080000
C	0.00000000	2.60810000	-3.21130000
C	-2.54640000	-1.47010000	-1.03690000
C	-3.12680000	-1.80520000	-2.26080000
C	-2.25870000	-1.30400000	-3.21130000
H	4.05690000	-2.34230000	-2.43320000
H	2.29360000	-1.32420000	-4.29860000
H	0.00000000	4.68460000	-2.43320000
H	0.00000000	3.32670000	-0.01820000
H	0.00000000	2.64840000	-4.29860000
H	2.88100000	-1.66330000	-0.01820000
H	0.00000000	0.00000000	-4.31910000
H	-4.05690000	-2.34230000	-2.43320000
H	-2.29360000	-1.32420000	-4.29860000
H	-2.88100000	-1.66330000	-0.01820000
B	0.00000000	0.00000000	-3.11270000
N	0.00000000	-1.62310000	1.24180000
N	0.00000000	-1.42540000	2.57270000
N	1.40560000	0.81150000	1.24180000
N	1.23450000	0.71270000	2.57270000
N	-1.40560000	0.81150000	1.24180000
N	-1.23450000	0.71270000	2.57270000
C	0.00000000	-2.94030000	1.03690000
C	0.00000000	-3.61050000	2.26080000
C	0.00000000	-2.60810000	3.21130000
C	2.54640000	1.47010000	1.03690000
C	3.12680000	1.80520000	2.26080000
C	2.25870000	1.30400000	3.21130000
C	-2.54640000	1.47010000	1.03690000
C	-3.12680000	1.80520000	2.26080000
C	-2.25870000	1.30400000	3.21130000
H	0.00000000	-4.68460000	2.43320000
H	0.00000000	-2.64840000	4.29860000
H	4.05690000	2.34230000	2.43320000
H	2.88100000	1.66330000	0.01820000
H	2.29360000	1.32420000	4.29860000
H	0.00000000	-3.32670000	0.01820000
H	0.00000000	0.00000000	4.31910000
H	-4.05690000	2.34230000	2.43320000
H	-2.29360000	1.32420000	4.29860000
H	-2.88100000	1.66330000	0.01820000
B	0.00000000	0.00000000	3.11270000

[Mn(Tb)$_2$] ^4E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.46190000	0.84400000	1.32860000
N	-1.25590000	0.72510000	2.65380000
N	1.46190000	0.84400000	1.32860000

N	1.25590000	0.72510000	2.65380000
N	0.00000000	-1.68810000	1.32860000
N	0.00000000	-1.45020000	2.65380000
C	-2.61340000	1.50890000	1.17700000
C	-3.16380000	1.82660000	2.42350000
C	-2.26110000	1.30540000	3.33800000
C	2.61340000	1.50890000	1.17700000
C	3.16380000	1.82660000	2.42350000
C	2.26110000	1.30540000	3.33800000
C	0.00000000	-3.01770000	1.17700000
C	0.00000000	-3.65330000	2.42350000
C	0.00000000	-2.61090000	3.33800000
H	-4.08480000	2.35840000	2.63360000
H	-2.26430000	1.30730000	4.42120000
H	4.08480000	2.35840000	2.63360000
H	2.98620000	1.72410000	0.18330000
H	2.26430000	1.30730000	4.42120000
H	-2.98620000	1.72410000	0.18330000
H	0.00000000	0.00000000	4.38110000
H	0.00000000	-4.71680000	2.63360000
H	0.00000000	-2.61460000	4.42120000
H	0.00000000	-3.44810000	0.18330000
B	0.00000000	0.00000000	3.17480000
N	-1.46190000	-0.84400000	-1.32860000
N	-1.25590000	-0.72510000	-2.65380000
N	0.00000000	1.68810000	-1.32860000
N	0.00000000	1.45020000	-2.65380000
N	1.46190000	-0.84400000	-1.32860000
N	1.25590000	-0.72510000	-2.65380000
C	-2.61340000	-1.50890000	-1.17700000
C	-3.16380000	-1.82660000	-2.42350000
C	-2.26110000	-1.30540000	-3.33800000
C	0.00000000	3.01770000	-1.17700000
C	0.00000000	3.65330000	-2.42350000
C	0.00000000	2.61090000	-3.33800000
C	2.61340000	-1.50890000	-1.17700000
C	3.16380000	-1.82660000	-2.42350000
C	2.26110000	-1.30540000	-3.33800000
H	-4.08480000	-2.35840000	-2.63360000
H	-2.26430000	-1.30730000	-4.42120000
H	0.00000000	4.71680000	-2.63360000
H	0.00000000	3.44810000	-0.18330000
H	0.00000000	2.61460000	-4.42120000
H	-2.98620000	-1.72410000	-0.18330000
H	0.00000000	0.00000000	-4.38110000
H	4.08480000	-2.35840000	-2.63360000
H	2.26430000	-1.30730000	-4.42120000
H	2.98620000	-1.72410000	-0.18330000
B	0.00000000	0.00000000	-3.17480000

$[Mn(Tb)_2]$ ^2E_g D_{3d} LDA

Mn	0.00000000	0.00000000	0.00000000
N	1.34970000	-0.77930000	-1.15090000
N	1.22470000	-0.70710000	-2.49110000
N	0.00000000	1.55850000	-1.15090000
N	0.00000000	1.41420000	-2.49110000
N	-1.34970000	-0.77930000	-1.15090000
N	-1.22470000	-0.70710000	-2.49110000
C	2.48630000	-1.43550000	-0.89840000
C	3.10430000	-1.79220000	-2.09610000
C	2.26730000	-1.30900000	-3.08470000
C	0.00000000	2.87090000	-0.89840000
C	0.00000000	3.58450000	-2.09610000
C	0.00000000	2.61810000	-3.08470000
C	-2.48630000	-1.43550000	-0.89840000
C	-3.10430000	-1.79220000	-2.09610000
C	-2.26730000	-1.30900000	-3.08470000
H	4.03930000	-2.33210000	-2.22710000
H	2.33740000	-1.34950000	-4.16950000
H	0.00000000	4.66420000	-2.22710000
H	0.00000000	3.21980000	0.13330000
H	0.00000000	2.69900000	-4.16950000
H	2.78840000	-1.60990000	0.13330000
H	0.00000000	0.00000000	-4.25660000
H	-4.03930000	-2.33210000	-2.22710000
H	-2.33740000	-1.34950000	-4.16950000
H	-2.78840000	-1.60990000	0.13330000
B	0.00000000	0.00000000	-3.05060000
N	0.00000000	-1.55850000	1.15090000
N	0.00000000	-1.41420000	2.49110000
N	1.34970000	0.77930000	1.15090000
N	1.22470000	0.70710000	2.49110000
N	-1.34970000	0.77930000	1.15090000
N	-1.22470000	0.70710000	2.49110000
C	0.00000000	-2.87090000	0.89840000
C	0.00000000	-3.58450000	2.09610000
C	0.00000000	-2.61810000	3.08470000
C	2.48630000	1.43550000	0.89840000
C	3.10430000	1.79220000	2.09610000
C	2.26730000	1.30900000	3.08470000
C	-2.48630000	1.43550000	0.89840000
C	-3.10430000	1.79220000	2.09610000
C	-2.26730000	1.30900000	3.08470000
H	0.00000000	-4.66420000	2.22710000
H	0.00000000	-2.69900000	4.16950000
H	4.03930000	2.33210000	2.22710000
H	2.78840000	1.60990000	-0.13330000
H	2.33740000	1.34950000	4.16950000
H	0.00000000	-3.21980000	-0.13330000
H	0.00000000	0.00000000	4.25660000
H	-4.03930000	2.33210000	2.22710000
H	-2.33740000	1.34950000	4.16950000
H	-2.78840000	1.60990000	-0.13330000
B	0.00000000	0.00000000	3.05060000

$[Mn(Tb)_2]$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.38630000	0.80040000	1.19550000
N	-1.24040000	0.71620000	2.53400000
N	1.38630000	0.80040000	1.19550000
N	1.24040000	0.71620000	2.53400000
N	0.00000000	-1.60070000	1.19550000
N	0.00000000	-1.43230000	2.53400000
C	-2.53250000	1.46220000	0.97470000
C	-3.13410000	1.80950000	2.18840000
C	-2.27480000	1.31340000	3.15710000
C	2.53250000	1.46220000	0.97470000
C	3.13410000	1.80950000	2.18840000

C	2.27480000	1.31340000	3.15710000
C	0.00000000	-2.92430000	0.97470000
C	0.00000000	-3.61890000	2.18840000
C	0.00000000	-2.62680000	3.15710000
H	-4.06340000	2.34600000	2.34080000
H	-2.32510000	1.34240000	4.23850000
H	4.06340000	2.34600000	2.34080000
H	2.86130000	1.65200000	-0.03810000
H	2.32510000	1.34240000	4.23850000
H	-2.86130000	1.65200000	-0.03810000
H	0.00000000	0.00000000	4.29320000
H	0.00000000	-4.69200000	2.34080000
H	0.00000000	-2.68480000	4.23850000
H	0.00000000	-3.30400000	-0.03810000
B	0.00000000	0.00000000	3.08800000
N	-1.38630000	-0.80040000	-1.19550000
N	-1.24040000	-0.71620000	-2.53400000
N	0.00000000	1.60070000	-1.19550000
N	0.00000000	1.43230000	-2.53400000
N	1.38630000	-0.80040000	-1.19550000
N	1.24040000	-0.71620000	-2.53400000
C	-2.53250000	-1.46220000	-0.97470000
C	-3.13410000	-1.80950000	-2.18840000
C	-2.27480000	-1.31340000	-3.15710000
C	0.00000000	2.92430000	-0.97470000
C	0.00000000	3.61890000	-2.18840000
C	0.00000000	2.62680000	-3.15710000
C	2.53250000	-1.46220000	-0.97470000
C	3.13410000	-1.80950000	-2.18840000
C	2.27480000	-1.31340000	-3.15710000
H	-4.06340000	-2.34600000	-2.34080000
H	-2.32510000	-1.34240000	-4.23850000
H	0.00000000	4.69200000	-2.34080000
H	0.00000000	3.30400000	0.03810000
H	0.00000000	2.68480000	-4.23850000
H	-2.86130000	-1.65200000	0.03810000
H	0.00000000	0.00000000	-4.29320000
H	4.06340000	-2.34600000	-2.34080000
H	2.32510000	-1.34240000	-4.23850000
H	2.86130000	-1.65200000	0.03810000
B	0.00000000	0.00000000	-3.08800000

$[Fe(Tb)_2]^+$ $^6A_{1g}$ D_{3d} LDA

Fe	0.00000000	0.00000000	0.00000000
N	1.41470000	-0.81680000	-1.26660000
N	1.23540000	-0.71320000	-2.59680000
N	0.00000000	1.63360000	-1.26660000
N	0.00000000	1.42650000	-2.59680000
N	-1.41470000	-0.81680000	-1.26660000
N	-1.23540000	-0.71320000	-2.59680000
C	2.55880000	-1.47730000	-1.06520000
C	3.13020000	-1.80720000	-2.28660000
C	2.25490000	-1.30190000	-3.23430000
C	0.00000000	2.95460000	-1.06520000
C	0.00000000	3.61450000	-2.28660000
C	0.00000000	2.60380000	-3.23430000
C	-2.55880000	-1.47730000	-1.06520000
C	-3.13020000	-1.80720000	-2.28660000
C	-2.25490000	-1.30190000	-3.23430000
H	4.05940000	-2.34370000	-2.46560000
H	2.29020000	-1.32230000	-4.32210000
H	0.00000000	4.68740000	-2.46560000
H	0.00000000	3.35110000	-0.05020000
H	0.00000000	2.64450000	-4.32210000
H	2.90210000	-1.67550000	-0.05020000
H	0.00000000	0.00000000	-4.34090000
H	-4.05940000	-2.34370000	-2.46560000
H	-2.29020000	-1.32230000	-4.32210000
H	-2.90210000	-1.67550000	-0.05020000
B	0.00000000	0.00000000	-3.13930000
N	0.00000000	-1.63360000	1.26660000
N	0.00000000	-1.42650000	2.59680000
N	1.41470000	0.81680000	1.26660000
N	1.23540000	0.71320000	2.59680000
N	-1.41470000	0.81680000	1.26660000
N	-1.23540000	0.71320000	2.59680000
C	0.00000000	-2.95460000	1.06520000
C	0.00000000	-3.61450000	2.28660000
C	0.00000000	-2.60380000	3.23430000
C	2.55880000	1.47730000	1.06520000
C	3.13020000	1.80720000	2.28660000
C	2.25490000	1.30190000	3.23430000
C	-2.55880000	1.47730000	1.06520000
C	-3.13020000	1.80720000	2.28660000
C	-2.25490000	1.30190000	3.23430000
H	0.00000000	-4.68740000	2.46560000
H	0.00000000	-2.64450000	4.32210000
H	4.05940000	2.34370000	2.46560000
H	2.90210000	1.67550000	0.05020000
H	2.29020000	1.32230000	4.32210000
H	0.00000000	-3.35110000	0.05020000
H	0.00000000	0.00000000	4.34090000
H	-4.05940000	2.34370000	2.46560000
H	-2.29020000	1.32230000	4.32210000
H	-2.90210000	1.67550000	0.05020000
B	0.00000000	0.00000000	3.13930000

$[Fe(Tb)_2]^+$ $^6A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.45040000	-0.83740000	-1.32320000
N	1.25170000	-0.72270000	-2.65280000
N	0.00000000	1.67480000	-1.32320000
N	0.00000000	1.44530000	-2.65280000
N	-1.45040000	-0.83740000	-1.32320000
N	-1.25170000	-0.72270000	-2.65280000
C	2.60380000	-1.50330000	-1.15120000
C	3.15940000	-1.82410000	-2.38730000
C	2.26430000	-1.30730000	-3.31590000
C	0.00000000	3.00660000	-1.15120000
C	0.00000000	3.64820000	-2.38730000
C	0.00000000	2.61460000	-3.31590000
C	-2.60380000	-1.50330000	-1.15120000
C	-3.15940000	-1.82410000	-2.38730000
C	-2.26430000	-1.30730000	-3.31590000
H	4.08190000	-2.35670000	-2.58540000
H	2.28220000	-1.31770000	-4.39890000
H	0.00000000	4.71330000	-2.58540000
H	0.00000000	3.42920000	-0.15450000

H	0.00000000	2.63530000	-4.39890000
H	2.96980000	-1.71460000	-0.15450000
H	0.00000000	0.00000000	-4.39180000
H	-4.08190000	-2.35670000	-2.58540000
H	-2.28220000	-1.31770000	-4.39890000
H	-2.96980000	-1.71460000	-0.15450000
B	0.00000000	0.00000000	-3.19200000
N	0.00000000	-1.67480000	1.32320000
N	0.00000000	-1.44530000	2.65280000
N	1.45040000	0.83740000	1.32320000
N	1.25170000	0.72270000	2.65280000
N	-1.45040000	0.83740000	1.32320000
N	-1.25170000	0.72270000	2.65280000
C	0.00000000	-3.00660000	1.15120000
C	0.00000000	-3.64820000	2.38730000
C	0.00000000	-2.61460000	3.31590000
C	2.60380000	1.50330000	1.15120000
C	3.15940000	1.82410000	2.38730000
C	2.26430000	1.30730000	3.31590000
C	-2.60380000	1.50330000	1.15120000
C	-3.15940000	1.82410000	2.38730000
C	-2.26430000	1.30730000	3.31590000
H	0.00000000	-4.71330000	2.58540000
H	0.00000000	-2.63530000	4.39890000
H	4.08190000	2.35670000	2.58540000
H	2.96980000	1.71460000	0.15450000
H	2.28220000	1.31770000	4.39890000
H	0.00000000	-3.42920000	0.15450000
H	0.00000000	0.00000000	4.39180000
H	-4.08190000	2.35670000	2.58540000
H	-2.28220000	1.31770000	4.39890000
H	-2.96980000	1.71460000	0.15450000
B	0.00000000	0.00000000	3.19200000

$[Fe(Tb)_2]^+$ ^4E_g D_{3d} LDA

Fe	0.00000000	0.00000000	0.00000000
N	-1.37760000	0.79530000	1.18630000
N	-1.22860000	0.70930000	2.52050000
N	1.37760000	0.79530000	1.18630000
N	1.22860000	0.70930000	2.52050000
N	0.00000000	-1.59070000	1.18630000
N	0.00000000	-1.41860000	2.52050000
C	-2.51700000	1.45320000	0.94890000
C	-3.11470000	1.79830000	2.15300000
C	-2.26110000	1.30540000	3.12750000
C	2.51700000	1.45320000	0.94890000
C	3.11470000	1.79830000	2.15300000
C	2.26110000	1.30540000	3.12750000
C	0.00000000	-2.90640000	0.94890000
C	0.00000000	-3.59660000	2.15300000
C	0.00000000	-2.61080000	3.12750000
H	-4.04770000	2.33700000	2.30360000
H	-2.32050000	1.33970000	4.21380000
H	4.04770000	2.33700000	2.30360000
H	2.83690000	1.63790000	-0.07630000
H	2.32050000	1.33970000	4.21380000
H	-2.83690000	1.63790000	-0.07630000
H	0.00000000	0.00000000	4.27790000
H	0.00000000	-4.67390000	2.30360000
H	0.00000000	-2.67950000	4.21380000
H	0.00000000	-3.27580000	-0.07630000
B	0.00000000	0.00000000	3.07670000
N	-1.37760000	-0.79530000	-1.18630000
N	-1.22860000	-0.70930000	-2.52050000
N	0.00000000	1.59070000	-1.18630000
N	0.00000000	1.41860000	-2.52050000
N	1.37760000	-0.79530000	-1.18630000
N	1.22860000	-0.70930000	-2.52050000
C	-2.51700000	-1.45320000	-0.94890000
C	-3.11470000	-1.79830000	-2.15300000
C	-2.26110000	-1.30540000	-3.12750000
C	0.00000000	2.90640000	-0.94890000
C	0.00000000	3.59660000	-2.15300000
C	0.00000000	2.61080000	-3.12750000
C	2.51700000	-1.45320000	-0.94890000
C	3.11470000	-1.79830000	-2.15300000
C	2.26110000	-1.30540000	-3.12750000
H	-4.04770000	-2.33700000	-2.30360000
H	-2.32050000	-1.33970000	-4.21380000
H	0.00000000	4.67390000	-2.30360000
H	0.00000000	3.27580000	0.07630000
H	0.00000000	2.67950000	-4.21380000
H	-2.83690000	-1.63790000	0.07630000
H	0.00000000	0.00000000	-4.27790000
H	4.04770000	-2.33700000	-2.30360000
H	2.32050000	-1.33970000	-4.21380000
H	2.83690000	-1.63790000	0.07630000
B	0.00000000	0.00000000	-3.07670000

$[Fe(Tb)_2]^+$ ^4E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.41560000	-0.81730000	-1.23410000
N	1.24460000	-0.71860000	-2.56650000
N	0.00000000	1.63460000	-1.23410000
N	0.00000000	1.43720000	-2.56650000
N	-1.41560000	-0.81730000	-1.23410000
N	-1.24460000	-0.71860000	-2.56650000
C	2.56430000	-1.48050000	-1.02550000
C	3.14500000	-1.81580000	-2.24640000
C	2.27050000	-1.31090000	-3.20070000
C	0.00000000	2.96100000	-1.02550000
C	0.00000000	3.63160000	-2.24640000
C	0.00000000	2.62170000	-3.20070000
C	-2.56430000	-1.48050000	-1.02550000
C	-3.14500000	-1.81580000	-2.24640000
C	-2.27050000	-1.31090000	-3.20070000
H	4.07160000	-2.35080000	-2.41700000
H	2.31070000	-1.33410000	-4.28290000
H	0.00000000	4.70150000	-2.41700000
H	0.00000000	3.35700000	-0.01840000
H	0.00000000	2.66820000	-4.28290000
H	2.90730000	-1.67850000	-0.01840000
H	0.00000000	0.00000000	-4.31780000
H	-4.07160000	-2.35080000	-2.41700000
H	-2.31070000	-1.33410000	-4.28290000
H	-2.90730000	-1.67850000	-0.01840000
B	0.00000000	0.00000000	-3.11830000
N	0.00000000	-1.63460000	1.23410000

N	0.00000000	-1.43720000	2.56650000
N	1.41560000	0.81730000	1.23410000
N	1.24460000	0.71860000	2.56650000
N	-1.41560000	0.81730000	1.23410000
N	-1.24460000	0.71860000	2.56650000
C	0.00000000	-2.96100000	1.02550000
C	0.00000000	-3.63160000	2.24640000
C	0.00000000	-2.62170000	3.20070000
C	2.56430000	1.48050000	1.02550000
C	3.14500000	1.81580000	2.24640000
C	2.27050000	1.31090000	3.20070000
C	-2.56430000	1.48050000	1.02550000
C	-3.14500000	1.81580000	2.24640000
C	-2.27050000	1.31090000	3.20070000
H	0.00000000	-4.70150000	2.41700000
H	0.00000000	-2.66820000	4.28290000
H	4.07160000	2.35080000	2.41700000
H	2.90730000	1.67850000	0.01840000
H	2.31070000	1.33410000	4.28290000
H	0.00000000	-3.35700000	0.01840000
H	0.00000000	0.00000000	4.31780000
H	-4.07160000	2.35080000	2.41700000
H	-2.31070000	1.33410000	4.28290000
H	-2.90730000	1.67850000	0.01840000
B	0.00000000	0.00000000	3.11830000

$[Fe(Tb)_2]^+$ ^2E_g D_{3d} LDA

Fe	0.00000000	0.00000000	0.00000000
N	-1.33520000	0.77090000	1.11600000
N	-1.22000000	0.70440000	2.45500000
N	1.33520000	0.77090000	1.11600000
N	1.22000000	0.70440000	2.45500000
N	0.00000000	-1.54180000	1.11600000
N	0.00000000	-1.40870000	2.45500000
C	-2.46760000	1.42460000	0.83760000
C	-3.09470000	1.78670000	2.02290000
C	-2.26850000	1.30970000	3.02630000
C	2.46760000	1.42460000	0.83760000
C	3.09470000	1.78670000	2.02290000
C	2.26850000	1.30970000	3.02630000
C	0.00000000	-2.84930000	0.83760000
C	0.00000000	-3.57350000	2.02290000
C	0.00000000	-2.61940000	3.02630000
H	-4.03130000	2.32740000	2.13860000
H	-2.35460000	1.35950000	4.10990000
H	4.03130000	2.32740000	2.13860000
H	2.76260000	1.59500000	-0.19690000
H	2.35460000	1.35950000	4.10990000
H	-2.76260000	1.59500000	-0.19690000
H	0.00000000	0.00000000	4.23040000
H	0.00000000	-4.65490000	2.13860000
H	0.00000000	-2.71890000	4.10990000
H	0.00000000	-3.19000000	-0.19690000
B	0.00000000	0.00000000	3.03040000
N	-1.33520000	-0.77090000	-1.11600000
N	-1.22000000	-0.70440000	-2.45500000
N	0.00000000	1.54180000	-1.11600000
N	0.00000000	1.40870000	-2.45500000
N	1.33520000	-0.77090000	-1.11600000
N	1.22000000	-0.70440000	-2.45500000
C	-2.46760000	-1.42460000	-0.83760000
C	-3.09470000	-1.78670000	-2.02290000
C	-2.26850000	-1.30970000	-3.02630000
C	0.00000000	2.84930000	-0.83760000
C	0.00000000	3.57350000	-2.02290000
C	0.00000000	2.61940000	-3.02630000
C	2.46760000	-1.42460000	-0.83760000
C	3.09470000	-1.78670000	-2.02290000
C	2.26850000	-1.30970000	-3.02630000
H	-4.03130000	-2.32740000	-2.13860000
H	-2.35460000	-1.35950000	-4.10990000
H	0.00000000	4.65490000	-2.13860000
H	0.00000000	3.19000000	0.19690000
H	0.00000000	2.71890000	-4.10990000
H	-2.76260000	-1.59500000	0.19690000
H	0.00000000	0.00000000	-4.23040000
H	4.03130000	-2.32740000	-2.13860000
H	2.35460000	-1.35950000	-4.10990000
H	2.76260000	-1.59500000	0.19690000
B	0.00000000	0.00000000	-3.03040000

$[Fe(Tb)_2]^+$ ^2E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.36510000	-0.78810000	-1.15140000
N	1.23380000	-0.71230000	-2.48990000
N	0.00000000	1.57620000	-1.15140000
N	0.00000000	1.42470000	-2.48990000
N	-1.36510000	-0.78810000	-1.15140000
N	-1.23380000	-0.71230000	-2.48990000
C	2.50720000	-1.44750000	-0.89750000
C	3.12210000	-1.80250000	-2.09620000
C	2.27730000	-1.31480000	-3.08450000
C	0.00000000	2.89510000	-0.89750000
C	0.00000000	3.60500000	-2.09620000
C	0.00000000	2.62960000	-3.08450000
C	-2.50720000	-1.44750000	-0.89750000
C	-3.12210000	-1.80250000	-2.09620000
C	-2.27730000	-1.31480000	-3.08450000
H	4.05320000	-2.34010000	-2.22820000
H	2.34720000	-1.35520000	-4.16440000
H	0.00000000	4.68030000	-2.22820000
H	0.00000000	3.25970000	0.12040000
H	0.00000000	2.71030000	-4.16440000
H	2.82300000	-1.62990000	0.12040000
H	0.00000000	0.00000000	-4.26210000
H	-4.05320000	-2.34010000	-2.22820000
H	-2.34720000	-1.35520000	-4.16440000
H	-2.82300000	-1.62990000	0.12040000
B	0.00000000	0.00000000	-3.06350000
N	0.00000000	-1.57620000	1.15140000
N	0.00000000	-1.42470000	2.48990000
N	1.36510000	0.78810000	1.15140000
N	1.23380000	0.71230000	2.48990000
N	-1.36510000	0.78810000	1.15140000
N	-1.23380000	0.71230000	2.48990000
C	0.00000000	-2.89510000	0.89750000
C	0.00000000	-3.60500000	2.09620000
C	0.00000000	-2.62960000	3.08450000

C	2.50720000	1.44750000	0.89750000
C	3.12210000	1.80250000	2.09620000
C	2.27730000	1.31480000	3.08450000
C	-2.50720000	1.44750000	0.89750000
C	-3.12210000	1.80250000	2.09620000
C	-2.27730000	1.31480000	3.08450000
H	0.00000000	-4.68030000	2.22820000
H	0.00000000	-2.71030000	4.16440000
H	4.05320000	2.34010000	2.22820000
H	2.82300000	1.62990000	-0.12040000
H	2.34720000	1.35520000	4.16440000
H	0.00000000	-3.25970000	-0.12040000
H	0.00000000	0.00000000	4.26210000
H	-4.05320000	2.34010000	2.22820000
H	-2.34720000	1.35520000	4.16440000
H	-2.82300000	1.62990000	-0.12040000
B	0.00000000	0.00000000	3.06350000

$[Fe(Tb)_2]$ $^5A_{1g}$ D_{3d} LDA

Fe	0.00000000	0.00000000	0.00000000
N	1.43150000	-0.82650000	-1.30300000
N	1.23900000	-0.71530000	-2.62810000
N	0.00000000	1.65290000	-1.30300000
N	0.00000000	1.43070000	-2.62810000
N	-1.43150000	-0.82650000	-1.30300000
N	-1.23900000	-0.71530000	-2.62810000
C	2.57380000	-1.48600000	-1.12530000
C	3.13600000	-1.81060000	-2.36060000
C	2.25130000	-1.29980000	-3.29050000
C	0.00000000	2.97190000	-1.12530000
C	0.00000000	3.62110000	-2.36060000
C	0.00000000	2.59950000	-3.29050000
C	-2.57380000	-1.48600000	-1.12530000
C	-3.13600000	-1.81060000	-2.36060000
C	-2.25130000	-1.29980000	-3.29050000
H	4.06300000	-2.34580000	-2.55430000
H	2.26710000	-1.30890000	-4.37840000
H	0.00000000	4.69160000	-2.55430000
H	0.00000000	3.37880000	-0.11430000
H	0.00000000	2.61790000	-4.37840000
H	2.92610000	-1.68940000	-0.11430000
H	0.00000000	0.00000000	-4.36360000
H	-4.06300000	-2.34580000	-2.55430000
H	-2.26710000	-1.30890000	-4.37840000
H	-2.92610000	-1.68940000	-0.11430000
B	0.00000000	0.00000000	-3.15660000
N	0.00000000	-1.65290000	1.30300000
N	0.00000000	-1.43070000	2.62810000
N	1.43150000	0.82650000	1.30300000
N	1.23900000	0.71530000	2.62810000
N	-1.43150000	0.82650000	1.30300000
N	-1.23900000	0.71530000	2.62810000
C	0.00000000	-2.97190000	1.12530000
C	0.00000000	-3.62110000	2.36060000
C	0.00000000	-2.59950000	3.29050000
C	2.57380000	1.48600000	1.12530000
C	3.13600000	1.81060000	2.36060000
C	2.25130000	1.29980000	3.29050000
C	-2.57380000	1.48600000	1.12530000
C	-3.13600000	1.81060000	2.36060000
C	-2.25130000	1.29980000	3.29050000
H	0.00000000	-4.69160000	2.55430000
H	0.00000000	-2.61790000	4.37840000
H	4.06300000	2.34580000	2.55430000
H	2.92610000	1.68940000	0.11430000
H	2.26710000	1.30890000	4.37840000
H	0.00000000	-3.37880000	0.11430000
H	0.00000000	0.00000000	4.36360000
H	-4.06300000	2.34580000	2.55430000
H	-2.26710000	1.30890000	4.37840000
H	-2.92610000	1.68940000	0.11430000
B	0.00000000	0.00000000	3.15660000

$[Fe(Tb)_2]$ $^5A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.72520000	-1.37560000
N	0.00000000	1.45660000	-2.69560000
N	-1.49400000	-0.86260000	-1.37560000
N	-1.26150000	-0.72830000	-2.69560000
N	1.49400000	-0.86260000	-1.37560000
N	1.26150000	-0.72830000	-2.69560000
C	0.00000000	3.05750000	-1.25610000
C	0.00000000	3.66480000	-2.51650000
C	0.00000000	2.60170000	-3.40680000
C	-2.64790000	-1.52880000	-1.25610000
C	-3.17380000	-1.83240000	-2.51650000
C	-2.25320000	-1.30090000	-3.40680000
C	2.64790000	-1.52880000	-1.25610000
C	3.17380000	-1.83240000	-2.51650000
C	2.25320000	-1.30090000	-3.40680000
H	0.00000000	4.72310000	-2.75120000
H	0.00000000	2.58070000	-4.48960000
H	-4.09030000	-2.36150000	-2.75120000
H	-3.04010000	-1.75520000	-0.27180000
H	-2.23490000	-1.29030000	-4.48960000
H	0.00000000	3.51040000	-0.27180000
H	0.00000000	0.00000000	-4.41150000
H	4.09030000	-2.36150000	-2.75120000
H	2.23490000	-1.29030000	-4.48960000
H	3.04010000	-1.75520000	-0.27180000
B	0.00000000	0.00000000	-3.20500000
N	1.49400000	0.86260000	1.37560000
N	1.26150000	0.72830000	2.69560000
N	-1.49400000	0.86260000	1.37560000
N	-1.26150000	0.72830000	2.69560000
N	0.00000000	-1.72520000	1.37560000
N	0.00000000	-1.45660000	2.69560000
C	2.64790000	1.52880000	1.25610000
C	3.17380000	1.83240000	2.51650000
C	2.25320000	1.30090000	3.40680000
C	-2.64790000	1.52880000	1.25610000
C	-3.17380000	1.83240000	2.51650000
C	-2.25320000	1.30090000	3.40680000
C	0.00000000	-3.05750000	1.25610000
C	0.00000000	-3.66480000	2.51650000
C	0.00000000	-2.60170000	3.40680000
H	4.09030000	2.36150000	2.75120000
H	2.23490000	1.29030000	4.48960000

H	-4.09030000	2.36150000	2.75120000
H	-3.04010000	1.75520000	0.27180000
H	-2.23490000	1.29030000	4.48960000
H	3.04010000	1.75520000	0.27180000
H	0.00000000	0.00000000	4.41150000
H	0.00000000	-4.72310000	2.75120000
H	0.00000000	-2.58070000	4.48960000
H	0.00000000	-3.51040000	0.27180000
B	0.00000000	0.00000000	3.20500000

$[Fe(Tb)_2]$ ^3E_g D_{3d} LDA

Fe	0.00000000	0.00000000	0.00000000
N	1.38070000	-0.79710000	-1.19920000
N	1.23050000	-0.71040000	-2.53200000
N	0.00000000	1.59430000	-1.19920000
N	0.00000000	1.42080000	-2.53200000
N	-1.38070000	-0.79710000	-1.19920000
N	-1.23050000	-0.71040000	-2.53200000
C	2.51820000	-1.45390000	-0.97290000
C	3.11690000	-1.79950000	-2.18450000
C	2.26160000	-1.30580000	-3.15190000
C	0.00000000	2.90770000	-0.97290000
C	0.00000000	3.59910000	-2.18450000
C	0.00000000	2.61150000	-3.15190000
C	-2.51820000	-1.45390000	-0.97290000
C	-3.11690000	-1.79950000	-2.18450000
C	-2.26160000	-1.30580000	-3.15190000
H	4.04950000	-2.33800000	-2.33910000
H	2.31170000	-1.33470000	-4.23840000
H	0.00000000	4.67590000	-2.33910000
H	0.00000000	3.27640000	0.05250000
H	0.00000000	2.66940000	-4.23840000
H	2.83740000	-1.63820000	0.05250000
H	0.00000000	0.00000000	-4.28580000
H	-4.04950000	-2.33800000	-2.33910000
H	-2.31170000	-1.33470000	-4.23840000
H	-2.83740000	-1.63820000	0.05250000
B	0.00000000	0.00000000	-3.07920000
N	0.00000000	-1.59430000	1.19920000
N	0.00000000	-1.42080000	2.53200000
N	1.38070000	0.79710000	1.19920000
N	1.23050000	0.71040000	2.53200000
N	-1.38070000	0.79710000	1.19920000
N	-1.23050000	0.71040000	2.53200000
C	0.00000000	-2.90770000	0.97290000
C	0.00000000	-3.59910000	2.18450000
C	0.00000000	-2.61150000	3.15190000
C	2.51820000	1.45390000	0.97290000
C	3.11690000	1.79950000	2.18450000
C	2.26160000	1.30580000	3.15190000
C	-2.51820000	1.45390000	0.97290000
C	-3.11690000	1.79950000	2.18450000
C	-2.26160000	1.30580000	3.15190000
H	0.00000000	-4.67590000	2.33910000
H	0.00000000	-2.66940000	4.23840000
H	4.04950000	2.33800000	2.33910000
H	2.83740000	1.63820000	-0.05250000
H	2.31170000	1.33470000	4.23840000
H	0.00000000	-3.27640000	-0.05250000
H	0.00000000	0.00000000	4.28580000
H	-4.04950000	2.33800000	2.33910000
H	-2.31170000	1.33470000	4.23840000
H	-2.83740000	1.63820000	-0.05250000
B	0.00000000	0.00000000	3.07920000

$[Fe(Tb)_2]$ ^3E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.64670000	-1.26460000
N	0.00000000	1.44160000	-2.59520000
N	-1.42610000	-0.82340000	-1.26460000
N	-1.24850000	-0.72080000	-2.59520000
N	1.42610000	-0.82340000	-1.26460000
N	1.24850000	-0.72080000	-2.59520000
C	0.00000000	2.97250000	-1.07790000
C	0.00000000	3.63710000	-2.30930000
C	0.00000000	2.61930000	-3.25100000
C	-2.57430000	-1.48630000	-1.07790000
C	-3.14980000	-1.81860000	-2.30930000
C	-2.26840000	-1.30970000	-3.25100000
C	2.57430000	-1.48630000	-1.07790000
C	3.14980000	-1.81860000	-2.30930000
C	2.26840000	-1.30970000	-3.25100000
H	0.00000000	4.70580000	-2.49120000
H	0.00000000	2.64920000	-4.33360000
H	-4.07530000	-2.35290000	-2.49120000
H	-2.92450000	-1.68840000	-0.07390000
H	-2.29420000	-1.32460000	-4.33360000
H	0.00000000	3.37690000	-0.07390000
H	0.00000000	0.00000000	-4.33870000
H	4.07530000	-2.35290000	-2.49120000
H	2.29420000	-1.32460000	-4.33360000
H	2.92450000	-1.68840000	-0.07390000
B	0.00000000	0.00000000	-3.13300000
N	1.42610000	0.82340000	1.26460000
N	1.24850000	0.72080000	2.59520000
N	-1.42610000	0.82340000	1.26460000
N	-1.24850000	0.72080000	2.59520000
N	0.00000000	-1.64670000	1.26460000
N	0.00000000	-1.44160000	2.59520000
C	2.57430000	1.48630000	1.07790000
C	3.14980000	1.81860000	2.30930000
C	2.26840000	1.30970000	3.25100000
C	-2.57430000	1.48630000	1.07790000
C	-3.14980000	1.81860000	2.30930000
C	-2.26840000	1.30970000	3.25100000
C	0.00000000	-2.97250000	1.07790000
C	0.00000000	-3.63710000	2.30930000
C	0.00000000	-2.61930000	3.25100000
H	4.07530000	2.35290000	2.49120000
H	2.29420000	1.32460000	4.33360000
H	-4.07530000	2.35290000	2.49120000
H	-2.92450000	1.68840000	0.07390000
H	-2.29420000	1.32460000	4.33360000
H	2.92450000	1.68840000	0.07390000
H	0.00000000	0.00000000	4.33870000
H	0.00000000	-4.70580000	2.49120000
H	0.00000000	-2.64920000	4.33360000
H	0.00000000	-3.37690000	0.07390000

B	0.00000000	0.00000000	3.13300000

$[Fe(Tb)_2]$ $^1A_{1g}$ D_{3d} LDA

Fe	0.00000000	0.00000000	0.00000000
N	1.33450000	-0.77050000	-1.11230000
N	1.22130000	-0.70510000	-2.45200000
N	0.00000000	1.54090000	-1.11230000
N	0.00000000	1.41020000	-2.45200000
N	-1.33450000	-0.77050000	-1.11230000
N	-1.22130000	-0.70510000	-2.45200000
C	2.46580000	-1.42360000	-0.84160000
C	3.09610000	-1.78750000	-2.03270000
C	2.27070000	-1.31100000	-3.03220000
C	0.00000000	2.84730000	-0.84160000
C	0.00000000	3.57500000	-2.03270000
C	0.00000000	2.62200000	-3.03220000
C	-2.46580000	-1.42360000	-0.84160000
C	-3.09610000	-1.78750000	-2.03270000
C	-2.27070000	-1.31100000	-3.03220000
H	4.03250000	-2.32820000	-2.14930000
H	2.35060000	-1.35710000	-4.11590000
H	0.00000000	4.65630000	-2.14930000
H	0.00000000	3.18450000	0.19370000
H	0.00000000	2.71420000	-4.11590000
H	2.75790000	-1.59230000	0.19370000
H	0.00000000	0.00000000	-4.22520000
H	-4.03250000	-2.32820000	-2.14930000
H	-2.35060000	-1.35710000	-4.11590000
H	-2.75790000	-1.59230000	0.19370000
B	0.00000000	0.00000000	-3.02000000
N	0.00000000	-1.54090000	1.11230000
N	0.00000000	-1.41020000	2.45200000
N	1.33450000	0.77050000	1.11230000
N	1.22130000	0.70510000	2.45200000
N	-1.33450000	0.77050000	1.11230000
N	-1.22130000	0.70510000	2.45200000
C	0.00000000	-2.84730000	0.84160000
C	0.00000000	-3.57500000	2.03270000
C	0.00000000	-2.62200000	3.03220000
C	2.46580000	1.42360000	0.84160000
C	3.09610000	1.78750000	2.03270000
C	2.27070000	1.31100000	3.03220000
C	-2.46580000	1.42360000	0.84160000
C	-3.09610000	1.78750000	2.03270000
C	-2.27070000	1.31100000	3.03220000
H	0.00000000	-4.65630000	2.14930000
H	0.00000000	-2.71420000	4.11590000
H	4.03250000	2.32820000	2.14930000
H	2.75790000	1.59230000	-0.19370000
H	2.35060000	1.35710000	4.11590000
H	0.00000000	-3.18450000	-0.19370000
H	0.00000000	0.00000000	4.22520000
H	-4.03250000	2.32820000	2.14930000
H	-2.35060000	1.35710000	4.11590000
H	-2.75790000	1.59230000	-0.19370000
B	0.00000000	0.00000000	3.02000000

$[Fe(Tb)_2]$ $^1A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.58050000	-1.15400000
N	0.00000000	1.42830000	-2.49280000
N	-1.36880000	-0.79030000	-1.15400000
N	-1.23690000	-0.71410000	-2.49280000
N	1.36880000	-0.79030000	-1.15400000
N	1.23690000	-0.71410000	-2.49280000
C	0.00000000	2.89870000	-0.91290000
C	0.00000000	3.60940000	-2.11890000
C	0.00000000	2.63190000	-3.10070000
C	-2.51030000	-1.44930000	-0.91290000
C	-3.12580000	-1.80470000	-2.11890000
C	-2.27930000	-1.31600000	-3.10070000
C	2.51030000	-1.44930000	-0.91290000
C	3.12580000	-1.80470000	-2.11890000
C	2.27930000	-1.31600000	-3.10070000
H	0.00000000	4.68450000	-2.25520000
H	0.00000000	2.70300000	-4.18120000
H	-4.05690000	-2.34230000	-2.25520000
H	-2.82770000	-1.63250000	0.10420000
H	-2.34080000	-1.35150000	-4.18120000
H	0.00000000	3.26510000	0.10420000
H	0.00000000	0.00000000	-4.25970000
H	4.05690000	-2.34230000	-2.25520000
H	2.34080000	-1.35150000	-4.18120000
H	2.82770000	-1.63250000	0.10420000
B	0.00000000	0.00000000	-3.05500000
N	1.36880000	0.79030000	1.15400000
N	1.23690000	0.71410000	2.49280000
N	-1.36880000	0.79030000	1.15400000
N	-1.23690000	0.71410000	2.49280000
N	0.00000000	-1.58050000	1.15400000
N	0.00000000	-1.42830000	2.49280000
C	2.51030000	1.44930000	0.91290000
C	3.12580000	1.80470000	2.11890000
C	2.27930000	1.31600000	3.10070000
C	-2.51030000	1.44930000	0.91290000
C	-3.12580000	1.80470000	2.11890000
C	-2.27930000	1.31600000	3.10070000
C	0.00000000	-2.89870000	0.91290000
C	0.00000000	-3.60940000	2.11890000
C	0.00000000	-2.63190000	3.10070000
H	4.05690000	2.34230000	2.25520000
H	2.34080000	1.35150000	4.18120000
H	-4.05690000	2.34230000	2.25520000
H	-2.82770000	1.63250000	-0.10420000
H	-2.34080000	1.35150000	4.18120000
H	2.82770000	1.63250000	-0.10420000
H	0.00000000	0.00000000	4.25970000
H	0.00000000	-4.68450000	2.25520000
H	0.00000000	-2.70300000	4.18120000
H	0.00000000	-3.26510000	-0.10420000
B	0.00000000	0.00000000	3.05500000

$[Co(Tb)_2]^+$ $^5A_{1g}$ D_{3d} LDA

Co	0.00000000	0.00000000	0.00000000
N	-1.39940000	-0.80800000	-1.21820000
N	-1.23280000	-0.71180000	-2.54990000
N	1.39940000	-0.80800000	-1.21820000

N	1.23280000	-0.71180000	-2.54990000
N	0.00000000	1.61590000	-1.21820000
N	0.00000000	1.42350000	-2.54990000
C	-2.54200000	-1.46760000	-1.00350000
C	-3.12470000	-1.80410000	-2.21700000
C	-2.25640000	-1.30270000	-3.17680000
C	2.54200000	-1.46760000	-1.00350000
C	3.12470000	-1.80410000	-2.21700000
C	2.25640000	-1.30270000	-3.17680000
C	0.00000000	2.93520000	-1.00350000
C	0.00000000	3.60810000	-2.21700000
C	0.00000000	2.60540000	-3.17680000
H	-4.05540000	-2.34140000	-2.38600000
H	-2.30160000	-1.32880000	-4.26410000
H	4.05540000	-2.34140000	-2.38600000
H	2.87550000	-1.66020000	0.01600000
H	2.30160000	-1.32880000	-4.26410000
H	-2.87550000	-1.66020000	0.01600000
H	0.00000000	0.00000000	-4.29820000
H	0.00000000	4.68280000	-2.38600000
H	0.00000000	2.65770000	-4.26410000
H	0.00000000	3.32030000	0.01600000
B	0.00000000	0.00000000	-3.09620000
N	-1.39940000	0.80800000	1.21820000
N	-1.23280000	0.71180000	2.54990000
N	0.00000000	-1.61590000	1.21820000
N	0.00000000	-1.42350000	2.54990000
N	1.39940000	0.80800000	1.21820000
N	1.23280000	0.71180000	2.54990000
C	-2.54200000	1.46760000	1.00350000
C	-3.12470000	1.80410000	2.21700000
C	-2.25640000	1.30270000	3.17680000
C	0.00000000	-2.93520000	1.00350000
C	0.00000000	-3.60810000	2.21700000
C	0.00000000	-2.60540000	3.17680000
C	2.54200000	1.46760000	1.00350000
C	3.12470000	1.80410000	2.21700000
C	2.25640000	1.30270000	3.17680000
H	-4.05540000	2.34140000	2.38600000
H	-2.30160000	1.32880000	4.26410000
H	0.00000000	-4.68280000	2.38600000
H	0.00000000	-3.32030000	-0.01600000
H	0.00000000	-2.65770000	4.26410000
H	-2.87550000	1.66020000	-0.01600000
H	0.00000000	0.00000000	4.29820000
H	4.05540000	2.34140000	2.38600000
H	2.30160000	1.32880000	4.26410000
H	2.87550000	1.66020000	-0.01600000
B	0.00000000	0.00000000	3.09620000

$[Co(Tb)_2]^+$ $^5A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.43750000	-0.82990000	-1.27350000
N	1.24940000	-0.72140000	-2.60410000
N	0.00000000	1.65980000	-1.27350000
N	0.00000000	1.44270000	-2.60410000
N	-1.43750000	-0.82990000	-1.27350000
N	-1.24940000	-0.72140000	-2.60410000
C	2.59000000	-1.49540000	-1.09030000
C	3.15530000	-1.82170000	-2.31980000
C	2.26550000	-1.30800000	-3.25880000
C	0.00000000	2.99070000	-1.09030000
C	0.00000000	3.64340000	-2.31980000
C	0.00000000	2.61600000	-3.25880000
C	-2.59000000	-1.49540000	-1.09030000
C	-3.15530000	-1.82170000	-2.31980000
C	-2.26550000	-1.30800000	-3.25880000
H	4.07900000	-2.35500000	-2.51000000
H	2.29170000	-1.32310000	-4.34160000
H	0.00000000	4.71010000	-2.51000000
H	0.00000000	3.40360000	-0.08960000
H	0.00000000	2.64630000	-4.34160000
H	2.94760000	-1.70180000	-0.08960000
H	0.00000000	0.00000000	-4.34660000
H	-4.07900000	-2.35500000	-2.51000000
H	-2.29170000	-1.32310000	-4.34160000
H	-2.94760000	-1.70180000	-0.08960000
B	0.00000000	0.00000000	-3.14620000
N	0.00000000	-1.65980000	1.27350000
N	0.00000000	-1.44270000	2.60410000
N	1.43750000	0.82990000	1.27350000
N	1.24940000	0.72140000	2.60410000
N	-1.43750000	0.82990000	1.27350000
N	-1.24940000	0.72140000	2.60410000
C	0.00000000	-2.99070000	1.09030000
C	0.00000000	-3.64340000	2.31980000
C	0.00000000	-2.61600000	3.25880000
C	2.59000000	1.49540000	1.09030000
C	3.15530000	1.82170000	2.31980000
C	2.26550000	1.30800000	3.25880000
C	-2.59000000	1.49540000	1.09030000
C	-3.15530000	1.82170000	2.31980000
C	-2.26550000	1.30800000	3.25880000
H	0.00000000	-4.71010000	2.51000000
H	0.00000000	-2.64630000	4.34160000
H	4.07900000	2.35500000	2.51000000
H	2.94760000	1.70180000	0.08960000
H	2.29170000	1.32310000	4.34160000
H	0.00000000	-3.40360000	0.08960000
H	0.00000000	0.00000000	4.34660000
H	-4.07900000	2.35500000	2.51000000
H	-2.29170000	1.32310000	4.34160000
H	-2.94760000	1.70180000	0.08960000
B	0.00000000	0.00000000	3.14620000

$[Co(Tb)_2]^+$ ^3E_g D_{3d} LDA

Co	0.00000000	0.00000000	0.00000000
N	-1.36270000	-0.78680000	-1.15680000
N	-1.22550000	-0.70750000	-2.49100000
N	1.36270000	-0.78680000	-1.15680000
N	1.22550000	-0.70750000	-2.49100000
N	0.00000000	1.57350000	-1.15680000
N	0.00000000	1.41510000	-2.49100000
C	-2.49720000	-1.44180000	-0.90060000
C	-3.10750000	-1.79410000	-2.09810000
C	-2.26500000	-1.30770000	-3.08470000
C	2.49720000	-1.44180000	-0.90060000
C	3.10750000	-1.79410000	-2.09810000

C	2.26500000	-1.30770000	-3.08470000
C	0.00000000	2.88360000	-0.90060000
C	0.00000000	3.58820000	-2.09810000
C	0.00000000	2.61540000	-3.08470000
H	-4.04210000	-2.33370000	-2.23410000
H	-2.33500000	-1.34810000	-4.17010000
H	4.04210000	-2.33370000	-2.23410000
H	2.80640000	-1.62030000	0.12890000
H	2.33500000	-1.34810000	-4.17010000
H	-2.80640000	-1.62030000	0.12890000
H	0.00000000	0.00000000	-4.25570000
H	0.00000000	4.66740000	-2.23410000
H	0.00000000	2.69620000	-4.17010000
H	0.00000000	3.24050000	0.12890000
B	0.00000000	0.00000000	-3.05510000
N	-1.36270000	0.78680000	1.15680000
N	-1.22550000	0.70750000	2.49100000
N	0.00000000	-1.57350000	1.15680000
N	0.00000000	-1.41510000	2.49100000
N	1.36270000	0.78680000	1.15680000
N	1.22550000	0.70750000	2.49100000
C	-2.49720000	1.44180000	0.90060000
C	-3.10750000	1.79410000	2.09810000
C	-2.26500000	1.30770000	3.08470000
C	0.00000000	-2.88360000	0.90060000
C	0.00000000	-3.58820000	2.09810000
C	0.00000000	-2.61540000	3.08470000
C	2.49720000	1.44180000	0.90060000
C	3.10750000	1.79410000	2.09810000
C	2.26500000	1.30770000	3.08470000
H	-4.04210000	2.33370000	2.23410000
H	-2.33500000	1.34810000	4.17010000
H	0.00000000	-4.66740000	2.23410000
H	0.00000000	-3.24050000	-0.12890000
H	0.00000000	-2.69620000	4.17010000
H	-2.80640000	1.62030000	-0.12890000
H	0.00000000	0.00000000	4.25570000
H	4.04210000	2.33370000	2.23410000
H	2.33500000	1.34810000	4.17010000
H	2.80640000	1.62030000	-0.12890000
B	0.00000000	0.00000000	3.05510000

$[Co(Tb)_2]^+$ ^3E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.39860000	-0.80750000	-1.20590000
N	1.24080000	-0.71640000	-2.53900000
N	0.00000000	1.61500000	-1.20590000
N	0.00000000	1.43280000	-2.53900000
N	-1.39860000	-0.80750000	-1.20590000
N	-1.24080000	-0.71640000	-2.53900000
C	2.54360000	-1.46860000	-0.97930000
C	3.13730000	-1.81130000	-2.19290000
C	2.27340000	-1.31260000	-3.16020000
C	0.00000000	2.93710000	-0.97930000
C	0.00000000	3.62260000	-2.19290000
C	0.00000000	2.62510000	-3.16020000
C	-2.54360000	-1.46860000	-0.97930000
C	-3.13730000	-1.81130000	-2.19290000
C	-2.27340000	-1.31260000	-3.16020000
H	4.06580000	-2.34740000	-2.34910000
H	2.32410000	-1.34180000	-4.24170000
H	0.00000000	4.69480000	-2.34910000
H	0.00000000	3.32130000	0.03200000
H	0.00000000	2.68370000	-4.24170000
H	2.87630000	-1.66060000	0.03200000
H	0.00000000	0.00000000	-4.29840000
H	-4.06580000	-2.34740000	-2.34910000
H	-2.32410000	-1.34180000	-4.24170000
H	-2.87630000	-1.66060000	0.03200000
B	0.00000000	0.00000000	-3.09920000
N	0.00000000	-1.61500000	1.20590000
N	0.00000000	-1.43280000	2.53900000
N	1.39860000	0.80750000	1.20590000
N	1.24080000	0.71640000	2.53900000
N	-1.39860000	0.80750000	1.20590000
N	-1.24080000	0.71640000	2.53900000
C	0.00000000	-2.93710000	0.97930000
C	0.00000000	-3.62260000	2.19290000
C	0.00000000	-2.62510000	3.16020000
C	2.54360000	1.46860000	0.97930000
C	3.13730000	1.81130000	2.19290000
C	2.27340000	1.31260000	3.16020000
C	-2.54360000	1.46860000	0.97930000
C	-3.13730000	1.81130000	2.19290000
C	-2.27340000	1.31260000	3.16020000
H	0.00000000	-4.69480000	2.34910000
H	0.00000000	-2.68370000	4.24170000
H	4.06580000	2.34740000	2.34910000
H	2.87630000	1.66060000	-0.03200000
H	2.32410000	1.34180000	4.24170000
H	0.00000000	-3.32130000	-0.03200000
H	0.00000000	0.00000000	4.29840000
H	-4.06580000	2.34740000	2.34910000
H	-2.32410000	1.34180000	4.24170000
H	-2.87630000	1.66060000	-0.03200000
B	0.00000000	0.00000000	3.09920000

$[Co(Tb)_2]^+$ $^1A_{1g}$ D_{3d} LDA

Co	0.00000000	0.00000000	0.00000000
N	-1.32920000	-0.76740000	-1.09320000
N	-1.21800000	-0.70320000	-2.42950000
N	1.32920000	-0.76740000	-1.09320000
N	1.21800000	-0.70320000	-2.42950000
N	0.00000000	1.53480000	-1.09320000
N	0.00000000	1.40640000	-2.42950000
C	-2.45600000	-1.41800000	-0.80130000
C	-3.08970000	-1.78390000	-1.98440000
C	-2.27130000	-1.31130000	-2.99300000
C	2.45600000	-1.41800000	-0.80130000
C	3.08970000	-1.78390000	-1.98440000
C	2.27130000	-1.31130000	-2.99300000
C	0.00000000	2.83590000	-0.80130000
C	0.00000000	3.56770000	-1.98440000
C	0.00000000	2.62270000	-2.99300000
H	-4.02710000	-2.32500000	-2.09060000
H	-2.36230000	-1.36390000	-4.07600000
H	4.02710000	-2.32500000	-2.09060000
H	2.74520000	-1.58490000	0.23520000

H	2.36230000	-1.36390000	-4.07600000
H	-2.74520000	-1.58490000	0.23520000
H	0.00000000	0.00000000	-4.20930000
H	0.00000000	4.65010000	-2.09060000
H	0.00000000	2.72780000	-4.07600000
H	0.00000000	3.16980000	0.23520000
B	0.00000000	0.00000000	-3.01010000
N	-1.32920000	0.76740000	1.09320000
N	-1.21800000	0.70320000	2.42950000
N	0.00000000	-1.53480000	1.09320000
N	0.00000000	-1.40640000	2.42950000
N	1.32920000	0.76740000	1.09320000
N	1.21800000	0.70320000	2.42950000
C	-2.45600000	1.41800000	0.80130000
C	-3.08970000	1.78390000	1.98440000
C	-2.27130000	1.31130000	2.99300000
C	0.00000000	-2.83590000	0.80130000
C	0.00000000	-3.56770000	1.98440000
C	0.00000000	-2.62270000	2.99300000
C	2.45600000	1.41800000	0.80130000
C	3.08970000	1.78390000	1.98440000
C	2.27130000	1.31130000	2.99300000
H	-4.02710000	2.32500000	2.09060000
H	-2.36230000	1.36390000	4.07600000
H	0.00000000	-4.65010000	2.09060000
H	0.00000000	-3.16980000	-0.23520000
H	0.00000000	-2.72780000	4.07600000
H	-2.74520000	1.58490000	-0.23520000
H	0.00000000	0.00000000	4.20930000
H	4.02710000	2.32500000	2.09060000
H	2.36230000	1.36390000	4.07600000
H	2.74520000	1.58490000	-0.23520000
B	0.00000000	0.00000000	3.01010000

$[Co(Tb)_2]^+$ $^1A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.35860014	-0.78438832	-1.12954101
N	-1.23162988	-0.71108193	-2.46590830
N	1.35860014	-0.78438832	-1.12954101
N	1.23162988	-0.71108193	-2.46590830
N	0.00000000	1.56877612	-1.12954101
N	0.00000000	1.42216333	-2.46590830
C	-2.49569092	-1.44088773	-0.86216415
C	-3.11705931	-1.79963498	-2.05870958
C	-2.28002685	-1.31637444	-3.05259600
C	2.49569092	-1.44088773	-0.86216415
C	3.11705931	-1.79963498	-2.05870958
C	2.28002685	-1.31637444	-3.05259600
C	0.00000000	2.88177547	-0.86216415
C	0.00000000	3.59927049	-2.05870958
C	0.00000000	2.63274836	-3.05259600
H	-4.04922673	-2.33782200	-2.18081194
H	-2.35460116	-1.35942936	-4.13199799
H	4.04922673	-2.33782200	-2.18081194
H	2.80538609	-1.61969038	0.15801233
H	2.35460116	-1.35942936	-4.13199799
H	-2.80538609	-1.61969038	0.15801233
H	0.00000000	0.00000000	-4.24275267
H	0.00000000	4.67564454	-2.18081194
H	0.00000000	2.71885926	-4.13199799
H	0.00000000	3.23938075	0.15801233
B	0.00000000	0.00000000	-3.04473190
N	-1.35860014	0.78438832	1.12954101
N	-1.23162988	0.71108193	2.46590830
N	0.00000000	-1.56877612	1.12954101
N	0.00000000	-1.42216333	2.46590830
N	1.35860014	0.78438832	1.12954101
N	1.23162988	0.71108193	2.46590830
C	-2.49569092	1.44088773	0.86216415
C	-3.11705931	1.79963498	2.05870958
C	-2.28002685	1.31637444	3.05259600
C	0.00000000	-2.88177547	0.86216415
C	0.00000000	-3.59927049	2.05870958
C	0.00000000	-2.63274836	3.05259600
C	2.49569092	1.44088773	0.86216415
C	3.11705931	1.79963498	2.05870958
C	2.28002685	1.31637444	3.05259600
H	-4.04922673	2.33782200	2.18081194
H	-2.35460116	1.35942936	4.13199799
H	0.00000000	-4.67564454	2.18081194
H	0.00000000	-3.23938075	-0.15801233
H	0.00000000	-2.71885926	4.13199799
H	-2.80538609	1.61969038	-0.15801233
H	0.00000000	0.00000000	4.24275267
H	4.04922673	2.33782200	2.18081194
H	2.35460116	1.35942936	4.13199799
H	2.80538609	1.61969038	-0.15801233
B	0.00000000	0.00000000	3.04473190

$[Co(Tb)_2]$ ^4E_g D_{3d} LDA

Co	0.00000000	0.00000000	0.00000000
N	-1.41070000	-0.81450000	-1.25100000
N	-1.23570000	-0.71340000	-2.57810000
N	1.41070000	-0.81450000	-1.25100000
N	1.23570000	-0.71340000	-2.57810000
N	0.00000000	1.62900000	-1.25100000
N	0.00000000	1.42680000	-2.57810000
C	-2.55060000	-1.47260000	-1.05380000
C	-3.12840000	-1.80620000	-2.27910000
C	-2.25470000	-1.30170000	-3.22430000
C	2.55060000	-1.47260000	-1.05380000
C	3.12840000	-1.80620000	-2.27910000
C	2.25470000	-1.30170000	-3.22430000
C	0.00000000	2.94520000	-1.05380000
C	0.00000000	3.61240000	-2.27910000
C	0.00000000	2.60350000	-3.22430000
H	-4.05780000	-2.34280000	-2.45760000
H	-2.28410000	-1.31870000	-4.31180000
H	4.05780000	-2.34280000	-2.45760000
H	2.88920000	-1.66810000	-0.03650000
H	2.28410000	-1.31870000	-4.31180000
H	-2.88920000	-1.66810000	-0.03650000
H	0.00000000	0.00000000	-4.32010000
H	0.00000000	4.68560000	-2.45760000
H	0.00000000	2.63740000	-4.31180000
H	0.00000000	3.33620000	-0.03650000
B	0.00000000	0.00000000	-3.11290000
N	-1.41070000	0.81450000	1.25100000

N	-1.23570000	0.71340000	2.57810000
N	0.00000000	-1.62900000	1.25100000
N	0.00000000	-1.42680000	2.57810000
N	1.41070000	0.81450000	1.25100000
N	1.23570000	0.71340000	2.57810000
C	-2.55060000	1.47260000	1.05380000
C	-3.12840000	1.80620000	2.27910000
C	-2.25470000	1.30170000	3.22430000
C	0.00000000	-2.94520000	1.05380000
C	0.00000000	-3.61240000	2.27910000
C	0.00000000	-2.60350000	3.22430000
C	2.55060000	1.47260000	1.05380000
C	3.12840000	1.80620000	2.27910000
C	2.25470000	1.30170000	3.22430000
H	-4.05780000	2.34280000	2.45760000
H	-2.28410000	1.31870000	4.31180000
H	0.00000000	-4.68560000	2.45760000
H	0.00000000	-3.33620000	0.03650000
H	0.00000000	-2.63740000	4.31180000
H	-2.88920000	1.66810000	0.03650000
H	0.00000000	0.00000000	4.32010000
H	4.05780000	2.34280000	2.45760000
H	2.28410000	1.31870000	4.31180000
H	2.88920000	1.66810000	0.03650000
B	0.00000000	0.00000000	3.11290000

$[Co(Tb)_2]$ ^4E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.46100000	-0.84350000	1.33470000
N	-1.25500000	-0.72460000	2.65920000
N	0.00000000	1.68700000	1.33470000
N	0.00000000	1.44910000	2.65920000
N	1.46100000	-0.84350000	1.33470000
N	1.25500000	-0.72460000	2.65920000
C	-2.61150000	-1.50770000	1.18190000
C	-3.16280000	-1.82600000	2.42820000
C	-2.26070000	-1.30520000	3.34330000
C	0.00000000	3.01550000	1.18190000
C	0.00000000	3.65210000	2.42820000
C	0.00000000	2.61040000	3.34330000
C	2.61150000	-1.50770000	1.18190000
C	3.16280000	-1.82600000	2.42820000
C	2.26070000	-1.30520000	3.34330000
H	-4.08390000	-2.35790000	2.63730000
H	-2.26390000	-1.30710000	4.42640000
H	0.00000000	4.71570000	2.63730000
H	0.00000000	3.44530000	0.18790000
H	0.00000000	2.61410000	4.42640000
H	-2.98370000	-1.72270000	0.18790000
H	0.00000000	0.00000000	4.39010000
H	4.08390000	-2.35790000	2.63730000
H	2.26390000	-1.30710000	4.42640000
H	2.98370000	-1.72270000	0.18790000
B	0.00000000	0.00000000	3.18420000
N	0.00000000	-1.68700000	-1.33470000
N	0.00000000	-1.44910000	-2.65920000
N	-1.46100000	0.84350000	-1.33470000
N	-1.25500000	0.72460000	-2.65920000
N	1.46100000	0.84350000	-1.33470000
N	1.25500000	0.72460000	-2.65920000
C	0.00000000	-3.01550000	-1.18190000
C	0.00000000	-3.65210000	-2.42820000
C	0.00000000	-2.61040000	-3.34330000
C	-2.61150000	1.50770000	-1.18190000
C	-3.16280000	1.82600000	-2.42820000
C	-2.26070000	1.30520000	-3.34330000
C	2.61150000	1.50770000	-1.18190000
C	3.16280000	1.82600000	-2.42820000
C	2.26070000	1.30520000	-3.34330000
H	0.00000000	-4.71570000	-2.63730000
H	0.00000000	-2.61410000	-4.42640000
H	-4.08390000	2.35790000	-2.63730000
H	-2.98370000	1.72270000	-0.18790000
H	-2.26390000	1.30710000	-4.42640000
H	0.00000000	-3.44530000	-0.18790000
H	0.00000000	0.00000000	-4.39010000
H	4.08390000	2.35790000	-2.63730000
H	2.26390000	1.30710000	-4.42640000
H	2.98370000	1.72270000	-0.18790000
B	0.00000000	0.00000000	-3.18420000

$[Co(Tb)_2]$ ^2E_g D_{3d} LDA

Co	0.00000000	0.00000000	0.00000000
N	-1.36570000	-0.78850000	1.16110000
N	-1.22740000	-0.70860000	2.49400000
N	0.00000000	1.57700000	1.16110000
N	0.00000000	1.41730000	2.49400000
N	1.36570000	-0.78850000	1.16110000
N	1.22740000	-0.70860000	2.49400000
C	-2.49860000	-1.44260000	0.91680000
C	-3.10970000	-1.79540000	2.12170000
C	-2.26550000	-1.30800000	3.10060000
C	0.00000000	2.88520000	0.91680000
C	0.00000000	3.59080000	2.12170000
C	0.00000000	2.61590000	3.10060000
C	2.49860000	-1.44260000	0.91680000
C	3.10970000	-1.79540000	2.12170000
C	2.26550000	-1.30800000	3.10060000
H	-4.04390000	-2.33470000	2.26230000
H	-2.32590000	-1.34290000	4.18630000
H	0.00000000	4.66950000	2.26230000
H	0.00000000	3.24160000	-0.11280000
H	0.00000000	2.68570000	4.18630000
H	-2.80730000	-1.62080000	-0.11280000
H	0.00000000	0.00000000	4.25540000
H	4.04390000	-2.33470000	2.26230000
H	2.32590000	-1.34290000	4.18630000
H	2.80730000	-1.62080000	-0.11280000
B	0.00000000	0.00000000	3.04950000
N	0.00000000	-1.57700000	-1.16110000
N	0.00000000	-1.41730000	-2.49400000
N	-1.36570000	0.78850000	-1.16110000
N	-1.22740000	0.70860000	-2.49400000
N	1.36570000	0.78850000	-1.16110000
N	1.22740000	0.70860000	-2.49400000
C	0.00000000	-2.88520000	-0.91680000
C	0.00000000	-3.59080000	-2.12170000
C	0.00000000	-2.61590000	-3.10060000

C	-2.49860000	1.44260000	-0.91680000
C	-3.10970000	1.79540000	-2.12170000
C	-2.26550000	1.30800000	-3.10060000
C	2.49860000	1.44260000	-0.91680000
C	3.10970000	1.79540000	-2.12170000
C	2.26550000	1.30800000	-3.10060000
H	0.00000000	-4.66950000	-2.26230000
H	0.00000000	-2.68570000	-4.18630000
H	-4.04390000	2.33470000	-2.26230000
H	-2.80730000	1.62080000	0.11280000
H	-2.32590000	1.34290000	-4.18630000
H	0.00000000	-3.24160000	0.11280000
H	0.00000000	0.00000000	-4.25540000
H	4.04390000	2.33470000	-2.26230000
H	2.32590000	1.34290000	-4.18630000
H	2.80730000	1.62080000	0.11280000
B	0.00000000	0.00000000	-3.04950000

$[Co(Tb)_2]$ ^2E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.40890000	-0.81340000	1.22350000
N	-1.24460000	-0.71860000	2.55500000
N	0.00000000	1.62690000	1.22350000
N	0.00000000	1.43720000	2.55500000
N	1.40890000	-0.81340000	1.22350000
N	1.24460000	-0.71860000	2.55500000
C	-2.55300000	-1.47390000	1.01780000
C	-3.14240000	-1.81430000	2.24170000
C	-2.27190000	-1.31170000	3.19580000
C	0.00000000	2.94790000	1.01780000
C	0.00000000	3.62850000	2.24170000
C	0.00000000	2.62340000	3.19580000
C	2.55300000	-1.47390000	1.01780000
C	3.14240000	-1.81430000	2.24170000
C	2.27190000	-1.31170000	3.19580000
H	-4.06990000	-2.34980000	2.40880000
H	-2.30870000	-1.33290000	4.27800000
H	0.00000000	4.69950000	2.40880000
H	0.00000000	3.33900000	0.00890000
H	0.00000000	2.66590000	4.27800000
H	-2.89170000	-1.66950000	0.00890000
H	0.00000000	0.00000000	4.30770000
H	4.06990000	-2.34980000	2.40880000
H	2.30870000	-1.33290000	4.27800000
H	2.89170000	-1.66950000	0.00890000
B	0.00000000	0.00000000	3.10250000
N	0.00000000	-1.62690000	-1.22350000
N	0.00000000	-1.43720000	-2.55500000
N	-1.40890000	0.81340000	-1.22350000
N	-1.24460000	0.71860000	-2.55500000
N	1.40890000	0.81340000	-1.22350000
N	1.24460000	0.71860000	-2.55500000
C	0.00000000	-2.94790000	-1.01780000
C	0.00000000	-3.62850000	-2.24170000
C	0.00000000	-2.62340000	-3.19580000
C	-2.55300000	1.47390000	-1.01780000
C	-3.14240000	1.81430000	-2.24170000
C	-2.27190000	1.31170000	-3.19580000
C	2.55300000	1.47390000	-1.01780000
C	3.14240000	1.81430000	-2.24170000
C	2.27190000	1.31170000	-3.19580000
H	0.00000000	-4.69950000	-2.40880000
H	0.00000000	-2.66590000	-4.27800000
H	-4.06990000	2.34980000	-2.40880000
H	-2.89170000	1.66950000	-0.00890000
H	-2.30870000	1.33290000	-4.27800000
H	0.00000000	-3.33900000	-0.00890000
H	0.00000000	0.00000000	-4.30770000
H	4.06990000	2.34980000	-2.40880000
H	2.30870000	1.33290000	-4.27800000
H	2.89170000	1.66950000	-0.00890000
B	0.00000000	0.00000000	-3.10250000

$[Mn(Tb)_2]^{2+}$ ^2A_g C_{2h} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.03591156	0.95152631	1.37809874
N	-2.37651703	1.08505414	1.23343226
N	-1.36740883	-1.39148745	0.00000000
N	-2.67338229	-1.03973222	0.00000000
N	-1.03591156	0.95152631	-1.37809874
N	-2.37651703	1.08505414	-1.23343226
C	-0.69427208	1.57153948	2.52600484
C	-1.82521647	2.10862105	3.12439742
C	-2.87670225	1.77101390	2.26757214
C	-1.31340629	-2.74642622	0.00000000
C	-2.59497516	-3.26410815	0.00000000
C	-3.43363378	-2.14202325	0.00000000
C	-0.69427208	1.57153948	-2.52600484
C	-1.82521647	2.10862105	-3.12439742
C	-2.87670225	1.77101390	-2.26757214
H	-1.88619886	2.66198276	4.05434388
H	-3.93871018	1.97553668	2.33811146
H	-2.89265482	-4.30635078	0.00000000
H	-0.36203185	-3.26099923	0.00000000
H	-4.51539167	-2.07138073	0.00000000
H	0.33542482	1.59828727	2.85644852
H	-4.22753354	0.61922046	0.00000000
H	-1.88619886	2.66198276	-4.05434388
H	-3.93871018	1.97553668	-2.33811146
H	0.33542482	1.59828727	-2.85644852
B	-3.04324967	0.45769122	0.00000000
N	1.36740883	1.39148745	0.00000000
N	2.67338229	1.03973222	0.00000000
N	1.03591156	-0.95152631	1.37809874
N	2.37651703	-1.08505414	1.23343226
N	1.03591156	-0.95152631	-1.37809874
N	2.37651703	-1.08505414	-1.23343226
C	1.31340629	2.74642622	0.00000000
C	2.59497516	3.26410815	0.00000000
C	3.43363378	2.14202325	0.00000000
C	0.69427208	-1.57153948	2.52600484
C	1.82521647	-2.10862105	3.12439742
C	2.87670225	-1.77101390	2.26757214
C	0.69427208	-1.57153948	-2.52600484
C	1.82521647	-2.10862105	-3.12439742
C	2.87670225	-1.77101390	-2.26757214
H	2.89265482	4.30635078	0.00000000
H	4.51539167	2.07138073	0.00000000

H	1.88619886	-2.66198276	4.05434388
H	-0.33542482	-1.59828727	2.85644852
H	3.93871018	-1.97553668	2.33811146
H	0.36203185	3.26099923	0.00000000
H	4.22753354	-0.61922046	0.00000000
H	1.88619886	-2.66198276	-4.05434388
H	3.93871018	-1.97553668	-2.33811146
H	-0.33542482	-1.59828727	-2.85644852
B	3.04324967	-0.45769122	0.00000000

$[Mn(Tb)_2]^{2+}$ ^2B_g C_{2h} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.14370000	-0.80720000	1.36970000
N	2.48940000	-0.74140000	1.23610000
N	1.19690000	1.57530000	0.00000000
N	2.53590000	1.39650000	0.00000000
N	1.14370000	-0.80720000	-1.36970000
N	2.48940000	-0.74140000	-1.23610000
C	0.88230000	-1.47100000	2.51840000
C	2.07200000	-1.82920000	3.12950000
C	3.07130000	-1.34760000	2.27730000
C	0.96690000	2.90500000	0.00000000
C	2.17610000	3.58660000	0.00000000
C	3.14870000	2.59030000	0.00000000
C	0.88230000	-1.47100000	-2.51840000
C	2.07200000	-1.82920000	-3.12950000
C	3.07130000	-1.34760000	-2.27730000
H	2.20460000	-2.36720000	4.06100000
H	4.15110000	-1.40440000	2.35370000
H	2.33140000	4.65910000	0.00000000
H	-0.04230000	3.29430000	0.00000000
H	4.23040000	2.65650000	0.00000000
H	-0.13630000	-1.64740000	2.83650000
H	4.27560000	-0.06920000	0.00000000
H	2.20460000	-2.36720000	-4.06100000
H	4.15110000	-1.40440000	-2.35370000
H	-0.13630000	-1.64740000	-2.83650000
B	3.08120000	-0.03740000	0.00000000
N	-1.19690000	-1.57530000	0.00000000
N	-2.53590000	-1.39650000	0.00000000
N	-1.14370000	0.80720000	1.36970000
N	-2.48940000	0.74140000	1.23610000
N	-1.14370000	0.80720000	-1.36970000
N	-2.48940000	0.74140000	-1.23610000
C	-0.96690000	-2.90500000	0.00000000
C	-2.17610000	-3.58660000	0.00000000
C	-3.14870000	-2.59030000	0.00000000
C	-0.88230000	1.47100000	2.51840000
C	-2.07200000	1.82920000	3.12950000
C	-3.07130000	1.34760000	2.27730000
C	-0.88230000	1.47100000	-2.51840000
C	-2.07200000	1.82920000	-3.12950000
C	-3.07130000	1.34760000	-2.27730000
H	-2.33140000	-4.65910000	0.00000000
H	-4.23040000	-2.65650000	0.00000000
H	-2.20460000	2.36720000	4.06100000
H	0.13630000	1.64740000	2.83650000
H	-4.15110000	1.40440000	2.35370000
H	0.04230000	-3.29430000	0.00000000
H	-4.27560000	0.06920000	0.00000000
H	-2.20460000	2.36720000	-4.06100000
H	-4.15110000	1.40440000	-2.35370000
H	0.13630000	1.64740000	-2.83650000
B	-3.08120000	0.03740000	0.00000000

$[Mn(Tb)_2]^{+}$ ^5A_g C_{2h} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.35056141	0.83804160	1.47800476
N	-2.67474175	0.71938842	1.25798344
N	-1.20298816	-1.58715391	0.00000000
N	-2.54142189	-1.42667350	0.00000000
N	-1.35056141	0.83804160	-1.47800476
N	-2.67474175	0.71938842	-1.25798344
C	-1.20048357	1.48579160	2.64183751
C	-2.44935352	1.79405375	3.18319483
C	-3.36007814	1.28697600	2.26854847
C	-0.94083164	-2.90563713	0.00000000
C	-2.13859471	-3.61206124	0.00000000
C	-3.12642840	-2.63496032	0.00000000
C	-1.20048357	1.48579160	-2.64183751
C	-2.44935352	1.79405375	-3.18319483
C	-3.36007814	1.28697600	-2.26854847
H	-2.66335809	2.31186215	4.11055891
H	-4.44319390	1.29092155	2.26862255
H	-2.27121446	-4.68713985	0.00000000
H	0.08008516	-3.26307890	0.00000000
H	-4.20620399	-2.71847401	0.00000000
H	-0.21133593	1.69311160	3.03039172
H	-4.37054210	-0.09438723	0.00000000
H	-2.66335809	2.31186215	-4.11055891
H	-4.44319390	1.29092155	-2.26862255
H	-0.21133593	1.69311160	-3.03039172
B	-3.17411891	-0.01099789	0.00000000
N	1.20298816	1.58715391	0.00000000
N	2.54142189	1.42667350	0.00000000
N	1.35056141	-0.83804160	1.47800476
N	2.67474175	-0.71938842	1.25798344
N	1.35056141	-0.83804160	-1.47800476
N	2.67474175	-0.71938842	-1.25798344
C	0.94083164	2.90563713	0.00000000
C	2.13859471	3.61206124	0.00000000
C	3.12642840	2.63496032	0.00000000
C	1.20048357	-1.48579160	2.64183751
C	2.44935352	-1.79405375	3.18319483
C	3.36007814	-1.28697600	2.26854847
C	1.20048357	-1.48579160	-2.64183751
C	2.44935352	-1.79405375	-3.18319483
C	3.36007814	-1.28697600	-2.26854847
H	2.27121446	4.68713985	0.00000000
H	4.20620399	2.71847401	0.00000000
H	2.66335809	-2.31186215	4.11055891
H	0.21133593	-1.69311160	3.03039172
H	4.44319390	-1.29092155	2.26862255
H	-0.08008516	3.26307890	0.00000000
H	4.37054210	0.09438723	0.00000000
H	2.66335809	-2.31186215	-4.11055891
H	4.44319390	-1.29092155	-2.26862255
H	0.21133593	-1.69311160	-3.03039172

B	3.17411891	0.01099789	0.00000000

$[Mn(Tb)_2]^+$ ^5B_g C_{2h} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.13620000	0.93380000	1.39120000
N	-2.47430000	0.98490000	1.23800000
N	-1.63530000	-1.61600000	0.00000000
N	-2.90250000	-1.15860000	0.00000000
N	-1.13620000	0.93380000	-1.39120000
N	-2.47430000	0.98490000	-1.23800000
C	-0.82720000	1.59180000	2.52120000
C	-1.99130000	2.07130000	3.11350000
C	-3.01240000	1.66380000	2.26420000
C	-1.71310000	-2.95260000	0.00000000
C	-3.04870000	-3.36690000	0.00000000
C	-3.77530000	-2.18680000	0.00000000
C	-0.82720000	1.59180000	-2.52120000
C	-1.99130000	2.07130000	-3.11350000
C	-3.01240000	1.66380000	-2.26420000
H	-2.08110000	2.63880000	4.03180000
H	-4.08360000	1.81220000	2.32090000
H	-3.43450000	-4.37950000	0.00000000
H	-0.81040000	-3.55220000	0.00000000
H	-4.84390000	-2.01000000	0.00000000
H	0.20310000	1.68340000	2.83840000
H	-4.32660000	0.59700000	0.00000000
H	-2.08110000	2.63880000	-4.03180000
H	-4.08360000	1.81220000	-2.32090000
H	0.20310000	1.68340000	-2.83840000
B	-3.15270000	0.35110000	0.00000000
N	1.63530000	1.61600000	0.00000000
N	2.90250000	1.15860000	0.00000000
N	1.13620000	-0.93380000	1.39120000
N	2.47430000	-0.98490000	1.23800000
N	1.13620000	-0.93380000	-1.39120000
N	2.47430000	-0.98490000	-1.23800000
C	1.71310000	2.95260000	0.00000000
C	3.04870000	3.36690000	0.00000000
C	3.77530000	2.18680000	0.00000000
C	0.82720000	-1.59180000	2.52120000
C	1.99130000	-2.07130000	3.11350000
C	3.01240000	-1.66380000	2.26420000
C	0.82720000	-1.59180000	-2.52120000
C	1.99130000	-2.07130000	-3.11350000
C	3.01240000	-1.66380000	-2.26420000
H	3.43450000	4.37950000	0.00000000
H	4.84390000	2.01000000	0.00000000
H	2.08110000	-2.63880000	4.03180000
H	-0.20310000	-1.68340000	2.83840000
H	4.08360000	-1.81220000	2.32090000
H	0.81040000	3.55220000	0.00000000
H	4.32660000	-0.59700000	0.00000000
H	2.08110000	-2.63880000	-4.03180000
H	4.08360000	-1.81220000	-2.32090000
H	-0.20310000	-1.68340000	-2.83840000
B	3.15270000	-0.35110000	0.00000000

$[Mn(Tb)_2]^+$ ^1A_g C_{2h} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.19051122	0.77741218	-1.37355310
N	-2.52827395	0.65835735	-1.23925903
N	-1.19051122	0.77741218	1.37355310
N	-2.52827395	0.65835735	1.23925903
N	-1.17970119	-1.63100789	0.00000000
N	-2.51812645	-1.48372093	0.00000000
C	-0.96050116	1.44978955	-2.51559116
C	-2.16886259	1.75922330	-3.13113966
C	-3.14059394	1.24365755	-2.28044173
C	-0.96050116	1.44978955	2.51559116
C	-2.16886259	1.75922330	3.13113966
C	-3.14059394	1.24365755	2.28044173
C	-0.92592948	-2.94731513	0.00000000
C	-2.12630139	-3.66250718	0.00000000
C	-3.11434728	-2.69275600	0.00000000
H	-2.32108360	2.29208204	-4.06197250
H	-4.22156971	1.25829248	-2.34631583
H	-2.32108360	2.29208204	4.06197250
H	0.05145878	1.66533932	2.83003463
H	-4.22156971	1.25829248	2.34631583
H	0.05145878	1.66533932	-2.83003463
H	-4.29091786	-0.06231697	0.00000000
H	-2.25487347	-4.73811603	0.00000000
H	-4.19413028	-2.77359153	0.00000000
H	0.09227581	-3.31196165	0.00000000
B	-3.09213983	-0.06379126	0.00000000
N	1.19051122	-0.77741218	-1.37355310
N	2.52827395	-0.65835735	-1.23925903
N	1.17970119	1.63100789	0.00000000
N	2.51812645	1.48372093	0.00000000
N	1.19051122	-0.77741218	1.37355310
N	2.52827395	-0.65835735	1.23925903
C	0.96050116	-1.44978955	-2.51559116
C	2.16886259	-1.75922330	-3.13113966
C	3.14059394	-1.24365755	-2.28044173
C	0.92592948	2.94731513	0.00000000
C	2.12630139	3.66250718	0.00000000
C	3.11434728	2.69275600	0.00000000
C	0.96050116	-1.44978955	2.51559116
C	2.16886259	-1.75922330	3.13113966
C	3.14059394	-1.24365755	2.28044173
H	2.32108360	-2.29208204	-4.06197250
H	4.22156971	-1.25829248	-2.34631583
H	2.25487347	4.73811603	0.00000000
H	-0.09227581	3.31196165	0.00000000
H	4.19413028	2.77359153	0.00000000
H	-0.05145878	-1.66533932	-2.83003463
H	4.29091786	0.06231697	0.00000000
H	2.32108360	-2.29208204	4.06197250
H	4.22156971	-1.25829248	2.34631583
H	-0.05145878	-1.66533932	2.83003463
B	3.09213983	0.06379126	0.00000000

$[Mn(Tb)_2]^+$ ^1B_g C_{2h} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.19335449	0.77422759	-1.38267929
N	-2.53065737	0.67500686	-1.23910081
N	-1.19335449	0.77422759	1.38267929

N	-2.53065737	0.67500686	1.23910081
N	-1.16356763	-1.61010539	0.00000000
N	-2.50488273	-1.46657559	0.00000000
C	-0.96667666	1.42754506	-2.53619256
C	-2.17609274	1.75069402	-3.14439926
C	-3.14639690	1.25446441	-2.28196893
C	-0.96667666	1.42754506	2.53619256
C	-2.17609274	1.75069402	3.14439926
C	-3.14639690	1.25446441	2.28196893
C	-0.90753051	-2.93079316	0.00000000
C	-2.10158087	-3.64596457	0.00000000
C	-3.09401735	-2.67307749	0.00000000
H	-2.32940914	2.27642792	-4.07912472
H	-4.22754042	1.27459008	-2.34260841
H	-2.32940914	2.27642792	4.07912472
H	0.04487317	1.62677871	2.86319870
H	-4.22754042	1.27459008	2.34260841
H	0.04487317	1.62677871	-2.86319870
H	-4.28612933	-0.05711992	0.00000000
H	-2.23148119	-4.72146441	0.00000000
H	-4.17364795	-2.75950166	0.00000000
H	0.11214271	-3.29133961	0.00000000
B	-3.08697188	-0.04413179	0.00000000
N	1.19335449	-0.77422759	-1.38267929
N	2.53065737	-0.67500686	-1.23910081
N	1.16356763	1.61010539	0.00000000
N	2.50488273	1.46657559	0.00000000
N	1.19335449	-0.77422759	1.38267929
N	2.53065737	-0.67500686	1.23910081
C	0.96667666	-1.42754506	-2.53619256
C	2.17609274	-1.75069402	-3.14439926
C	3.14639690	-1.25446441	-2.28196893
C	0.90753051	2.93079316	0.00000000
C	2.10158087	3.64596457	0.00000000
C	3.09401735	2.67307749	0.00000000
C	0.96667666	-1.42754506	2.53619256
C	2.17609274	-1.75069402	3.14439926
C	3.14639690	-1.25446441	2.28196893
H	2.32940914	-2.27642792	-4.07912472
H	4.22754042	-1.27459008	-2.34260841
H	2.23148119	4.72146441	0.00000000
H	-0.11214271	3.29133961	0.00000000
H	4.17364795	2.75950166	0.00000000
H	-0.04487317	-1.62677871	-2.86319870
H	4.28612933	0.05711992	0.00000000
H	2.32940914	-2.27642792	4.07912472
H	4.22754042	-1.27459008	2.34260841
H	-0.04487317	-1.62677871	2.86319870
B	3.08697188	0.04413179	0.00000000

$[Mn(Tb)_2]$ ^4A_g C_{2h} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.39120000	0.90900000	1.48850000
N	-2.71060000	0.77480000	1.26110000
N	-1.24760000	-1.56590000	0.00000000
N	-2.58650000	-1.38530000	0.00000000
N	-1.39120000	0.90900000	-1.48850000
N	-2.71060000	0.77480000	-1.26110000
C	-1.26880000	1.56180000	2.64930000
C	-2.52950000	1.86150000	3.18150000
C	-3.42210000	1.34120000	2.25800000
C	-1.03280000	-2.88920000	0.00000000
C	-2.24740000	-3.57690000	0.00000000
C	-3.20970000	-2.57660000	0.00000000
C	-1.26880000	1.56180000	-2.64930000
C	-2.52950000	1.86150000	-3.18150000
C	-3.42210000	1.34120000	-2.25800000
H	-2.76170000	2.38050000	4.10460000
H	-4.50510000	1.33230000	2.24070000
H	-2.40720000	-4.64870000	0.00000000
H	-0.01930000	-3.26810000	0.00000000
H	-4.29130000	-2.63140000	0.00000000
H	-0.28470000	1.78340000	3.04450000
H	-4.39650000	-0.03840000	0.00000000
H	-2.76170000	2.38050000	-4.10460000
H	-4.50510000	1.33230000	-2.24070000
H	-0.28470000	1.78340000	-3.04450000
B	-3.19280000	0.03680000	0.00000000
N	1.24760000	1.56590000	0.00000000
N	2.58650000	1.38530000	0.00000000
N	1.39120000	-0.90900000	1.48850000
N	2.71060000	-0.77480000	1.26110000
N	1.39120000	-0.90900000	-1.48850000
N	2.71060000	-0.77480000	-1.26110000
C	1.03280000	2.88920000	0.00000000
C	2.24740000	3.57690000	0.00000000
C	3.20970000	2.57660000	0.00000000
C	1.26880000	-1.56180000	2.64930000
C	2.52950000	-1.86150000	3.18150000
C	3.42210000	-1.34120000	2.25800000
C	1.26880000	-1.56180000	-2.64930000
C	2.52950000	-1.86150000	-3.18150000
C	3.42210000	-1.34120000	-2.25800000
H	2.40720000	4.64870000	0.00000000
H	4.29130000	2.63140000	0.00000000
H	2.76170000	-2.38050000	4.10460000
H	0.28470000	-1.78340000	3.04450000
H	4.50510000	-1.33230000	2.24070000
H	0.01930000	3.26810000	0.00000000
H	4.39650000	0.03840000	0.00000000
H	2.76170000	-2.38050000	-4.10460000
H	4.50510000	-1.33230000	-2.24070000
H	0.28470000	-1.78340000	-3.04450000
B	3.19280000	-0.03680000	0.00000000

$[Mn(Tb)_2]$ ^4B_g C_{2h} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.27150000	0.71570000	1.39780000
N	-2.60620000	0.59160000	1.24250000
N	-1.51960000	-1.95570000	0.00000000
N	-2.81560000	-1.59710000	0.00000000
N	-1.27150000	0.71570000	-1.39780000
N	-2.60620000	0.59160000	-1.24250000
C	-1.07120000	1.38930000	2.53970000
C	-2.29530000	1.70200000	3.13670000
C	-3.24490000	1.17080000	2.27780000
C	-1.50210000	-3.29130000	0.00000000
C	-2.80560000	-3.80960000	0.00000000

C	-3.61550000	-2.68550000	0.00000000
C	-1.07120000	1.38930000	-2.53970000
C	-2.29530000	1.70200000	-3.13670000
C	-3.24490000	1.17080000	-2.27780000
H	-2.46690000	2.24040000	4.06130000
H	-4.32620000	1.15820000	2.33250000
H	-3.11760000	-4.84810000	0.00000000
H	-0.55450000	-3.81890000	0.00000000
H	-4.69410000	-2.58420000	0.00000000
H	-0.06380000	1.61160000	2.86600000
H	-4.39580000	0.00980000	0.00000000
H	-2.46690000	2.24040000	-4.06130000
H	-4.32620000	1.15820000	-2.33250000
H	-0.06380000	1.61160000	-2.86600000
B	-3.19550000	-0.10710000	0.00000000
N	1.51960000	1.95570000	0.00000000
N	2.81560000	1.59710000	0.00000000
N	1.27150000	-0.71570000	1.39780000
N	2.60620000	-0.59160000	1.24250000
N	1.27150000	-0.71570000	-1.39780000
N	2.60620000	-0.59160000	-1.24250000
C	1.50210000	3.29130000	0.00000000
C	2.80560000	3.80960000	0.00000000
C	3.61550000	2.68550000	0.00000000
C	1.07120000	-1.38930000	2.53970000
C	2.29530000	-1.70200000	3.13670000
C	3.24490000	-1.17080000	2.27780000
C	1.07120000	-1.38930000	-2.53970000
C	2.29530000	-1.70200000	-3.13670000
C	3.24490000	-1.17080000	-2.27780000
H	3.11760000	4.84810000	0.00000000
H	4.69410000	2.58420000	0.00000000
H	2.46690000	-2.24040000	4.06130000
H	0.06380000	-1.61160000	2.86600000
H	4.32620000	-1.15820000	2.33250000
H	0.55450000	3.81890000	0.00000000
H	4.39580000	-0.00980000	0.00000000
H	2.46690000	-2.24040000	-4.06130000
H	4.32620000	-1.15820000	-2.33250000
H	0.06380000	-1.61160000	-2.86600000
B	3.19550000	0.10710000	0.00000000

$[Mn(Tb)_2]$ ^2A_g C_{2h} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.19160000	0.79350000	1.40010000
N	-2.52990000	0.72840000	1.24440000
N	-1.21860000	-1.58810000	0.00000000
N	-2.55570000	-1.41430000	0.00000000
N	-1.19160000	0.79350000	-1.40010000
N	-2.52990000	0.72840000	-1.24440000
C	-0.96860000	1.45100000	2.54760000
C	-2.18050000	1.80460000	3.14750000
C	-3.15030000	1.32630000	2.27810000
C	-1.00450000	-2.91320000	0.00000000
C	-2.22390000	-3.60200000	0.00000000
C	-3.18780000	-2.60810000	0.00000000
C	-0.96860000	1.45100000	-2.54760000
C	-2.18050000	1.80460000	-3.14750000
C	-3.15030000	1.32630000	-2.27810000
H	-2.33190000	2.33990000	4.07770000
H	-4.23150000	1.37250000	2.32080000
H	-2.38030000	-4.67460000	0.00000000
H	0.00540000	-3.30040000	0.00000000
H	-4.26930000	-2.65930000	0.00000000
H	0.04510000	1.62980000	2.87950000
H	-4.29690000	0.04110000	0.00000000
H	-2.33190000	2.33990000	-4.07770000
H	-4.23150000	1.37250000	-2.32080000
H	0.04510000	1.62980000	-2.87950000
B	-3.09190000	0.01950000	0.00000000
N	1.21860000	1.58810000	0.00000000
N	2.55570000	1.41430000	0.00000000
N	1.19160000	-0.79350000	1.40010000
N	2.52990000	-0.72840000	1.24440000
N	1.19160000	-0.79350000	-1.40010000
N	2.52990000	-0.72840000	-1.24440000
C	1.00450000	2.91320000	0.00000000
C	2.22390000	3.60200000	0.00000000
C	3.18780000	2.60810000	0.00000000
C	0.96860000	-1.45100000	2.54760000
C	2.18050000	-1.80460000	3.14750000
C	3.15030000	-1.32630000	2.27810000
C	0.96860000	-1.45100000	-2.54760000
C	2.18050000	-1.80460000	-3.14750000
C	3.15030000	-1.32630000	-2.27810000
H	2.38030000	4.67460000	0.00000000
H	4.26930000	2.65930000	0.00000000
H	2.33190000	-2.33990000	4.07770000
H	-0.04510000	-1.62980000	2.87950000
H	4.23150000	-1.37250000	2.32080000
H	-0.00540000	3.30040000	0.00000000
H	4.29690000	-0.04110000	0.00000000
H	2.33190000	-2.33990000	-4.07770000
H	4.23150000	-1.37250000	-2.32080000
H	-0.04510000	-1.62980000	-2.87950000
B	3.09190000	-0.01950000	0.00000000

$[Mn(Tb)_2]$ ^2B_g C_{2h} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.19280000	-0.81140000	1.38090000
N	2.53200000	-0.73450000	1.23940000
N	1.21760000	1.60160000	0.00000000
N	2.55320000	1.41660000	0.00000000
N	1.19280000	-0.81140000	-1.38090000
N	2.53200000	-0.73450000	-1.23940000
C	0.96600000	-1.45480000	2.53670000
C	2.17740000	-1.80160000	3.14590000
C	3.15070000	-1.32080000	2.28480000
C	1.01010000	2.92610000	0.00000000
C	2.22960000	3.60690000	0.00000000
C	3.18760000	2.60180000	0.00000000
C	0.96600000	-1.45480000	-2.53670000
C	2.17740000	-1.80160000	-3.14590000
C	3.15070000	-1.32080000	-2.28480000
H	2.32380000	-2.32710000	4.08240000
H	4.23170000	-1.34660000	2.34230000
H	2.39500000	4.67800000	0.00000000
H	0.00050000	3.31440000	0.00000000

H	4.26970000	2.64850000	0.00000000
H	-0.04820000	-1.63350000	2.86720000
H	4.29780000	-0.03500000	0.00000000
H	2.32380000	-2.32710000	-4.08240000
H	4.23170000	-1.34660000	-2.34230000
H	-0.04820000	-1.63350000	-2.86720000
B	3.09260000	-0.02780000	0.00000000
N	-1.21760000	-1.60160000	0.00000000
N	-2.55320000	-1.41660000	0.00000000
N	-1.19280000	0.81140000	1.38090000
N	-2.53200000	0.73450000	1.23940000
N	-1.19280000	0.81140000	-1.38090000
N	-2.53200000	0.73450000	-1.23940000
C	-1.01010000	-2.92610000	0.00000000
C	-2.22960000	-3.60690000	0.00000000
C	-3.18760000	-2.60180000	0.00000000
C	-0.96600000	1.45480000	2.53670000
C	-2.17740000	1.80160000	3.14590000
C	-3.15070000	1.32080000	2.28480000
C	-0.96600000	1.45480000	-2.53670000
C	-2.17740000	1.80160000	-3.14590000
C	-3.15070000	1.32080000	-2.28480000
H	-2.39500000	-4.67800000	0.00000000
H	-4.26970000	-2.64850000	0.00000000
H	-2.32380000	2.32710000	4.08240000
H	0.04820000	1.63350000	2.86720000
H	-4.23170000	1.34660000	2.34230000
H	-0.00050000	-3.31440000	0.00000000
H	-4.29780000	0.03500000	0.00000000
H	-2.32380000	2.32710000	-4.08240000
H	-4.23170000	1.34660000	-2.34230000
H	0.04820000	1.63350000	-2.86720000
B	-3.09260000	0.02780000	0.00000000

$[Fe(Tb)_2]^+$ ^4A_g C_{2h} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	-1.00900000	-1.64130000	0.00000000
N	-2.35750000	-1.61770000	0.00000000
N	-1.35660000	0.72600000	-1.45470000
N	-2.66930000	0.50230000	-1.25390000
N	-1.35660000	0.72600000	1.45470000
N	-2.66930000	0.50230000	1.25390000
C	-0.61920000	-2.93020000	0.00000000
C	-1.73890000	-3.75150000	0.00000000
C	-2.82080000	-2.87540000	0.00000000
C	-1.24270000	1.39110000	-2.61380000
C	-2.50450000	1.60070000	-3.17100000
C	-3.38510000	1.01990000	-2.26910000
C	-1.24270000	1.39110000	2.61380000
C	-2.50450000	1.60070000	3.17100000
C	-3.38510000	1.01990000	2.26910000
H	-1.76510000	-4.83440000	0.00000000
H	-3.88670000	-3.06690000	0.00000000
H	-2.74690000	2.10240000	-4.10020000
H	-0.26850000	1.67770000	-2.98850000
H	-4.46520000	0.93970000	-2.28170000
H	0.43130000	-3.18550000	0.00000000
H	-4.29810000	-0.44930000	0.00000000
H	-2.74690000	2.10240000	4.10020000
H	-4.46520000	0.93970000	2.28170000
H	-0.26850000	1.67770000	2.98850000
B	-3.11240000	-0.26670000	0.00000000
N	1.35660000	-0.72600000	1.45470000
N	2.66930000	-0.50230000	1.25390000
N	1.35660000	-0.72600000	-1.45470000
N	2.66930000	-0.50230000	-1.25390000
N	1.00900000	1.64130000	0.00000000
N	2.35750000	1.61770000	0.00000000
C	1.24270000	-1.39110000	2.61380000
C	2.50450000	-1.60070000	3.17100000
C	3.38510000	-1.01990000	2.26910000
C	1.24270000	-1.39110000	-2.61380000
C	2.50450000	-1.60070000	-3.17100000
C	3.38510000	-1.01990000	-2.26910000
C	0.61920000	2.93020000	0.00000000
C	1.73890000	3.75150000	0.00000000
C	2.82080000	2.87540000	0.00000000
H	2.74690000	-2.10240000	4.10020000
H	4.46520000	-0.93970000	2.28170000
H	2.74690000	-2.10240000	-4.10020000
H	0.26850000	-1.67770000	-2.98850000
H	4.46520000	-0.93970000	-2.28170000
H	0.26850000	-1.67770000	2.98850000
H	4.29810000	0.44930000	0.00000000
H	1.76510000	4.83440000	0.00000000
H	3.88670000	3.06690000	0.00000000
H	-0.43130000	3.18550000	0.00000000
B	3.11240000	0.26670000	0.00000000

$[Fe(Tb)_2]^+$ ^4B_g C_{2h} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	-1.57220000	-1.58600000	0.00000000
N	-2.84220000	-1.13800000	0.00000000
N	-1.07760000	0.91370000	-1.37180000
N	-2.41460000	1.00210000	-1.23080000
N	-1.07760000	0.91370000	1.37180000
N	-2.41460000	1.00210000	1.23080000
C	-1.63660000	-2.92400000	0.00000000
C	-2.96790000	-3.34830000	0.00000000
C	-3.70510000	-2.17330000	0.00000000
C	-0.74540000	1.55370000	-2.50720000
C	-1.89130000	2.05980000	-3.11030000
C	-2.93030000	1.68140000	-2.26680000
C	-0.74540000	1.55370000	2.50720000
C	-1.89130000	2.05980000	3.11030000
C	-2.93030000	1.68140000	2.26680000
H	-3.34540000	-4.36410000	0.00000000
H	-4.77520000	-2.00570000	0.00000000
H	-1.96040000	2.62500000	-4.03180000
H	0.28870000	1.62000000	-2.81690000
H	-3.99800000	1.84870000	-2.33700000
H	-0.72860000	-3.51500000	0.00000000
H	-4.27470000	0.61460000	0.00000000
H	-1.96040000	2.62500000	4.03180000
H	-3.99800000	1.84870000	2.33700000
H	0.28870000	1.62000000	2.81690000
B	-3.09980000	0.37200000	0.00000000
N	1.07760000	-0.91370000	1.37180000

N	2.41460000	-1.00210000	1.23080000
N	1.07760000	-0.91370000	-1.37180000
N	2.41460000	-1.00210000	-1.23080000
N	1.57220000	1.58600000	0.00000000
N	2.84220000	1.13800000	0.00000000
C	0.74540000	-1.55370000	2.50720000
C	1.89130000	-2.05980000	3.11030000
C	2.93030000	-1.68140000	2.26680000
C	0.74540000	-1.55370000	-2.50720000
C	1.89130000	-2.05980000	-3.11030000
C	2.93030000	-1.68140000	-2.26680000
C	1.63660000	2.92400000	0.00000000
C	2.96790000	3.34830000	0.00000000
C	3.70510000	2.17330000	0.00000000
H	1.96040000	-2.62500000	4.03180000
H	3.99800000	-1.84870000	2.33700000
H	1.96040000	-2.62500000	-4.03180000
H	-0.28870000	-1.62000000	-2.81690000
H	3.99800000	-1.84870000	-2.33700000
H	-0.28870000	-1.62000000	2.81690000
H	4.27470000	-0.61460000	0.00000000
H	3.34540000	4.36410000	0.00000000
H	4.77520000	2.00570000	0.00000000
H	0.72860000	3.51500000	0.00000000
B	3.09980000	-0.37200000	0.00000000

$[Fe(Tb)_2]^+$ ^2A_g C_{2h} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.18150000	1.57800000	0.00000000
N	2.51690000	1.41780000	0.00000000
N	1.14140000	-0.79210000	-1.36200000
N	2.48120000	-0.71710000	-1.23540000
N	1.14140000	-0.79210000	1.36200000
N	2.48120000	-0.71710000	1.23540000
C	0.93660000	2.89590000	0.00000000
C	2.14310000	3.59940000	0.00000000
C	3.12310000	2.62040000	0.00000000
C	0.88190000	-1.45770000	-2.50060000
C	2.07660000	-1.81080000	-3.12060000
C	3.06940000	-1.32420000	-2.27820000
C	0.88190000	-1.45770000	2.50060000
C	2.07660000	-1.81080000	3.12060000
C	3.06940000	-1.32420000	2.27820000
H	2.28110000	4.67380000	0.00000000
H	4.20360000	2.69150000	0.00000000
H	2.20500000	-2.35170000	-4.05050000
H	-0.13770000	-1.64020000	-2.81070000
H	4.14890000	-1.37240000	-2.34970000
H	-0.07830000	3.26890000	0.00000000
H	4.26480000	-0.03790000	0.00000000
H	2.20500000	-2.35170000	4.05050000
H	4.14890000	-1.37240000	2.34970000
H	-0.13770000	-1.64020000	2.81070000
B	3.06650000	-0.01150000	0.00000000
N	-1.14140000	0.79210000	1.36200000
N	-2.48120000	0.71710000	1.23540000
N	-1.14140000	0.79210000	-1.36200000
N	-2.48120000	0.71710000	-1.23540000
N	-1.18150000	-1.57800000	0.00000000
N	-2.51690000	-1.41780000	0.00000000
C	-0.88190000	1.45770000	2.50060000
C	-2.07660000	1.81080000	3.12060000
C	-3.06940000	1.32420000	2.27820000
C	-0.88190000	1.45770000	-2.50060000
C	-2.07660000	1.81080000	-3.12060000
C	-3.06940000	1.32420000	-2.27820000
C	-0.93660000	-2.89590000	0.00000000
C	-2.14310000	-3.59940000	0.00000000
C	-3.12310000	-2.62040000	0.00000000
H	-2.20500000	2.35170000	4.05050000
H	-4.14890000	1.37240000	2.34970000
H	-2.20500000	2.35170000	-4.05050000
H	0.13770000	1.64020000	-2.81070000
H	-4.14890000	1.37240000	-2.34970000
H	0.13770000	1.64020000	2.81070000
H	-4.26480000	0.03790000	0.00000000
H	-2.28110000	-4.67380000	0.00000000
H	-4.20360000	-2.69150000	0.00000000
H	0.07830000	-3.26890000	0.00000000
B	-3.06650000	0.01150000	0.00000000

$[Fe(Tb)_2]^+$ ^2B_g C_{2h} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	-1.13850000	-1.57160000	0.00000000
N	-2.48000000	-1.42810000	0.00000000
N	-1.16350000	0.78290000	-1.37030000
N	-2.50020000	0.70950000	-1.23390000
N	-1.16350000	0.78290000	1.37030000
N	-2.50020000	0.70950000	1.23390000
C	-0.87410000	-2.89080000	0.00000000
C	-2.06570000	-3.60700000	0.00000000
C	-3.06230000	-2.63610000	0.00000000
C	-0.91290000	1.42050000	-2.52390000
C	-2.11470000	1.76580000	-3.14180000
C	-3.09950000	1.29310000	-2.28740000
C	-0.91290000	1.42050000	2.52390000
C	-2.11470000	1.76580000	3.14180000
C	-3.09950000	1.29310000	2.28740000
H	-2.19240000	-4.68290000	0.00000000
H	-4.14170000	-2.72640000	0.00000000
H	-2.24830000	2.28930000	-4.08080000
H	0.10380000	1.59860000	-2.84610000
H	-4.17960000	1.32700000	-2.35670000
H	0.14700000	-3.24620000	0.00000000
H	-4.26550000	-0.01800000	0.00000000
H	-2.24830000	2.28930000	4.08080000
H	-4.17960000	1.32700000	2.35670000
H	0.10380000	1.59860000	2.84610000
B	-3.06700000	-0.00300000	0.00000000
N	1.16350000	-0.78290000	1.37030000
N	2.50020000	-0.70950000	1.23390000
N	1.16350000	-0.78290000	-1.37030000
N	2.50020000	-0.70950000	-1.23390000
N	1.13850000	1.57160000	0.00000000
N	2.48000000	1.42810000	0.00000000
C	0.91290000	-1.42050000	2.52390000
C	2.11470000	-1.76580000	3.14180000
C	3.09950000	-1.29310000	2.28740000

C	0.91290000	-1.42050000	-2.52390000
C	2.11470000	-1.76580000	-3.14180000
C	3.09950000	-1.29310000	-2.28740000
C	0.87410000	2.89080000	0.00000000
C	2.06570000	3.60700000	0.00000000
C	3.06230000	2.63610000	0.00000000
H	2.24830000	-2.28930000	4.08080000
H	4.17960000	-1.32700000	2.35670000
H	2.24830000	-2.28930000	-4.08080000
H	-0.10380000	-1.59860000	-2.84610000
H	4.17960000	-1.32700000	-2.35670000
H	-0.10380000	-1.59860000	2.84610000
H	4.26550000	0.01800000	0.00000000
H	2.19240000	4.68290000	0.00000000
H	4.14170000	2.72640000	0.00000000
H	-0.14700000	3.24620000	0.00000000
B	3.06700000	0.00300000	0.00000000

$[Fe(Tb)_2]$ ^3A_g C_{2h} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	-1.24250000	2.06940000	0.00000000
N	-2.57460000	1.88970000	0.00000000
N	-1.29840000	-0.56840000	1.37580000
N	-2.61340000	-0.30110000	1.23880000
N	-1.29840000	-0.56840000	-1.37580000
N	-2.61340000	-0.30110000	-1.23880000
C	-1.04490000	3.39020000	0.00000000
C	-2.26790000	4.07940000	0.00000000
C	-3.22220000	3.07580000	0.00000000
C	-1.15610000	-1.27510000	2.50490000
C	-2.39840000	-1.45890000	3.11750000
C	-3.29730000	-0.82230000	2.27520000
C	-1.15610000	-1.27510000	-2.50490000
C	-2.39840000	-1.45890000	-3.11750000
C	-3.29730000	-0.82230000	-2.27520000
H	-2.43610000	5.15060000	0.00000000
H	-4.30460000	3.12040000	0.00000000
H	-2.61460000	-1.98680000	4.03880000
H	-0.17480000	-1.61290000	2.80980000
H	-4.37190000	-0.70510000	2.33820000
H	-0.03570000	3.78650000	0.00000000
H	-4.33570000	0.47700000	0.00000000
H	-2.61460000	-1.98680000	-4.03880000
H	-4.37190000	-0.70510000	-2.33820000
H	-0.17480000	-1.61290000	-2.80980000
B	-3.13010000	0.46030000	0.00000000
N	1.29840000	0.56840000	-1.37580000
N	2.61340000	0.30110000	-1.23880000
N	1.29840000	0.56840000	1.37580000
N	2.61340000	0.30110000	1.23880000
N	1.24250000	-2.06940000	0.00000000
N	2.57460000	-1.88970000	0.00000000
C	1.15610000	1.27510000	-2.50490000
C	2.39840000	1.45890000	-3.11750000
C	3.29730000	0.82230000	-2.27520000
C	1.15610000	1.27510000	2.50490000
C	2.39840000	1.45890000	3.11750000
C	3.29730000	0.82230000	2.27520000
C	1.04490000	-3.39020000	0.00000000
C	2.26790000	-4.07940000	0.00000000
C	3.22220000	-3.07580000	0.00000000
H	2.61460000	1.98680000	-4.03880000
H	4.37190000	0.70510000	-2.33820000
H	2.61460000	1.98680000	4.03880000
H	0.17480000	1.61290000	2.80980000
H	4.37190000	0.70510000	2.33820000
H	0.17480000	1.61290000	-2.80980000
H	4.33570000	-0.47700000	0.00000000
H	2.43610000	-5.15060000	0.00000000
H	4.30460000	-3.12040000	0.00000000
H	0.03570000	-3.78650000	0.00000000
B	3.13010000	-0.46030000	0.00000000

$[Fe(Tb)_2]$ ^3B_g C_{2h} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.03320000	1.64750000	0.00000000
N	2.38190000	1.62110000	0.00000000
N	1.39990000	-0.74120000	-1.47410000
N	2.70630000	-0.50600000	-1.25780000
N	1.39990000	-0.74120000	1.47410000
N	2.70630000	-0.50600000	1.25780000
C	0.66690000	2.93710000	0.00000000
C	1.79870000	3.75920000	0.00000000
C	2.86830000	2.87930000	0.00000000
C	1.31520000	-1.40630000	-2.63150000
C	2.59000000	-1.60360000	-3.17630000
C	3.44910000	-1.01410000	-2.26140000
C	1.31520000	-1.40630000	2.63150000
C	2.59000000	-1.60360000	3.17630000
C	3.44910000	-1.01410000	2.26140000
H	1.83200000	4.84230000	0.00000000
H	3.93660000	3.05430000	0.00000000
H	2.85230000	-2.10350000	-4.10180000
H	0.34760000	-1.70570000	-3.01460000
H	4.52820000	-0.92110000	-2.25360000
H	-0.38110000	3.20270000	0.00000000
H	4.32040000	0.45650000	0.00000000
H	2.85230000	-2.10350000	4.10180000
H	4.52820000	-0.92110000	2.25360000
H	0.34760000	-1.70570000	3.01460000
B	3.12850000	0.27540000	0.00000000
N	-1.39990000	0.74120000	1.47410000
N	-2.70630000	0.50600000	1.25780000
N	-1.39990000	0.74120000	-1.47410000
N	-2.70630000	0.50600000	-1.25780000
N	-1.03320000	-1.64750000	0.00000000
N	-2.38190000	-1.62110000	0.00000000
C	-1.31520000	1.40630000	2.63150000
C	-2.59000000	1.60360000	3.17630000
C	-3.44910000	1.01410000	2.26140000
C	-1.31520000	1.40630000	-2.63150000
C	-2.59000000	1.60360000	-3.17630000
C	-3.44910000	1.01410000	-2.26140000
C	-0.66690000	-2.93710000	0.00000000
C	-1.79870000	-3.75920000	0.00000000
C	-2.86830000	-2.87930000	0.00000000
H	-2.85230000	2.10350000	4.10180000
H	-4.52820000	0.92110000	2.25360000

H	-2.85230000	2.10350000	-4.10180000
H	-0.34760000	1.70570000	-3.01460000
H	-4.52820000	0.92110000	-2.25360000
H	-0.34760000	1.70570000	3.01460000
H	-4.32040000	-0.45650000	0.00000000
H	-1.83200000	-4.84230000	0.00000000
H	-3.93660000	-3.05430000	0.00000000
H	0.38110000	-3.20270000	0.00000000
B	-3.12850000	-0.27540000	0.00000000

$[Co(Tb)_2]^+$ ^3A_g C_{2h} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.12500000	1.92320000	0.00000000
N	-2.46560000	1.81970000	0.00000000
N	-1.24160000	-0.61710000	1.34400000
N	-2.55730000	-0.35280000	1.22970000
N	-1.24160000	-0.61710000	-1.34400000
N	-2.55730000	-0.35280000	-1.22970000
C	-0.83930000	3.22940000	0.00000000
C	-2.01790000	3.98550000	0.00000000
C	-3.03300000	3.04420000	0.00000000
C	-1.05950000	-1.33170000	2.46740000
C	-2.28470000	-1.52760000	3.09460000
C	-3.20940000	-0.89120000	2.27220000
C	-1.05950000	-1.33170000	-2.46740000
C	-2.28470000	-1.52760000	-3.09460000
C	-3.20940000	-0.89120000	-2.27220000
H	-2.11790000	5.06450000	0.00000000
H	-4.11020000	3.15790000	0.00000000
H	-2.47830000	-2.06430000	4.01550000
H	-0.07120000	-1.66320000	2.75410000
H	-4.28390000	-0.78780000	2.35970000
H	0.19010000	3.56640000	0.00000000
H	-4.28040000	0.46110000	0.00000000
H	-2.47830000	-2.06430000	-4.01550000
H	-4.28390000	-0.78780000	-2.35970000
H	-0.07120000	-1.66320000	-2.75410000
B	-3.08140000	0.42250000	0.00000000
N	1.24160000	0.61710000	-1.34400000
N	2.55730000	0.35280000	-1.22970000
N	1.24160000	0.61710000	1.34400000
N	2.55730000	0.35280000	1.22970000
N	1.12500000	-1.92320000	0.00000000
N	2.46560000	-1.81970000	0.00000000
C	1.05950000	1.33170000	-2.46740000
C	2.28470000	1.52760000	-3.09460000
C	3.20940000	0.89120000	-2.27220000
C	1.05950000	1.33170000	2.46740000
C	2.28470000	1.52760000	3.09460000
C	3.20940000	0.89120000	2.27220000
C	0.83930000	-3.22940000	0.00000000
C	2.01790000	-3.98550000	0.00000000
C	3.03300000	-3.04420000	0.00000000
H	2.47830000	2.06430000	-4.01550000
H	4.28390000	0.78780000	-2.35970000
H	2.47830000	2.06430000	4.01550000
H	0.07120000	1.66320000	2.75410000
H	4.28390000	0.78780000	2.35970000
H	0.07120000	1.66320000	-2.75410000
H	4.28040000	-0.46110000	0.00000000
H	2.11790000	-5.06450000	0.00000000
H	4.11020000	-3.15790000	0.00000000
H	-0.19010000	-3.56640000	0.00000000
B	3.08140000	-0.42250000	0.00000000

$[Co(Tb)_2]^+$ ^3B_g C_{2h} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.98980000	1.65130000	0.00000000
N	2.33360000	1.64130000	0.00000000
N	1.31660000	-0.70210000	-1.42740000
N	2.63170000	-0.47530000	-1.24910000
N	1.31660000	-0.70210000	1.42740000
N	2.63170000	-0.47530000	1.24910000
C	0.58400000	2.92820000	0.00000000
C	1.69900000	3.76620000	0.00000000
C	2.78780000	2.90820000	0.00000000
C	1.18110000	-1.38670000	-2.57340000
C	2.43250000	-1.60230000	-3.14780000
C	3.32940000	-1.00800000	-2.26730000
C	1.18110000	-1.38670000	2.57340000
C	2.43250000	-1.60230000	3.14780000
C	3.32940000	-1.00800000	2.26730000
H	1.70770000	4.84940000	0.00000000
H	3.85200000	3.10760000	0.00000000
H	2.66010000	-2.11690000	-4.07370000
H	0.20020000	-1.67840000	-2.92530000
H	4.40950000	-0.93100000	-2.29780000
H	-0.46860000	3.17410000	0.00000000
H	4.27480000	0.46830000	0.00000000
H	2.66010000	-2.11690000	4.07370000
H	4.40950000	-0.93100000	2.29780000
H	0.20020000	-1.67840000	2.92530000
B	3.08750000	0.29900000	0.00000000
N	-1.31660000	0.70210000	1.42740000
N	-2.63170000	0.47530000	1.24910000
N	-1.31660000	0.70210000	-1.42740000
N	-2.63170000	0.47530000	-1.24910000
N	-0.98980000	-1.65130000	0.00000000
N	-2.33360000	-1.64130000	0.00000000
C	-1.18110000	1.38670000	2.57340000
C	-2.43250000	1.60230000	3.14780000
C	-3.32940000	1.00800000	2.26730000
C	-1.18110000	1.38670000	-2.57340000
C	-2.43250000	1.60230000	-3.14780000
C	-3.32940000	1.00800000	-2.26730000
C	-0.58400000	-2.92820000	0.00000000
C	-1.69900000	-3.76620000	0.00000000
C	-2.78780000	-2.90820000	0.00000000
H	-2.66010000	2.11690000	4.07370000
H	-4.40950000	0.93100000	2.29780000
H	-2.66010000	2.11690000	-4.07370000
H	-0.20020000	1.67840000	-2.92530000
H	-4.40950000	0.93100000	-2.29780000
H	-0.20020000	1.67840000	2.92530000
H	-4.27480000	-0.46830000	0.00000000
H	-1.70770000	-4.84940000	0.00000000
H	-3.85200000	-3.10760000	0.00000000
H	0.46860000	-3.17410000	0.00000000

B	-3.08750000	-0.29900000	0.00000000

$[Co(Tb)_2]$ ^4A_g C_{2h} OPBE

Co	0.000000	0.000000	0.000000
N	-1.341900	-1.691000	0.000000
N	-2.667100	-1.451400	0.000000
N	-1.349000	0.840100	-1.461400
N	-2.672900	0.721000	-1.255700
N	-1.349000	0.840100	1.461400
N	-2.672900	0.721000	1.255700
C	-1.191000	-3.020500	0.000000
C	-2.437200	-3.654600	0.000000
C	-3.351700	-2.611100	0.000000
C	-1.196300	1.481100	-2.624400
C	-2.443200	1.785300	-3.184200
C	-3.358000	1.280200	-2.273700
C	-1.196300	1.481100	2.624400
C	-2.443200	1.785300	3.184200
C	-3.358000	1.280200	2.273700
H	-2.647800	-4.717900	0.000000
H	-4.434800	-2.613900	0.000000
H	-2.651900	2.299700	-4.115200
H	-0.202500	1.692000	-2.999500
H	-4.441000	1.275700	-2.279800
H	-0.197300	-3.450900	0.000000
H	-4.401800	-0.006300	0.000000
H	-2.651900	2.299700	4.115200
H	-4.441000	1.275700	2.279800
H	-0.202500	1.692000	2.999500
B	-3.195900	-0.000900	0.000000
N	1.349000	-0.840100	1.461400
N	2.672900	-0.721000	1.255700
N	1.349000	-0.840100	-1.461400
N	2.672900	-0.721000	-1.255700
N	1.341900	1.691000	0.000000
N	2.667100	1.451400	0.000000
C	1.196300	-1.481100	2.624400
C	2.443200	-1.785300	3.184200
C	3.358000	-1.280200	2.273700
C	1.196300	-1.481100	-2.624400
C	2.443200	-1.785300	-3.184200
C	3.358000	-1.280200	-2.273700
C	1.191000	3.020500	0.000000
C	2.437200	3.654600	0.000000
C	3.351700	2.611100	0.000000
H	2.651900	-2.299700	4.115200
H	4.441000	-1.275700	2.279800
H	2.651900	-2.299700	-4.115200
H	0.202500	-1.692000	-2.999500
H	4.441000	-1.275700	-2.279800
H	0.202500	-1.692000	2.999500
H	4.401800	0.006300	0.000000
H	2.647800	4.717900	0.000000
H	4.434800	2.613900	0.000000
H	0.197300	3.450900	0.000000
B	3.195900	0.000900	0.000000

$[Co(Tb)_2]$ ^4B_g C_{2h} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.38810000	-1.67890000	0.00000000
N	-2.70630000	-1.41270000	0.00000000
N	-1.32300000	0.84940000	-1.46440000
N	-2.64970000	0.75720000	-1.25680000
N	-1.32300000	0.84940000	1.46440000
N	-2.64970000	0.75720000	1.25680000
C	-1.26600000	-3.00990000	0.00000000
C	-2.52750000	-3.61880000	0.00000000
C	-3.41920000	-2.55830000	0.00000000
C	-1.15750000	1.50590000	-2.61770000
C	-2.39720000	1.84300000	-3.17130000
C	-3.32180000	1.34590000	-2.26500000
C	-1.15750000	1.50590000	2.61770000
C	-2.39720000	1.84300000	3.17130000
C	-3.32180000	1.34590000	2.26500000
H	-2.75950000	-4.67760000	0.00000000
H	-4.50200000	-2.53630000	0.00000000
H	-2.59650000	2.37460000	-4.09470000
H	-0.15930000	1.70090000	-2.98970000
H	-4.40470000	1.37080000	-2.26710000
H	-0.28240000	-3.46350000	0.00000000
H	-4.39860000	0.08210000	0.00000000
H	-2.59650000	2.37460000	4.09470000
H	-4.40470000	1.37080000	2.26710000
H	-0.15930000	1.70090000	2.98970000
B	-3.19320000	0.04690000	0.00000000
N	1.32300000	-0.84940000	1.46440000
N	2.64970000	-0.75720000	1.25680000
N	1.32300000	-0.84940000	-1.46440000
N	2.64970000	-0.75720000	-1.25680000
N	1.38810000	1.67890000	0.00000000
N	2.70630000	1.41270000	0.00000000
C	1.15750000	-1.50590000	2.61770000
C	2.39720000	-1.84300000	3.17130000
C	3.32180000	-1.34590000	2.26500000
C	1.15750000	-1.50590000	-2.61770000
C	2.39720000	-1.84300000	-3.17130000
C	3.32180000	-1.34590000	-2.26500000
C	1.26600000	3.00990000	0.00000000
C	2.52750000	3.61880000	0.00000000
C	3.41920000	2.55830000	0.00000000
H	2.59650000	-2.37460000	4.09470000
H	4.40470000	-1.37080000	2.26710000
H	2.59650000	-2.37460000	-4.09470000
H	0.15930000	-1.70090000	-2.98970000
H	4.40470000	-1.37080000	-2.26710000
H	0.15930000	-1.70090000	2.98970000
H	4.39860000	-0.08210000	0.00000000
H	2.75950000	4.67760000	0.00000000
H	4.50200000	2.53630000	0.00000000
H	0.28240000	3.46350000	0.00000000
B	3.19320000	-0.04690000	0.00000000

$[Co(Tb)_2]$ ^2A_g C_{2h} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.63540000	-1.62160000	0.00000000
N	-2.88730000	-1.13630000	0.00000000
N	-1.05090000	0.91910000	-1.35030000

N	-2.38990000	0.99500000	-1.23210000
N	-1.05090000	0.91910000	1.35030000
N	-2.38990000	0.99500000	1.23210000
C	-1.74830000	-2.95210000	0.00000000
C	-3.09790000	-3.33690000	0.00000000
C	-3.79280000	-2.13790000	0.00000000
C	-0.71550000	1.57030000	-2.47040000
C	-1.86150000	2.07580000	-3.09240000
C	-2.90520000	1.68680000	-2.26760000
C	-0.71550000	1.57030000	2.47040000
C	-1.86150000	2.07580000	3.09240000
C	-2.90520000	1.68680000	2.26760000
H	-3.51050000	-4.33970000	0.00000000
H	-4.85570000	-1.92860000	0.00000000
H	-1.92060000	2.64650000	-4.01170000
H	0.32250000	1.64470000	-2.76390000
H	-3.97270000	1.85230000	-2.33960000
H	-0.85830000	-3.57080000	0.00000000
H	-4.25840000	0.66080000	0.00000000
H	-1.92060000	2.64650000	4.01170000
H	-3.97270000	1.85230000	2.33960000
H	0.32250000	1.64470000	2.76390000
B	-3.08480000	0.38510000	0.00000000
N	1.05090000	-0.91910000	1.35030000
N	2.38990000	-0.99500000	1.23210000
N	1.05090000	-0.91910000	-1.35030000
N	2.38990000	-0.99500000	-1.23210000
N	1.63540000	1.62160000	0.00000000
N	2.88730000	1.13630000	0.00000000
C	0.71550000	-1.57030000	2.47040000
C	1.86150000	-2.07580000	3.09240000
C	2.90520000	-1.68680000	2.26760000
C	0.71550000	-1.57030000	-2.47040000
C	1.86150000	-2.07580000	-3.09240000
C	2.90520000	-1.68680000	-2.26760000
C	1.74830000	2.95210000	0.00000000
C	3.09790000	3.33690000	0.00000000
C	3.79280000	2.13790000	0.00000000
H	1.92060000	-2.64650000	4.01170000
H	3.97270000	-1.85230000	2.33960000
H	1.92060000	-2.64650000	-4.01170000
H	-0.32250000	-1.64470000	-2.76390000
H	3.97270000	-1.85230000	-2.33960000
H	-0.32250000	-1.64470000	2.76390000
H	4.25840000	-0.66080000	0.00000000
H	3.51050000	4.33970000	0.00000000
H	4.85570000	1.92860000	0.00000000
H	0.85830000	3.57080000	0.00000000
B	3.08480000	-0.38510000	0.00000000

$[Co(Tb)_2]$ ^2B_g C_{2h} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.00470000	-1.62770000	0.00000000
N	-2.35110000	-1.60180000	0.00000000
N	-1.34320000	0.72600000	-1.45740000
N	-2.65610000	0.52220000	-1.25360000
N	-1.34320000	0.72600000	1.45740000
N	-2.65610000	0.52220000	1.25360000
C	-0.62960000	-2.91260000	0.00000000
C	-1.75860000	-3.73760000	0.00000000
C	-2.83160000	-2.86070000	0.00000000
C	-1.23100000	1.38250000	-2.61620000
C	-2.49640000	1.60760000	-3.17470000
C	-3.37820000	1.03990000	-2.26870000
C	-1.23100000	1.38250000	2.61620000
C	-2.49640000	1.60760000	3.17470000
C	-3.37820000	1.03990000	2.26870000
H	-1.78730000	-4.82080000	0.00000000
H	-3.89950000	-3.03880000	0.00000000
H	-2.73680000	2.11030000	-4.10460000
H	-0.25360000	1.65660000	-2.99220000
H	-4.45870000	0.96480000	-2.27450000
H	0.41970000	-3.17190000	0.00000000
H	-4.28730000	-0.42540000	0.00000000
H	-2.73680000	2.11030000	4.10460000
H	-4.45870000	0.96480000	2.27450000
H	-0.25360000	1.65660000	2.99220000
B	-3.09460000	-0.25070000	0.00000000
N	1.34320000	-0.72600000	1.45740000
N	2.65610000	-0.52220000	1.25360000
N	1.34320000	-0.72600000	-1.45740000
N	2.65610000	-0.52220000	-1.25360000
N	1.00470000	1.62770000	0.00000000
N	2.35110000	1.60180000	0.00000000
C	1.23100000	-1.38250000	2.61620000
C	2.49640000	-1.60760000	3.17470000
C	3.37820000	-1.03990000	2.26870000
C	1.23100000	-1.38250000	-2.61620000
C	2.49640000	-1.60760000	-3.17470000
C	3.37820000	-1.03990000	-2.26870000
C	0.62960000	2.91260000	0.00000000
C	1.75860000	3.73760000	0.00000000
C	2.83160000	2.86070000	0.00000000
H	2.73680000	-2.11030000	4.10460000
H	4.45870000	-0.96480000	2.27450000
H	2.73680000	-2.11030000	-4.10460000
H	0.25360000	-1.65660000	-2.99220000
H	4.45870000	-0.96480000	-2.27450000
H	0.25360000	-1.65660000	2.99220000
H	4.28730000	0.42540000	0.00000000
H	1.78730000	4.82080000	0.00000000
H	3.89950000	3.03880000	0.00000000
H	-0.41970000	3.17190000	0.00000000
B	3.09460000	0.25070000	0.00000000

$[Cr(Tb^{3CH3})_2]^+$ $^4A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	1.47246850	0.85013013	1.23024556
N	1.24771475	0.72036846	2.55718026
N	0.00000000	-1.70026026	1.23024556
N	0.00000000	-1.44073692	2.55718026
N	-1.47246850	0.85013013	1.23024556
N	-1.24771475	0.72036846	2.55718026
C	2.64157609	1.52511476	1.08492396
C	3.14910682	1.81813767	2.35832656
C	2.23974800	1.29311922	3.25562544
C	0.00000000	-3.05022899	1.08492396
C	0.00000000	-3.63627533	2.35832656
C	0.00000000	-2.58623844	3.25562544
C	-2.64157609	1.52511476	1.08492396
C	-3.14910682	1.81813767	2.35832656
C	-2.23974800	1.29311922	3.25562544
H	4.06666048	2.34788748	2.58547801
H	2.22673659	1.28560702	4.33807496
H	0.00000000	-4.69577497	2.58547801
C	0.00000000	-3.79134755	-0.20599177
H	0.00000000	-2.57121351	4.33807496
C	3.28340354	1.89567377	-0.20599177
H	0.00000000	0.00000000	4.28184988
H	-4.06666048	2.34788748	2.58547801
H	-2.22673659	1.28560702	4.33807496
C	-3.28340354	1.89567377	-0.20599177
B	0.00000000	0.00000000	3.08225215
N	0.00000000	1.70026026	-1.23024556
N	0.00000000	1.44073692	-2.55718026
N	1.47246850	-0.85013013	-1.23024556
N	1.24771475	-0.72036846	-2.55718026
N	-1.47246850	-0.85013013	-1.23024556
N	-1.24771475	-0.72036846	-2.55718026
C	0.00000000	3.05022899	-1.08492396
C	0.00000000	3.63627533	-2.35832656
C	0.00000000	2.58623844	-3.25562544
C	2.64157609	-1.52511476	-1.08492396
C	3.14910682	-1.81813767	-2.35832656
C	2.23974800	-1.29311922	-3.25562544
C	-2.64157609	-1.52511476	-1.08492396
C	-3.14910682	-1.81813767	-2.35832656
C	-2.23974800	-1.29311922	-3.25562544
H	0.00000000	4.69577497	-2.58547801
H	0.00000000	2.57121351	-4.33807496
H	4.06666048	-2.34788748	-2.58547801
C	3.28340354	-1.89567377	0.20599177
H	2.22673659	-1.28560702	-4.33807496
C	0.00000000	3.79134755	0.20599177
H	0.00000000	0.00000000	-4.28184988
H	-4.06666048	-2.34788748	-2.58547801
H	-2.22673659	-1.28560702	-4.33807496
C	-3.28340354	-1.89567377	0.20599177
B	0.00000000	0.00000000	-3.08225215
H	-0.87939363	-3.56768338	-0.81453026
H	0.00000000	-4.86384378	0.00272685
H	0.87939363	-3.56768338	-0.81453026
H	4.21221227	2.43192189	0.00272685
H	2.65000747	2.54541930	-0.81453026
H	3.52940163	1.02226461	-0.81453026
H	-4.21221227	2.43192189	0.00272685
H	-3.52940163	1.02226461	-0.81453026
H	-2.65000747	2.54541930	-0.81453026
H	3.52940163	-1.02226461	0.81453026
H	4.21221227	-2.43192189	-0.00272685
H	2.65000747	-2.54541930	0.81453026
H	-2.65000747	-2.54541930	0.81453026
H	-4.21221227	-2.43192189	-0.00272685
H	-3.52940163	-1.02226461	0.81453026
H	-0.87939363	3.56768338	0.81453026
H	0.00000000	4.86384378	-0.00272685
H	0.87939363	3.56768338	0.81453026

$[Cr(Tb^{3CH3})_2]^+$ $^2A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	1.45180307	0.83819877	1.19979775
N	1.24505299	0.71883173	2.53160883
N	0.00000000	-1.67639807	1.19979775
N	0.00000000	-1.43766346	2.53160883
N	-1.45180307	0.83819877	1.19979775
N	-1.24505299	0.71883173	2.53160883
C	2.62628499	1.51628650	1.04499595
C	3.14475592	1.81562566	2.30909773
C	2.24097357	1.29382673	3.21815228
C	0.00000000	-3.03257246	1.04499595
C	0.00000000	-3.63125132	2.30909773
C	0.00000000	-2.58765346	3.21815228
C	-2.62628499	1.51628650	1.04499595
C	-3.14475592	1.81562566	2.30909773
C	-2.24097357	1.29382673	3.21815228
H	4.06387066	2.34627667	2.52808451
H	2.23900239	1.29268847	4.30087221
H	0.00000000	-4.69255334	2.52808451
C	0.00000000	-3.76063622	-0.25176931
H	0.00000000	-2.58537694	4.30087221
C	3.25680656	1.88031811	-0.25176931
H	0.00000000	0.00000000	4.25701559
H	-4.06387066	2.34627667	2.52808451
H	-2.23900239	1.29268847	4.30087221
C	-3.25680656	1.88031811	-0.25176931
B	0.00000000	0.00000000	3.05595204
N	0.00000000	1.67639807	-1.19979775
N	0.00000000	1.43766346	-2.53160883
N	1.45180307	-0.83819877	-1.19979775
N	1.24505299	-0.71883173	-2.53160883
N	-1.45180307	-0.83819877	-1.19979775
N	-1.24505299	-0.71883173	-2.53160883
C	0.00000000	3.03257246	-1.04499595
C	0.00000000	3.63125132	-2.30909773
C	0.00000000	2.58765346	-3.21815228
C	2.62628499	-1.51628650	-1.04499595
C	3.14475592	-1.81562566	-2.30909773
C	2.24097357	-1.29382673	-3.21815228
C	-2.62628499	-1.51628650	-1.04499595
C	-3.14475592	-1.81562566	-2.30909773
C	-2.24097357	-1.29382673	-3.21815228
H	0.00000000	4.69255334	-2.52808451
H	0.00000000	2.58537694	-4.30087221

H	4.06387066	-2.34627667	-2.52808451
C	3.25680656	-1.88031811	0.25176931
H	2.23900239	-1.29268847	-4.30087221
C	0.00000000	3.76063622	0.25176931
H	0.00000000	0.00000000	-4.25701559
H	-4.06387066	-2.34627667	-2.52808451
H	-2.23900239	-1.29268847	-4.30087221
C	-3.25680656	-1.88031811	0.25176931
B	0.00000000	0.00000000	-3.05595204
H	-0.87910205	-3.52923441	-0.85817256
H	0.00000000	-4.83547459	-0.05496458
H	0.87910205	-3.52923441	-0.85817256
H	4.18764363	2.41773729	-0.05496458
H	2.61685558	2.52594187	-0.85817256
H	3.49595763	1.00329255	-0.85817256
H	-4.18764363	2.41773729	-0.05496458
H	-3.49595763	1.00329255	-0.85817256
H	-2.61685558	2.52594187	-0.85817256
H	3.49595763	-1.00329255	0.85817256
H	4.18764363	-2.41773729	0.05496458
H	2.61685558	-2.52594187	0.85817256
H	-2.61685558	-2.52594187	0.85817256
H	-4.18764363	-2.41773729	0.05496458
H	-3.49595763	-1.00329255	0.85817256
H	-0.87910205	3.52923441	0.85817256
H	0.00000000	4.83547459	0.05496458
H	0.87910205	3.52923441	0.85817256

$[Cr(Tb^{3CF3})_2]^+$ $^4A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	1.53502413	0.88624648	1.16557269
N	1.26130403	0.72821457	2.47685592
N	0.00000000	-1.77249348	1.16557269
N	0.00000000	-1.45642861	2.47685592
N	-1.53502413	0.88624648	1.16557269
N	-1.26130403	0.72821457	2.47685592
C	2.71448719	1.56720975	1.10436328
C	3.16777143	1.82891383	2.39815932
C	2.21924979	1.28128417	3.23556274
C	0.00000000	-3.13442003	1.10436328
C	0.00000000	-3.65782713	2.39815932
C	0.00000000	-2.56256887	3.23556274
C	-2.71448719	1.56720975	1.10436328
C	-3.16777143	1.82891383	2.39815932
C	-2.21924979	1.28128417	3.23556274
H	4.07118124	2.35049791	2.68262173
H	2.16017985	1.24718029	4.31540289
H	0.00000000	-4.70099530	2.68262173
C	0.00000000	-4.05721414	-0.11373236
H	0.00000000	-2.49436057	4.31540289
C	3.51365067	2.02860733	-0.11373236
H	0.00000000	0.00000000	4.17152224
H	-4.07118124	2.35049791	2.68262173
H	-2.16017985	1.24718029	4.31540289
C	-3.51365067	2.02860733	-0.11373236
B	0.00000000	0.00000000	2.97410473
N	0.00000000	1.77249348	-1.16557269
N	0.00000000	1.45642861	-2.47685592
N	1.53502413	-0.88624648	-1.16557269
N	1.26130403	-0.72821457	-2.47685592
N	-1.53502413	-0.88624648	-1.16557269
N	-1.26130403	-0.72821457	-2.47685592
C	0.00000000	3.13442003	-1.10436328
C	0.00000000	3.65782713	-2.39815932
C	0.00000000	2.56256887	-3.23556274
C	2.71448719	-1.56720975	-1.10436328
C	3.16777143	-1.82891383	-2.39815932
C	2.21924979	-1.28128417	-3.23556274
C	-2.71448719	-1.56720975	-1.10436328
C	-3.16777143	-1.82891383	-2.39815932
C	-2.21924979	-1.28128417	-3.23556274
H	0.00000000	4.70099530	-2.68262173
H	0.00000000	2.49436057	-4.31540289
H	4.07118124	-2.35049791	-2.68262173
C	3.51365067	-2.02860733	0.11373236
H	2.16017985	-1.24718029	-4.31540289
C	0.00000000	4.05721414	0.11373236
H	0.00000000	0.00000000	-4.17152224
H	-4.07118124	-2.35049791	-2.68262173
H	-2.16017985	-1.24718029	-4.31540289
C	-3.51365067	-2.02860733	0.11373236
B	0.00000000	0.00000000	-2.97410473
F	-1.07825579	-3.91915126	-0.90479043
F	0.00000000	-5.33467024	0.33110409
F	1.07825579	-3.91915126	-0.90479043
F	4.61995974	2.66733485	0.33110409
F	2.85495676	2.89337239	-0.90479043
F	3.93321256	1.02577887	-0.90479043
F	-4.61995974	2.66733485	0.33110409
F	-3.93321256	1.02577887	-0.90479043
F	-2.85495676	2.89337239	-0.90479043
F	3.93321256	-1.02577887	0.90479043
F	4.61995974	-2.66733485	-0.33110409
F	2.85495676	-2.89337239	0.90479043
F	-2.85495676	-2.89337239	0.90479043
F	-4.61995974	-2.66733485	-0.33110409
F	-3.93321256	-1.02577887	0.90479043
F	-1.07825579	3.91915126	0.90479043
F	0.00000000	5.33467024	-0.33110409
F	1.07825579	3.91915126	0.90479043

$[Cr(Tb^{3CF3})_2]^+$ $^2A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	1.51422376	0.87423733	1.14916396
N	1.25865867	0.72668684	2.46648722
N	0.00000000	-1.74847518	1.14916396
N	0.00000000	-1.45337367	2.46648722
N	-1.51422376	0.87423733	1.14916396
N	-1.25865867	0.72668684	2.46648722
C	2.69935484	1.55847356	1.07763137
C	3.16380419	1.82662302	2.36281346
C	2.22019331	1.28182922	3.21332777
C	0.00000000	-3.11694660	1.07763137
C	0.00000000	-3.65324604	2.36281346
C	0.00000000	-2.56365845	3.21332777
C	-2.69935484	1.55847356	1.07763137
C	-3.16380419	1.82662302	2.36281346
C	-2.22019331	1.28182922	3.21332777

H	4.06909258	2.34929192	2.63917627
H	2.17239643	1.25423369	4.29404159
H	0.00000000	-4.69858384	2.63917627
C	0.00000000	-4.03623279	-0.14362506
H	0.00000000	-2.50846738	4.29404159
C	3.49548031	2.01811639	-0.14362506
H	0.00000000	0.00000000	4.15887173
H	-4.06909258	2.34929192	2.63917627
H	-2.17239643	1.25423369	4.29404159
C	-3.49548031	2.01811639	-0.14362506
B	0.00000000	0.00000000	2.95941265
N	0.00000000	1.74847518	-1.14916396
N	0.00000000	1.45337367	-2.46648722
N	1.51422376	-0.87423733	-1.14916396
N	1.25865867	-0.72668684	-2.46648722
N	-1.51422376	-0.87423733	-1.14916396
N	-1.25865867	-0.72668684	-2.46648722
C	0.00000000	3.11694660	-1.07763137
C	0.00000000	3.65324604	-2.36281346
C	0.00000000	2.56365845	-3.21332777
C	2.69935484	-1.55847356	-1.07763137
C	3.16380419	-1.82662302	-2.36281346
C	2.22019331	-1.28182922	-3.21332777
C	-2.69935484	-1.55847356	-1.07763137
C	-3.16380419	-1.82662302	-2.36281346
C	-2.22019331	-1.28182922	-3.21332777
H	0.00000000	4.69858384	-2.63917627
H	0.00000000	2.50846738	-4.29404159
H	4.06909258	-2.34929192	-2.63917627
C	3.49548031	-2.01811639	0.14362506
H	2.17239643	-1.25423369	-4.29404159
C	0.00000000	4.03623279	0.14362506
H	0.00000000	0.00000000	-4.15887173
H	-4.06909258	-2.34929192	-2.63917627
H	-2.17239643	-1.25423369	-4.29404159
C	-3.49548031	-2.01811639	0.14362506
B	0.00000000	0.00000000	-2.95941265
F	-1.07847593	-3.89735022	-0.93437250
F	0.00000000	-5.31564949	0.29675202
F	1.07847593	-3.89735022	-0.93437250
F	4.60348751	2.65782448	0.29675202
F	2.83596618	2.88266290	-0.93437250
F	3.91444264	1.01468732	-0.93437250
F	-4.60348751	2.65782448	0.29675202
F	-3.91444264	1.01468732	-0.93437250
F	-2.83596618	2.88266290	-0.93437250
F	3.91444264	-1.01468732	0.93437250
F	4.60348751	-2.65782448	-0.29675202
F	2.83596618	-2.88266290	0.93437250
F	-2.83596618	-2.88266290	0.93437250
F	-4.60348751	-2.65782448	-0.29675202
F	-3.91444264	-1.01468732	0.93437250
F	-1.07847593	3.89735022	0.93437250
F	0.00000000	5.31564949	-0.29675202
F	1.07847593	3.89735022	0.93437250

$[Cr(Tb^{3NH2})_2]^+$ $^4A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	0.00000000	1.66860858	1.24497944
N	0.00000000	1.43702527	2.59455076
N	1.44505712	-0.83430403	1.24497944
N	1.24450000	-0.71851263	2.59455076
N	-1.44505712	-0.83430403	1.24497944
N	-1.24450000	-0.71851263	2.59455076
C	0.00000000	3.01679187	1.08168275
C	0.00000000	3.64191583	2.34543051
C	0.00000000	2.60427862	3.25424640
C	2.61261846	-1.50839593	1.08168275
C	3.15399165	-1.82095765	2.34543051
C	2.25537143	-1.30213958	3.25424640
C	-2.61261846	-1.50839593	1.08168275
C	-3.15399165	-1.82095765	2.34543051
C	-2.25537143	-1.30213958	3.25424640
H	0.00000000	4.70497789	2.55337706
H	0.00000000	2.62139433	4.33692294
H	4.07463042	-2.35248868	2.55337706
N	3.13173922	-1.80811029	-0.12788997
H	2.27019421	-1.31069743	4.33692294
N	0.00000000	3.61622057	-0.12788997
H	0.00000000	0.00000000	4.32686434
H	-4.07463042	-2.35248868	2.55337706
H	-2.27019421	-1.31069743	4.33692294
N	-3.13173922	-1.80811029	-0.12788997
B	0.00000000	0.00000000	3.12500650
N	-1.44505712	0.83430403	-1.24497944
N	-1.24450000	0.71851263	-2.59455076
N	1.44505712	0.83430403	-1.24497944
N	1.24450000	0.71851263	-2.59455076
N	0.00000000	-1.66860858	-1.24497944
N	0.00000000	-1.43702527	-2.59455076
C	-2.61261846	1.50839593	-1.08168275
C	-3.15399165	1.82095765	-2.34543051
C	-2.25537143	1.30213958	-3.25424640
C	2.61261846	1.50839593	-1.08168275
C	3.15399165	1.82095765	-2.34543051
C	2.25537143	1.30213958	-3.25424640
C	0.00000000	-3.01679187	-1.08168275
C	0.00000000	-3.64191583	-2.34543051
C	0.00000000	-2.60427862	-3.25424640
H	-4.07463042	2.35248868	-2.55337706
H	-2.27019421	1.31069743	-4.33692294
H	4.07463042	2.35248868	-2.55337706
N	3.13173922	1.80811029	0.12788997
H	2.27019421	1.31069743	-4.33692294
N	-3.13173922	1.80811029	0.12788997
H	0.00000000	0.00000000	-4.32686434
H	0.00000000	-4.70497789	-2.55337706
H	0.00000000	-2.62139433	-4.33692294
N	0.00000000	-3.61622057	0.12788997
B	0.00000000	0.00000000	-3.12500650
H	0.00000000	4.61671165	-0.18717052
H	3.99818918	-2.30835583	-0.18717052
H	-3.99818918	-2.30835583	-0.18717052
H	-3.99818918	2.30835583	0.18717052
H	3.99818918	2.30835583	0.18717052
H	0.00000000	-4.61671165	0.18717052
H	2.66603625	-1.53923691	-0.97520117
H	0.00000000	3.07847330	-0.97520117
H	-2.66603625	-1.53923691	-0.97520117

H	2.66603625	1.53923691	0.97520117
H	-2.66603625	1.53923691	0.97520117
H	0.00000000	-3.07847330	0.97520117

$[Cr(Tb^{3NH2})_2]^+$ $^2A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	0.00000000	1.64211744	1.22408540
N	0.00000000	1.43493978	2.57619572
N	1.42211570	-0.82105872	1.22408540
N	1.24269445	-0.71747016	2.57619572
N	-1.42211570	-0.82105872	1.22408540
N	-1.24269445	-0.71747016	2.57619572
C	0.00000000	2.99690856	1.05220863
C	0.00000000	3.63803855	2.30652223
C	0.00000000	2.60868191	3.22533639
C	2.59539903	-1.49845428	1.05220863
C	3.15063402	-1.81901927	2.30652223
C	2.25918468	-1.30434095	3.22533639
C	-2.59539903	-1.49845428	1.05220863
C	-3.15063402	-1.81901927	2.30652223
C	-2.25918468	-1.30434095	3.22533639
H	0.00000000	4.70296649	2.50476367
H	0.00000000	2.63783216	4.30785841
H	4.07288837	-2.35148324	2.50476367
N	3.09642987	-1.78772426	-0.16536366
H	2.28442961	-1.31891608	4.30785841
N	0.00000000	3.57544905	-0.16536366
H	0.00000000	0.00000000	4.31030956
H	-4.07288837	-2.35148324	2.50476367
H	-2.28442961	-1.31891608	4.30785841
N	-3.09642987	-1.78772426	-0.16536366
B	0.00000000	0.00000000	3.10708432
N	-1.42211570	0.82105872	-1.22408540
N	-1.24269445	0.71747016	-2.57619572
N	1.42211570	0.82105872	-1.22408540
N	1.24269445	0.71747016	-2.57619572
N	0.00000000	-1.64211744	-1.22408540
N	0.00000000	-1.43493978	-2.57619572
C	-2.59539903	1.49845428	-1.05220863
C	-3.15063402	1.81901927	-2.30652223
C	-2.25918468	1.30434095	-3.22533639
C	2.59539903	1.49845428	-1.05220863
C	3.15063402	1.81901927	-2.30652223
C	2.25918468	1.30434095	-3.22533639
C	0.00000000	-2.99690856	-1.05220863
C	0.00000000	-3.63803855	-2.30652223
C	0.00000000	-2.60868191	-3.22533639
H	-4.07288837	2.35148324	-2.50476367
H	-2.28442961	1.31891608	-4.30785841
H	4.07288837	2.35148324	-2.50476367
N	3.09642987	1.78772426	0.16536366
H	2.28442961	1.31891608	-4.30785841
N	-3.09642987	1.78772426	0.16536366
H	0.00000000	0.00000000	-4.31030956
H	0.00000000	-4.70296649	-2.50476367
H	0.00000000	-2.63783216	-4.30785841
N	0.00000000	-3.57544905	0.16536366
B	0.00000000	0.00000000	-3.10708432
H	0.00000000	4.57491882	-0.24495403
H	3.96199610	-2.28745915	-0.24495403
H	-3.96199610	-2.28745915	-0.24495403
H	-3.96199610	2.28745915	0.24495403
H	3.96199610	2.28745915	0.24495403
H	0.00000000	-4.57491882	0.24495403
H	2.61337730	-1.50883409	-1.00023284
H	0.00000000	3.01766819	-1.00023284
H	-2.61337730	-1.50883409	-1.00023284
H	2.61337730	1.50883409	1.00023284
H	-2.61337730	1.50883409	1.00023284
H	0.00000000	-3.01766819	1.00023284

$[Cr(Tb^{3NO2})_2]^+$ $^4A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	0.00000000	1.72080609	1.22458918
N	0.00000000	1.43963993	2.53752080
N	1.49026209	-0.86040305	1.22458918
N	1.24676488	-0.71981970	2.53752080
N	-1.49026209	-0.86040305	1.22458918
N	-1.24676488	-0.71981970	2.53752080
C	0.00000000	3.08101599	1.17776599
C	0.00000000	3.64227091	2.44804486
C	0.00000000	2.55144821	3.29116974
C	2.66823816	-1.54050800	1.17776599
C	3.15429910	-1.82113545	2.44804486
C	2.20961929	-1.27572411	3.29116974
C	-2.66823816	-1.54050800	1.17776599
C	-3.15429910	-1.82113545	2.44804486
C	-2.20961929	-1.27572411	3.29116974
H	0.00000000	4.69394243	2.69655179
H	0.00000000	2.48885977	4.37140995
H	4.06507348	-2.34697095	2.69655179
N	3.38075469	-1.95187928	-0.02113216
H	2.15541566	-1.24442962	4.37140995
N	0.00000000	3.90375908	-0.02113216
H	0.00000000	0.00000000	4.24222244
H	-4.06507348	-2.34697095	2.69655179
H	-2.15541566	-1.24442962	4.37140995
N	-3.38075469	-1.95187928	-0.02113216
B	0.00000000	0.00000000	3.04362592
N	-1.49026209	0.86040305	-1.22458918
N	-1.24676488	0.71981970	-2.53752080
N	1.49026209	0.86040305	-1.22458918
N	1.24676488	0.71981970	-2.53752080
N	0.00000000	-1.72080609	-1.22458918
N	0.00000000	-1.43963993	-2.53752080
C	-2.66823816	1.54050800	-1.17776599
C	-3.15429910	1.82113545	-2.44804486
C	-2.20961929	1.27572411	-3.29116974
C	2.66823816	1.54050800	-1.17776599
C	3.15429910	1.82113545	-2.44804486
C	2.20961929	1.27572411	-3.29116974
C	0.00000000	-3.08101599	-1.17776599
C	0.00000000	-3.64227091	-2.44804486
C	0.00000000	-2.55144821	-3.29116974
H	-4.06507348	2.34697095	-2.69655179
H	-2.15541566	1.24442962	-4.37140995
H	4.06507348	2.34697095	-2.69655179
N	3.38075469	1.95187928	0.02113216

H	2.15541566	1.24442962	-4.37140995
N	-3.38075469	1.95187928	0.02113216
H	0.00000000	0.00000000	-4.24222244
H	0.00000000	-4.69394243	-2.69655179
H	0.00000000	-2.48885977	-4.37140995
N	0.00000000	-3.90375908	0.02113216
B	0.00000000	0.00000000	-3.04362592
O	0.00000000	5.11062453	0.17742096
O	4.42593055	-2.55531226	0.17742096
O	-4.42593055	-2.55531226	0.17742096
O	-4.42593055	2.55531226	-0.17742096
O	4.42593055	2.55531226	-0.17742096
O	0.00000000	-5.11062453	-0.17742096
O	2.90992717	-1.68004727	-1.11479548
O	0.00000000	3.36009455	-1.11479548
O	-2.90992717	-1.68004727	-1.11479548
O	2.90992717	1.68004727	1.11479548
O	-2.90992717	1.68004727	1.11479548
O	0.00000000	-3.36009455	1.11479548

$[Cr(Tb^{3NO2})_2]^+$ $^2A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	0.00000000	1.73886162	1.27042281
N	0.00000000	1.44090149	2.57754670
N	1.50589875	-0.86943081	1.27042281
N	1.24785710	-0.72045048	2.57754670
N	-1.50589875	-0.86943081	1.27042281
N	-1.24785710	-0.72045048	2.57754670
C	0.00000000	3.09313257	1.23042706
C	0.00000000	3.64462945	2.50782443
C	0.00000000	2.55014114	3.34047901
C	2.67873122	-1.54656655	1.23042706
C	3.15634173	-1.82231446	2.50782443
C	2.20848685	-1.27507057	3.34047901
C	-2.67873122	-1.54656655	1.23042706
C	-3.15634173	-1.82231446	2.50782443
C	-2.20848685	-1.27507057	3.34047901
H	0.00000000	4.69496585	2.76204488
H	0.00000000	2.47654952	4.41990111
H	4.06595932	-2.34748266	2.76204488
N	3.38854682	-1.95637834	0.03178556
H	2.14475486	-1.23827476	4.41990111
N	0.00000000	3.91275668	0.03178556
H	0.00000000	0.00000000	4.28440051
H	-4.06595932	-2.34748266	2.76204488
H	-2.14475486	-1.23827476	4.41990111
N	-3.38854682	-1.95637834	0.03178556
B	0.00000000	0.00000000	3.08745820
N	-1.50589875	0.86943081	-1.27042281
N	-1.24785710	0.72045048	-2.57754670
N	1.50589875	0.86943081	-1.27042281
N	1.24785710	0.72045048	-2.57754670
N	0.00000000	-1.73886162	-1.27042281
N	0.00000000	-1.44090149	-2.57754670
C	-2.67873122	1.54656655	-1.23042706
C	-3.15634173	1.82231446	-2.50782443
C	-2.20848685	1.27507057	-3.34047901
C	2.67873122	1.54656655	-1.23042706
C	3.15634173	1.82231446	-2.50782443
C	2.20848685	1.27507057	-3.34047901
C	0.00000000	-3.09313257	-1.23042706
C	0.00000000	-3.64462945	-2.50782443
C	0.00000000	-2.55014114	-3.34047901
H	-4.06595932	2.34748266	-2.76204488
H	-2.14475486	1.23827476	-4.41990111
H	4.06595932	2.34748266	-2.76204488
N	3.38854682	1.95637834	-0.03178556
H	2.14475486	1.23827476	-4.41990111
N	-3.38854682	1.95637834	-0.03178556
H	0.00000000	0.00000000	-4.28440051
H	0.00000000	-4.69496585	-2.76204488
H	0.00000000	-2.47654952	-4.41990111
N	0.00000000	-3.91275668	-0.03178556
B	0.00000000	0.00000000	-3.08745820
O	0.00000000	5.12001743	0.22559249
O	4.43406560	-2.56000871	0.22559249
O	-4.43406560	-2.56000871	0.22559249
O	-4.43406560	2.56000871	-0.22559249
O	4.43406560	2.56000871	-0.22559249
O	0.00000000	-5.12001743	-0.22559249
O	2.91161895	-1.68102414	-1.05870905
O	0.00000000	3.36204827	-1.05870905
O	-2.91161895	-1.68102414	-1.05870905
O	2.91161895	1.68102414	1.05870905
O	-2.91161895	1.68102414	1.05870905
O	0.00000000	-3.36204827	1.05870905

$[Cr(Tb^{5CH3})_2]^+$ $^4A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	1.40604565	0.81178118	1.25088664
N	1.25122108	0.72239309	2.59114233
N	0.00000000	-1.62356184	1.25088664
N	0.00000000	-1.44478618	2.59114233
N	-1.40604565	0.81178118	1.25088664
N	-1.25122108	0.72239309	2.59114233
C	2.54842502	1.47133395	1.02005000
C	3.14318215	1.81471706	2.22880620
C	2.29186455	1.32320877	3.21730665
C	0.00000000	-2.94266736	1.02005000
C	0.00000000	-3.62943413	2.22880620
C	0.00000000	-2.64641754	3.21730665
C	-2.54842502	1.47133395	1.02005000
C	-3.14318215	1.81471706	2.22880620
C	-2.29186455	1.32320877	3.21730665
H	4.07286455	2.35146948	2.37662657
C	2.43884406	1.40806710	4.69651793
H	0.00000000	-4.70293897	2.37662657
H	0.00000000	-3.32241448	0.00721692
C	0.00000000	-2.81613421	4.69651793
H	2.87729545	1.66120751	0.00721692
H	0.00000000	0.00000000	4.33522111
H	-4.07286455	2.35146948	2.37662657
C	-2.43884406	1.40806710	4.69651793
H	-2.87729545	1.66120751	0.00721692
B	0.00000000	0.00000000	3.14087388
N	0.00000000	1.62356184	-1.25088664
N	0.00000000	1.44478618	-2.59114233
N	1.40604565	-0.81178118	-1.25088664

N	1.25122108	-0.72239309	-2.59114233
N	-1.40604565	-0.81178118	-1.25088664
N	-1.25122108	-0.72239309	-2.59114233
C	0.00000000	2.94266736	-1.02005000
C	0.00000000	3.62943413	-2.22880620
C	0.00000000	2.64641754	-3.21730665
C	2.54842502	-1.47133395	-1.02005000
C	3.14318215	-1.81471706	-2.22880620
C	2.29186455	-1.32320877	-3.21730665
C	-2.54842502	-1.47133395	-1.02005000
C	-3.14318215	-1.81471706	-2.22880620
C	-2.29186455	-1.32320877	-3.21730665
H	0.00000000	4.70293897	-2.37662657
C	0.00000000	2.81613421	-4.69651793
H	4.07286455	-2.35146948	-2.37662657
H	2.87729545	-1.66120751	-0.00721692
C	2.43884406	-1.40806710	-4.69651793
H	0.00000000	3.32241448	-0.00721692
H	0.00000000	0.00000000	-4.33522111
H	-4.07286455	-2.35146948	-2.37662657
C	-2.43884406	-1.40806710	-4.69651793
H	-2.87729545	-1.66120751	-0.00721692
B	0.00000000	0.00000000	-3.14087388
H	-3.36116137	-1.94056758	-4.93956957
H	-1.60663981	-1.94896192	-5.15941150
H	-2.49117016	-0.41691018	-5.15941150
H	3.36116137	-1.94056758	-4.93956957
H	2.49117016	-0.41691018	-5.15941150
H	1.60663981	-1.94896192	-5.15941150
H	0.88453035	2.36587157	-5.15941150
H	0.00000000	3.88113517	-4.93956957
H	-0.88453035	2.36587157	-5.15941150
H	-2.49117016	0.41691018	5.15941150
H	-3.36116137	1.94056758	4.93956957
H	-1.60663981	1.94896192	5.15941150
H	-0.88453035	-2.36587157	5.15941150
H	0.88453035	-2.36587157	5.15941150
H	0.00000000	-3.88113517	4.93956957
H	2.49117016	0.41691018	5.15941150
H	1.60663981	1.94896192	5.15941150
H	3.36116137	1.94056758	4.93956957

$[Cr(Tb^{5CH3})_2]^+$ $^2A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	1.39300989	0.80425469	1.21474437
N	1.24987221	0.72161414	2.55949224
N	0.00000000	-1.60850939	1.21474437
N	0.00000000	-1.44322776	2.55949224
N	-1.39300989	0.80425469	1.21474437
N	-1.24987221	0.72161414	2.55949224
C	2.53975128	1.46632581	0.98210905
C	3.14013673	1.81295861	2.18318159
C	2.29035851	1.32233880	3.17931702
C	0.00000000	-2.93265216	0.98210905
C	0.00000000	-3.62591774	2.18318159
C	0.00000000	-2.64467813	3.17931702
C	-2.53975128	1.46632581	0.98210905
C	-3.14013673	1.81295861	2.18318159
C	-2.29035851	1.32233880	3.17931702
H	4.07029646	2.34998673	2.32850372
C	2.44677484	1.41264607	4.65623696
H	0.00000000	-4.69997346	2.32850372
H	0.00000000	-3.30756259	-0.03237718
C	0.00000000	-2.82529215	4.65623696
H	2.86443327	1.65378156	-0.03237718
H	0.00000000	0.00000000	4.30229199
H	-4.07029646	2.34998673	2.32850372
C	-2.44677484	1.41264607	4.65623696
H	-2.86443327	1.65378156	-0.03237718
B	0.00000000	0.00000000	3.10668479
N	0.00000000	1.60850939	-1.21474437
N	0.00000000	1.44322776	-2.55949224
N	1.39300989	-0.80425469	-1.21474437
N	1.24987221	-0.72161414	-2.55949224
N	-1.39300989	-0.80425469	-1.21474437
N	-1.24987221	-0.72161414	-2.55949224
C	0.00000000	2.93265216	-0.98210905
C	0.00000000	3.62591774	-2.18318159
C	0.00000000	2.64467813	-3.17931702
C	2.53975128	-1.46632581	-0.98210905
C	3.14013673	-1.81295861	-2.18318159
C	2.29035851	-1.32233880	-3.17931702
C	-2.53975128	-1.46632581	-0.98210905
C	-3.14013673	-1.81295861	-2.18318159
C	-2.29035851	-1.32233880	-3.17931702
H	0.00000000	4.69997346	-2.32850372
C	0.00000000	2.82529215	-4.65623696
H	4.07029646	-2.34998673	-2.32850372
H	2.86443327	-1.65378156	0.03237718
C	2.44677484	-1.41264607	-4.65623696
H	0.00000000	3.30756259	0.03237718
H	0.00000000	0.00000000	-4.30229199
H	-4.07029646	-2.34998673	-2.32850372
C	-2.44677484	-1.41264607	-4.65623696
H	-2.86443327	-1.65378156	0.03237718
B	0.00000000	0.00000000	-3.10668479
H	-3.37006478	-1.94570801	-4.89389311
H	-1.61569985	-1.95351708	-5.12139752
H	-2.49964546	-0.42247871	-5.12139752
H	3.37006478	-1.94570801	-4.89389311
H	2.49964546	-0.42247871	-5.12139752
H	1.61569985	-1.95351708	-5.12139752
H	0.88394508	2.37599579	-5.12139752
H	0.00000000	3.89141602	-4.89389311
H	-0.88394508	2.37599579	-5.12139752
H	-2.49964546	0.42247871	5.12139752
H	-3.37006478	1.94570801	4.89389311
H	-1.61569985	1.95351708	5.12139752
H	-0.88394508	-2.37599579	5.12139752
H	0.88394508	-2.37599579	5.12139752
H	0.00000000	-3.89141602	4.89389311
H	2.49964546	0.42247871	5.12139752
H	1.61569985	1.95351708	5.12139752
H	3.37006478	1.94570801	4.89389311

$[Cr(Tb^{5CF3})_2]^+$ $^4A_{2g}$ D_{3d} OPBE

[Cr	0.00000000	0.00000000	0.00000000
N	1.40314681	0.81010740	1.26281694

N	1.25433476	0.72419071	2.60122262
N	0.00000000	-1.62021426	1.26281694
N	0.00000000	-1.44838088	2.60122262
N	-1.40314681	0.81010740	1.26281694
N	-1.25433476	0.72419071	2.60122262
C	2.54350526	1.46849332	1.01239969
C	3.15477801	1.82141221	2.20862708
C	2.30930305	1.33327689	3.19581465
C	0.00000000	-2.93698718	1.01239969
C	0.00000000	-3.64282390	2.20862708
C	0.00000000	-2.66655379	3.19581465
C	-2.54350526	1.46849332	1.01239969
C	-3.15477801	1.82141221	2.20862708
C	-2.30930305	1.33327689	3.19581465
H	4.08438157	2.35811860	2.34701646
C	2.51827674	1.45392772	4.68822731
H	0.00000000	-4.71623719	2.34701646
H	0.00000000	-3.30705035	-0.00404239
C	0.00000000	-2.90785544	4.68822731
H	2.86398982	1.65352544	-0.00404239
H	0.00000000	0.00000000	4.34836957
H	-4.08438157	2.35811860	2.34701646
C	-2.51827674	1.45392772	4.68822731
H	-2.86398982	1.65352544	-0.00404239
B	0.00000000	0.00000000	3.16456409
N	0.00000000	1.62021426	-1.26281694
N	0.00000000	1.44838088	-2.60122262
N	1.40314681	-0.81010740	-1.26281694
N	1.25433476	-0.72419071	-2.60122262
N	-1.40314681	-0.81010740	-1.26281694
N	-1.25433476	-0.72419071	-2.60122262
C	0.00000000	2.93698718	-1.01239969
C	0.00000000	3.64282390	-2.20862708
C	0.00000000	2.66655379	-3.19581465
C	2.54350526	-1.46849332	-1.01239969
C	3.15477801	-1.82141221	-2.20862708
C	2.30930305	-1.33327689	-3.19581465
C	-2.54350526	-1.46849332	-1.01239969
C	-3.15477801	-1.82141221	-2.20862708
C	-2.30930305	-1.33327689	-3.19581465
H	0.00000000	4.71623719	-2.34701646
C	0.00000000	2.90785544	-4.68822731
H	4.08438157	-2.35811860	-2.34701646
H	2.86398982	-1.65352544	0.00404239
C	2.51827674	-1.45392772	-4.68822731
H	0.00000000	3.30705035	0.00404239
H	0.00000000	0.00000000	-4.34836957
H	-4.08438157	-2.35811860	-2.34701646
C	-2.51827674	-1.45392772	-4.68822731
H	-2.86398982	-1.65352544	0.00404239
B	0.00000000	0.00000000	-3.16456409
F	-3.66778149	-2.11759431	-4.92079330
F	-1.52049928	-2.13584933	-5.28496991
F	-2.60994982	-0.24886624	-5.28496991
F	3.66778149	-2.11759431	-4.92079330
F	2.60994982	-0.24886624	-5.28496991
F	1.52049928	-2.13584933	-5.28496991
F	1.08945001	2.38471610	-5.28496991
F	0.00000000	4.23518914	-4.92079330
F	-1.08945001	2.38471610	-5.28496991
F	-2.60994982	0.24886624	5.28496991
F	-3.66778149	2.11759431	4.92079330
F	-1.52049928	2.13584933	5.28496991
F	-1.08945001	-2.38471610	5.28496991
F	1.08945001	-2.38471610	5.28496991
F	0.00000000	-4.23518914	4.92079330
F	2.60994982	0.24886624	5.28496991
F	1.52049928	2.13584933	5.28496991
F	3.66778149	2.11759431	4.92079330

$Cr(Tb^{5CF3})_2]^+$ $^2A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	1.40055173	0.80860877	1.23927755
N	1.25398127	0.72398644	2.57944116
N	0.00000000	-1.61721753	1.23927755
N	0.00000000	-1.44797289	2.57944116
N	-1.40055173	0.80860877	1.23927755
N	-1.25398127	0.72398644	2.57944116
C	2.54201880	1.46763553	0.98900106
C	3.15401705	1.82097247	2.18394678
C	2.30913530	1.33317953	3.17264039
C	0.00000000	-2.93527052	0.98900106
C	0.00000000	-3.64194546	2.18394678
C	0.00000000	-2.66635958	3.17264039
C	-2.54201880	1.46763553	0.98900106
C	-3.15401705	1.82097247	2.18394678
C	-2.30913530	1.33317953	3.17264039
H	4.08371639	2.35773494	2.32162389
C	2.51919327	1.45445690	4.66482339
H	0.00000000	-4.71546936	2.32162389
H	0.00000000	-3.30445209	-0.02756855
C	0.00000000	-2.90891432	4.66482339
H	2.86173923	1.65222578	-0.02756855
H	0.00000000	0.00000000	4.32680931
H	-4.08371639	2.35773494	2.32162389
C	-2.51919327	1.45445690	4.66482339
H	-2.86173923	1.65222578	-0.02756855
B	0.00000000	0.00000000	3.14290221
N	0.00000000	1.61721753	-1.23927755
N	0.00000000	1.44797289	-2.57944116
N	1.40055173	-0.80860877	-1.23927755
N	1.25398127	-0.72398644	-2.57944116
N	-1.40055173	-0.80860877	-1.23927755
N	-1.25398127	-0.72398644	-2.57944116
C	0.00000000	2.93527052	-0.98900106
C	0.00000000	3.64194546	-2.18394678
C	0.00000000	2.66635958	-3.17264039
C	2.54201880	-1.46763553	-0.98900106
C	3.15401705	-1.82097247	-2.18394678
C	2.30913530	-1.33317953	-3.17264039
C	-2.54201880	-1.46763553	-0.98900106
C	-3.15401705	-1.82097247	-2.18394678
C	-2.30913530	-1.33317953	-3.17264039
H	0.00000000	4.71546936	-2.32162389
C	0.00000000	2.90891432	-4.66482339
H	4.08371639	-2.35773494	-2.32162389
H	2.86173923	-1.65222578	0.02756855
C	2.51919327	-1.45445690	-4.66482339
H	0.00000000	3.30445209	0.02756855

H	0.00000000	0.00000000	-4.32680931
H	-4.08371639	-2.35773494	-2.32162389
C	-2.51919327	-1.45445690	-4.66482339
H	-2.86173923	-1.65222578	0.02756855
B	0.00000000	0.00000000	-3.14290221
F	-3.66880280	-2.11818434	-4.89654005
F	-1.52163119	-2.13659442	-5.26171045
F	-2.61116057	-0.24947426	-5.26171045
F	3.66880280	-2.11818434	-4.89654005
F	2.61116057	-0.24947426	-5.26171045
F	1.52163119	-2.13659442	-5.26171045
F	1.08952939	2.38606815	-5.26171045
F	0.00000000	4.23636868	-4.89654005
F	-1.08952939	2.38606815	-5.26171045
F	-2.61116057	0.24947426	5.26171045
F	-3.66880280	2.11818434	4.89654005
F	-1.52163119	2.13659442	5.26171045
F	-1.08952939	-2.38606815	5.26171045
F	1.08952939	-2.38606815	5.26171045
F	0.00000000	-4.23636868	4.89654005
F	2.61116057	0.24947426	5.26171045
F	1.52163119	2.13659442	5.26171045
F	3.66880280	2.11818434	4.89654005

$[Cr(Tb^{5NH2})_2]^+$ $^4A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	0.00000000	1.62350574	-1.24662306
N	0.00000000	1.44180480	-2.60020502
N	-1.40599749	-0.81175314	-1.24662306
N	-1.24863976	-0.72090240	-2.60020502
N	1.40599749	-0.81175314	-1.24662306
N	1.24863976	-0.72090240	-2.60020502
C	0.00000000	2.94182227	-1.02801253
C	0.00000000	3.64011134	-2.22836063
C	0.00000000	2.64778705	-3.21670074
C	-2.54769264	-1.47091113	-1.02801253
C	-3.15242899	-1.82005593	-2.22836063
C	-2.29305096	-1.32389352	-3.21670074
C	2.54769264	-1.47091113	-1.02801253
C	3.15242899	-1.82005593	-2.22836063
C	2.29305096	-1.32389352	-3.21670074
H	0.00000000	4.71349711	-2.37374732
N	0.00000000	2.79504755	-4.56778922
H	-4.08200821	-2.35674856	-2.37374732
H	-2.88041389	-1.66300777	-0.01685747
N	-2.42058215	-1.39752378	-4.56778922
H	0.00000000	3.32601553	-0.01685747
H	0.00000000	0.00000000	-4.34349321
H	4.08200821	-2.35674856	-2.37374732
N	2.42058215	-1.39752378	-4.56778922
H	2.88041389	-1.66300777	-0.01685747
B	0.00000000	0.00000000	-3.13611552
N	1.40599749	0.81175314	1.24662306
N	1.24863976	0.72090240	2.60020502
N	-1.40599749	0.81175314	1.24662306
N	-1.24863976	0.72090240	2.60020502
N	0.00000000	-1.62350574	1.24662306
N	0.00000000	-1.44180480	2.60020502
C	2.54769264	1.47091113	1.02801253
C	3.15242899	1.82005593	2.22836063
C	2.29305096	1.32389352	3.21670074
C	-2.54769264	1.47091113	1.02801253
C	-3.15242899	1.82005593	2.22836063
C	-2.29305096	1.32389352	3.21670074
C	0.00000000	-2.94182227	1.02801253
C	0.00000000	-3.64011134	2.22836063
C	0.00000000	-2.64778705	3.21670074
H	4.08200821	2.35674856	2.37374732
N	2.42058215	1.39752378	4.56778922
H	-4.08200821	2.35674856	2.37374732
H	-2.88041389	1.66300777	0.01685747
N	-2.42058215	1.39752378	4.56778922
H	2.88041389	1.66300777	0.01685747
H	0.00000000	0.00000000	4.34349321
H	0.00000000	-4.71349711	2.37374732
N	0.00000000	-2.79504755	4.56778922
H	0.00000000	-3.32601553	0.01685747
B	0.00000000	0.00000000	3.13611552
H	0.00000000	3.71522117	-4.96555164
H	0.00000000	2.00550504	-5.18409126
H	-3.21747546	-1.85761058	-4.96555164
H	-1.73681847	-1.00275226	-5.18409126
H	3.21747546	-1.85761058	-4.96555164
H	1.73681847	-1.00275226	-5.18409126
H	3.21747546	1.85761058	4.96555164
H	1.73681847	1.00275226	5.18409126
H	-3.21747546	1.85761058	4.96555164
H	-1.73681847	1.00275226	5.18409126
H	0.00000000	-3.71522117	4.96555164
H	0.00000000	-2.00550504	5.18409126

$[Cr(Tb^{5NH2})_2]^+$ $^2A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	0.00000000	1.62010684	-1.22566606
N	0.00000000	1.44150846	-2.58065350
N	-1.40305368	-0.81005342	-1.22566606
N	-1.24838311	-0.72075423	-2.58065350
N	1.40305368	-0.81005342	-1.22566606
N	1.24838311	-0.72075423	-2.58065350
C	0.00000000	2.93952511	-1.00684280
C	0.00000000	3.63938742	-2.20587430
C	0.00000000	2.64799343	-3.19568341
C	-2.54570346	-1.46976282	-1.00684280
C	-3.15180192	-1.81969345	-2.20587430
C	-2.29322982	-1.32399671	-3.19568341
C	2.54570346	-1.46976282	-1.00684280
C	3.15180192	-1.81969345	-2.20587430
C	2.29322982	-1.32399671	-3.19568341
H	0.00000000	4.71292719	-2.35046352
N	0.00000000	2.79710129	-4.54627075
H	-4.08151501	-2.35646386	-2.35046352
H	-2.87715522	-1.66112654	0.00468110
N	-2.42236071	-1.39855038	-4.54627075
H	0.00000000	3.32225308	0.00468110
H	0.00000000	0.00000000	-4.32435392
H	4.08151501	-2.35646386	-2.35046352
N	2.42236071	-1.39855038	-4.54627075
H	2.87715522	-1.66112654	0.00468110

B	0.00000000	0.00000000	-3.11651003
N	1.40305368	0.81005342	1.22566606
N	1.24838311	0.72075423	2.58065350
N	-1.40305368	0.81005342	1.22566606
N	-1.24838311	0.72075423	2.58065350
N	0.00000000	-1.62010684	1.22566606
N	0.00000000	-1.44150846	2.58065350
C	2.54570346	1.46976282	1.00684280
C	3.15180192	1.81969345	2.20587430
C	2.29322982	1.32399671	3.19568341
C	-2.54570346	1.46976282	1.00684280
C	-3.15180192	1.81969345	2.20587430
C	-2.29322982	1.32399671	3.19568341
C	0.00000000	-2.93952511	1.00684280
C	0.00000000	-3.63938742	2.20587430
C	0.00000000	-2.64799343	3.19568341
H	4.08151501	2.35646386	2.35046352
N	2.42236071	1.39855038	4.54627075
H	-4.08151501	2.35646386	2.35046352
H	-2.87715522	1.66112654	-0.00468110
N	-2.42236071	1.39855038	4.54627075
H	2.87715522	1.66112654	-0.00468110
H	0.00000000	0.00000000	4.32435392
H	0.00000000	-4.71292719	2.35046352
N	0.00000000	-2.79710129	4.54627075
H	0.00000000	-3.32225308	-0.00468110
B	0.00000000	0.00000000	3.11651003
H	0.00000000	3.71774217	-4.94310236
H	0.00000000	2.00798053	-5.16322898
H	-3.21965937	-1.85887108	-4.94310236
H	-1.73896217	-1.00399000	-5.16322898
H	3.21965937	-1.85887108	-4.94310236
H	1.73896217	-1.00399000	-5.16322898
H	3.21965937	1.85887108	4.94310236
H	1.73896217	1.00399000	5.16322898
H	-3.21965937	1.85887108	4.94310236
H	-1.73896217	1.00399000	5.16322898
H	0.00000000	-3.71774217	4.94310236
H	0.00000000	-2.00798053	5.16322898

$[Cr(Tb^{5NO2})_2]^+$ $^4A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	-1.40317750	-0.81012486	-1.23382597
N	-1.25995727	-0.72743668	-2.57094786
N	1.40317750	-0.81012486	-1.23382597
N	1.25995727	-0.72743668	-2.57094786
N	0.00000000	1.62024972	-1.23382597
N	0.00000000	1.45487336	-2.57094786
C	-2.54158011	-1.46738205	-0.95889193
C	-3.16883137	-1.82952556	-2.13824862
C	-2.33114537	-1.34588719	-3.13112908
C	2.54158011	-1.46738205	-0.95889193
C	3.16883137	-1.82952556	-2.13824862
C	2.33114537	-1.34588719	-3.13112908
C	0.00000000	2.93476357	-0.95889193
C	0.00000000	3.65905165	-2.13824862
C	0.00000000	2.69177491	-3.13112908
H	-4.09735488	-2.36560910	-2.27960245
N	-2.60249212	-1.50254958	-4.56360184
H	4.09735488	-2.36560910	-2.27960245
H	2.84672541	-1.64355786	0.06351979
N	2.60249212	-1.50254958	-4.56360184
H	-2.84672541	-1.64355786	0.06351979
H	0.00000000	0.00000000	-4.30602957
H	0.00000000	4.73121820	-2.27960245
N	0.00000000	3.00509917	-4.56360184
H	0.00000000	3.28711571	0.06351979
B	0.00000000	0.00000000	-3.13927947
N	-1.40317750	0.81012486	1.23382597
N	-1.25995727	0.72743668	2.57094786
N	0.00000000	-1.62024972	1.23382597
N	0.00000000	-1.45487336	2.57094786
N	1.40317750	0.81012486	1.23382597
N	1.25995727	0.72743668	2.57094786
C	-2.54158011	1.46738205	0.95889193
C	-3.16883137	1.82952556	2.13824862
C	-2.33114537	1.34588719	3.13112908
C	0.00000000	-2.93476357	0.95889193
C	0.00000000	-3.65905165	2.13824862
C	0.00000000	-2.69177491	3.13112908
C	2.54158011	1.46738205	0.95889193
C	3.16883137	1.82952556	2.13824862
C	2.33114537	1.34588719	3.13112908
H	-4.09735488	2.36560910	2.27960245
N	-2.60249212	1.50254958	4.56360184
H	0.00000000	-4.73121820	2.27960245
H	0.00000000	-3.28711571	-0.06351979
N	0.00000000	-3.00509917	4.56360184
H	-2.84672541	1.64355786	-0.06351979
H	0.00000000	0.00000000	4.30602957
H	4.09735488	2.36560910	2.27960245
N	2.60249212	1.50254958	4.56360184
H	2.84672541	1.64355786	-0.06351979
B	0.00000000	0.00000000	3.13927947
O	-3.63992189	-2.10150996	-4.80645874
O	-1.81408628	-1.04736349	-5.37029763
O	3.63992189	-2.10150996	-4.80645874
O	1.81408628	-1.04736349	-5.37029763
O	0.00000000	4.20301993	-4.80645874
O	0.00000000	2.09472644	-5.37029763
O	-3.63992189	2.10150996	4.80645874
O	-1.81408628	1.04736349	5.37029763
O	0.00000000	-4.20301993	4.80645874
O	0.00000000	-2.09472644	5.37029763
O	3.63992189	2.10150996	4.80645874
O	1.81408628	1.04736349	5.37029763

$[Cr(Tb^{5NO2})_2]^+$ $^2A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	-1.40004583	-0.80831666	-1.20934782
N	-1.25953710	-0.72719432	-2.54843508
N	1.40004583	-0.80831666	-1.20934782
N	1.25953710	-0.72719432	-2.54843508
N	0.00000000	1.61663385	-1.20934782
N	0.00000000	1.45438810	-2.54843508
C	-2.53949621	-1.46617870	-0.93382110
C	-3.16781429	-1.82893817	-2.11153311
C	-2.33115807	-1.34589460	-3.10649535

C	2.53949621	-1.46617870	-0.93382110
C	3.16781429	-1.82893817	-2.11153311
C	2.33115807	-1.34589460	-3.10649535
C	0.00000000	2.93235740	-0.93382110
C	0.00000000	3.65787687	-2.11153311
C	0.00000000	2.69178972	-3.10649535
H	-4.09649337	-2.36511167	-2.25153330
N	-2.60406589	-1.50345818	-4.53837172
H	4.09649337	-2.36511167	-2.25153330
H	2.84344081	-1.64166129	0.08890231
N	2.60406589	-1.50345818	-4.53837172
H	-2.84344081	-1.64166129	0.08890231
H	0.00000000	0.00000000	-4.28411211
H	0.00000000	4.73022282	-2.25153330
N	0.00000000	3.00691636	-4.53837172
H	0.00000000	3.28332310	0.08890231
B	0.00000000	0.00000000	-3.11721278
N	-1.40004583	0.80831666	1.20934782
N	-1.25953710	0.72719432	2.54843508
N	0.00000000	-1.61663385	1.20934782
N	0.00000000	-1.45438810	2.54843508
N	1.40004583	0.80831666	1.20934782
N	1.25953710	0.72719432	2.54843508
C	-2.53949621	1.46617870	0.93382110
C	-3.16781429	1.82893817	2.11153311
C	-2.33115807	1.34589460	3.10649535
C	0.00000000	-2.93235740	0.93382110
C	0.00000000	-3.65787687	2.11153311
C	0.00000000	-2.69178972	3.10649535
C	2.53949621	1.46617870	0.93382110
C	3.16781429	1.82893817	2.11153311
C	2.33115807	1.34589460	3.10649535
H	-4.09649337	2.36511167	2.25153330
N	-2.60406589	1.50345818	4.53837172
H	0.00000000	-4.73022282	2.25153330
H	0.00000000	-3.28332310	-0.08890231
N	0.00000000	-3.00691636	4.53837172
H	-2.84344081	1.64166129	-0.08890231
H	0.00000000	0.00000000	4.28411211
H	4.09649337	2.36511167	2.25153330
N	2.60406589	1.50345818	4.53837172
H	2.84344081	1.64166129	-0.08890231
B	0.00000000	0.00000000	3.11721278
O	-3.64184598	-2.10262071	-4.77982578
O	-1.81638133	-1.04868802	-5.34608724
O	3.64184598	-2.10262071	-4.77982578
O	1.81638133	-1.04868802	-5.34608724
O	0.00000000	4.20524142	-4.77982578
O	0.00000000	2.09737603	-5.34608724
O	-3.64184598	2.10262071	4.77982578
O	-1.81638133	1.04868802	5.34608724
O	0.00000000	-4.20524142	4.77982578
O	0.00000000	-2.09737603	5.34608724
O	3.64184598	2.10262071	4.77982578
O	1.81638133	1.04868802	5.34608724

$[Cr(Tb^{3,5\text{-}CH3})_2]^+$ $^4A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	1.46850000	-0.84790000	1.23650000
N	1.25520000	-0.72470000	2.57150000
N	-1.46850000	-0.84790000	1.23650000
N	-1.25520000	-0.72470000	2.57150000
N	0.00000000	1.69570000	1.23650000
N	0.00000000	1.44940000	2.57150000
C	2.63360000	-1.52050000	1.07490000
C	3.15050000	-1.81900000	2.33870000
C	2.25900000	-1.30420000	3.26800000
C	-2.63360000	-1.52050000	1.07490000
C	-3.15050000	-1.81900000	2.33870000
C	-2.25900000	-1.30420000	3.26800000
C	0.00000000	3.04100000	1.07490000
C	0.00000000	3.63790000	2.33870000
C	0.00000000	2.60840000	3.26800000
H	4.07150000	-2.35070000	2.54870000
C	2.34150000	-1.35180000	4.75440000
H	-4.07150000	-2.35070000	2.54870000
C	-3.27230000	-1.88930000	-0.21850000
C	-2.34150000	-1.35180000	4.75440000
C	3.27230000	-1.88930000	-0.21850000
H	0.00000000	0.00000000	4.28130000
H	0.00000000	4.70130000	2.54870000
C	0.00000000	2.70370000	4.75440000
C	0.00000000	3.77860000	-0.21850000
B	0.00000000	0.00000000	3.08750000
N	1.46850000	0.84790000	-1.23650000
N	1.25520000	0.72470000	-2.57150000
N	0.00000000	-1.69570000	-1.23650000
N	0.00000000	-1.44940000	-2.57150000
N	-1.46850000	0.84790000	-1.23650000
N	-1.25520000	0.72470000	-2.57150000
C	2.63360000	1.52050000	-1.07490000
C	3.15050000	1.81900000	-2.33870000
C	2.25900000	1.30420000	-3.26800000
C	0.00000000	-3.04100000	-1.07490000
C	0.00000000	-3.63790000	-2.33870000
C	0.00000000	-2.60840000	-3.26800000
C	-2.63360000	1.52050000	-1.07490000
C	-3.15050000	1.81900000	-2.33870000
C	-2.25900000	1.30420000	-3.26800000
H	4.07150000	2.35070000	-2.54870000
C	2.34150000	1.35180000	-4.75440000
H	0.00000000	-4.70130000	-2.54870000
C	0.00000000	-3.77860000	0.21850000
C	0.00000000	-2.70370000	-4.75440000
C	3.27230000	1.88930000	0.21850000
H	0.00000000	0.00000000	-4.28130000
H	-4.07150000	2.35070000	-2.54870000
C	-2.34150000	1.35180000	-4.75440000
C	-3.27230000	1.88930000	0.21850000
B	0.00000000	0.00000000	-3.08750000
H	-3.51710000	-1.01540000	-0.82680000
H	-4.20140000	-2.42570000	-0.01070000
H	-2.63790000	-2.53820000	-0.82680000
H	4.20140000	-2.42570000	-0.01070000
H	3.51710000	-1.01540000	-0.82680000
H	2.63790000	-2.53820000	-0.82680000
H	0.00000000	4.85130000	-0.01070000
H	-0.87920000	3.55360000	-0.82680000
H	0.87920000	3.55360000	-0.82680000

H	0.87920000	-3.55360000	0.82680000
H	0.00000000	-4.85130000	0.01070000
H	-0.87920000	-3.55360000	0.82680000
H	-3.51710000	1.01540000	0.82680000
H	-4.20140000	2.42570000	0.01070000
H	-2.63790000	2.53820000	0.82680000
H	2.63790000	2.53820000	0.82680000
H	4.20140000	2.42570000	0.01070000
H	3.51710000	1.01540000	0.82680000
H	-3.25330000	1.87830000	-5.04650000
H	-2.37650000	0.35090000	-5.19670000
H	-1.49220000	1.88260000	-5.19670000
H	0.00000000	-3.75660000	-5.04650000
H	0.88430000	-2.23360000	-5.19670000
H	-0.88430000	-2.23360000	-5.19670000
H	2.37650000	0.35090000	-5.19670000
H	3.25330000	1.87830000	-5.04650000
H	1.49220000	1.88260000	-5.19670000
H	-0.88430000	2.23360000	5.19670000
H	0.00000000	3.75660000	5.04650000
H	0.88430000	2.23360000	5.19670000
H	-2.37650000	-0.35090000	5.19670000
H	-1.49220000	-1.88260000	5.19670000
H	-3.25330000	-1.87830000	5.04650000
H	1.49220000	-1.88260000	5.19670000
H	2.37650000	-0.35090000	5.19670000
H	3.25330000	-1.87830000	5.04650000

$[Cr(Tb^{3,5\text{-}CH3})_2]^+$ $^2A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	1.40400000	0.81060000	-1.16730000
N	1.23170000	0.71110000	-2.50660000
N	-1.40400000	0.81060000	-1.16730000
N	-1.23170000	0.71110000	-2.50660000
N	0.00000000	-1.62120000	-1.16730000
N	0.00000000	-1.42230000	-2.50660000
C	2.55650000	1.47600000	-0.95530000
C	3.11320000	1.79740000	-2.19130000
C	2.25140000	1.29990000	-3.15490000
C	-2.55650000	1.47600000	-0.95530000
C	-3.11320000	1.79740000	-2.19130000
C	-2.25140000	1.29990000	-3.15490000
C	0.00000000	-2.95190000	-0.95530000
C	0.00000000	-3.59480000	-2.19130000
C	0.00000000	-2.59970000	-3.15490000
H	4.04460000	2.33510000	-2.36330000
C	2.34310000	1.35280000	-4.62480000
H	-4.04460000	2.33510000	-2.36330000
C	-3.10100000	1.79040000	0.37590000
C	-2.34310000	1.35280000	-4.62480000
C	3.10100000	1.79040000	0.37590000
H	0.00000000	0.00000000	-4.24520000
H	0.00000000	-4.67030000	-2.36330000
C	0.00000000	-2.70560000	-4.62480000
C	0.00000000	-3.58070000	0.37590000
B	0.00000000	0.00000000	-3.04330000
N	1.40400000	-0.81060000	1.16730000
N	1.23170000	-0.71110000	2.50660000
N	0.00000000	1.62120000	1.16730000
N	0.00000000	1.42230000	2.50660000
N	-1.40400000	-0.81060000	1.16730000
N	-1.23170000	-0.71110000	2.50660000
C	2.55650000	-1.47600000	0.95530000
C	3.11320000	-1.79740000	2.19130000
C	2.25140000	-1.29990000	3.15490000
C	0.00000000	2.95190000	0.95530000
C	0.00000000	3.59480000	2.19130000
C	0.00000000	2.59970000	3.15490000
C	-2.55650000	-1.47600000	0.95530000
C	-3.11320000	-1.79740000	2.19130000
C	-2.25140000	-1.29990000	3.15490000
H	4.04460000	-2.33510000	2.36330000
C	2.34310000	-1.35280000	4.62480000
H	0.00000000	4.67030000	2.36330000
C	0.00000000	3.58070000	-0.37590000
C	0.00000000	2.70560000	4.62480000
C	3.10100000	-1.79040000	-0.37590000
H	0.00000000	0.00000000	4.24520000
H	-4.04460000	-2.33510000	2.36330000
C	-2.34310000	-1.35280000	4.62480000
C	-3.10100000	-1.79040000	-0.37590000
B	0.00000000	0.00000000	3.04330000
H	-3.29250000	0.87750000	0.96610000
H	-4.04700000	2.33650000	0.26540000
H	-2.40620000	2.41260000	0.96610000
H	4.04700000	2.33650000	0.26540000
H	3.29250000	0.87750000	0.96610000
H	2.40620000	2.41260000	0.96610000
H	0.00000000	-4.67310000	0.26540000
H	-0.88630000	-3.29010000	0.96610000
H	0.88630000	-3.29010000	0.96610000
H	0.88630000	3.29010000	-0.96610000
H	0.00000000	4.67310000	-0.26540000
H	-0.88630000	3.29010000	-0.96610000
H	-3.29250000	-0.87750000	-0.96610000
H	-4.04700000	-2.33650000	-0.26540000
H	-2.40620000	-2.41260000	-0.96610000
H	2.40620000	-2.41260000	-0.96610000
H	4.04700000	-2.33650000	-0.26540000
H	3.29250000	-0.87750000	-0.96610000
H	-3.25790000	-1.88100000	4.92340000
H	-2.36940000	-0.34420000	5.06700000
H	-1.48280000	-1.87990000	5.06700000
H	0.00000000	3.76190000	4.92340000
H	0.88660000	2.22410000	5.06700000
H	-0.88660000	2.22410000	5.06700000
H	2.36940000	-0.34420000	5.06700000
H	3.25790000	-1.88100000	4.92340000
H	1.48280000	-1.87990000	5.06700000
H	-0.88660000	-2.22410000	-5.06700000
H	0.00000000	-3.76190000	-4.92340000
H	0.88660000	-2.22410000	-5.06700000
H	-2.36940000	0.34420000	-5.06700000
H	-1.48280000	1.87990000	-5.06700000
H	-3.25790000	1.88100000	-4.92340000
H	1.48280000	1.87990000	-5.06700000
H	2.36940000	0.34420000	-5.06700000
H	3.25790000	1.88100000	-4.92340000

$[Cr(Tb^{3,5\text{-}CF3})_2]^+$ $^4A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	1.51956739	0.87732243	1.17700027
N	1.27824564	0.73799535	2.50298034
N	0.00000000	-1.75464486	1.17700027
N	0.00000000	-1.47599124	2.50298034
N	-1.51956739	0.87732243	1.17700027
N	-1.27824564	0.73799535	2.50298034
C	2.69412392	1.55545302	1.05221604
C	3.19099490	1.84232159	2.31729681
C	2.28052375	1.31666073	3.20877843
C	0.00000000	-3.11090604	1.05221604
C	0.00000000	-3.68464372	2.31729681
C	0.00000000	-2.63332199	3.20877843
C	-2.69412392	1.55545302	1.05221604
C	-3.19099490	1.84232159	2.31729681
C	-2.28052375	1.31666073	3.20877843
H	4.10263183	2.36865557	2.55851908
C	2.42549450	1.40035964	4.71497563
H	0.00000000	-4.73731115	2.55851908
C	0.00000000	-4.01230445	-0.18928776
C	0.00000000	-2.80071980	4.71497563
C	3.47475773	2.00615222	-0.18928776
H	0.00000000	0.00000000	4.19388368
H	-4.10263183	2.36865557	2.55851908
C	-2.42549450	1.40035964	4.71497563
C	-3.47475773	2.00615222	-0.18928776
B	0.00000000	0.00000000	3.00929501
N	0.00000000	1.75464486	-1.17700027
N	0.00000000	1.47599124	-2.50298034
N	1.51956739	-0.87732243	-1.17700027
N	1.27824564	-0.73799535	-2.50298034
N	-1.51956739	-0.87732243	-1.17700027
N	-1.27824564	-0.73799535	-2.50298034
C	0.00000000	3.11090604	-1.05221604
C	0.00000000	3.68464372	-2.31729681
C	0.00000000	2.63332199	-3.20877843
C	2.69412392	-1.55545302	-1.05221604
C	3.19099490	-1.84232159	-2.31729681
C	2.28052375	-1.31666073	-3.20877843
C	-2.69412392	-1.55545302	-1.05221604
C	-3.19099490	-1.84232159	-2.31729681
C	-2.28052375	-1.31666073	-3.20877843
H	0.00000000	4.73731115	-2.55851908
C	0.00000000	2.80071980	-4.71497563
H	4.10263183	-2.36865557	-2.55851908
C	3.47475773	-2.00615222	0.18928776
C	2.42549450	-1.40035964	-4.71497563
C	0.00000000	4.01230445	0.18928776
H	0.00000000	0.00000000	-4.19388368
H	-4.10263183	-2.36865557	-2.55851908
C	-2.42549450	-1.40035964	-4.71497563
C	-3.47475773	-2.00615222	0.18928776
B	0.00000000	0.00000000	-3.00929501
F	-1.07874211	-3.85925316	-0.97408302
F	0.00000000	-5.29343781	0.23405774
F	1.07874211	-3.85925316	-0.97408302
F	4.58425139	2.64671864	0.23405774
F	2.80284021	2.86384483	-0.97408302
F	3.88158232	0.99540833	-0.97408302
F	-4.58425139	2.64671864	0.23405774
F	-3.88158232	0.99540833	-0.97408302
F	-2.80284021	2.86384483	-0.97408302
F	3.88158232	-0.99540833	0.97408302
F	4.58425139	-2.64671864	-0.23405774
F	2.80284021	-2.86384483	0.97408302
F	-2.80284021	-2.86384483	0.97408302
F	-4.58425139	-2.64671864	-0.23405774
F	-3.88158232	-0.99540833	0.97408302
F	-1.07874211	3.85925316	0.97408302
F	0.00000000	5.29343781	-0.23405774
F	1.07874211	3.85925316	0.97408302
F	-3.56586089	-2.05875086	-4.99947455
F	-1.41067489	-2.07171676	-5.28632143
F	-2.49949677	-0.18582218	-5.28632143
F	3.56586089	-2.05875086	-4.99947455
F	2.49949677	-0.18582218	-5.28632143
F	1.41067489	-2.07171676	-5.28632143
F	1.08882188	2.25753894	-5.28632143
F	0.00000000	4.11750118	-4.99947455
F	-1.08882188	2.25753894	-5.28632143
F	-2.49949677	0.18582218	5.28632143
F	-3.56586089	2.05875086	4.99947455
F	-1.41067489	2.07171676	5.28632143
F	-1.08882188	-2.25753894	5.28632143
F	1.08882188	-2.25753894	5.28632143
F	0.00000000	-4.11750118	4.99947455
F	2.49949677	0.18582218	5.28632143
F	1.41067489	2.07171676	5.28632143
F	3.56586089	2.05875086	4.99947455

$[Cr(Tb^{3,5\text{-}CF3})_2]^+$ $^2A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	1.50143196	0.86685213	1.15433085
N	1.27595536	0.73667294	2.48559581
N	0.00000000	-1.73370479	1.15433085
N	0.00000000	-1.47334641	2.48559581
N	-1.50143196	0.86685213	1.15433085
N	-1.27595536	0.73667294	2.48559581
C	2.68199571	1.54845095	1.02280913
C	3.18691812	1.83996781	2.28021524
C	2.28000304	1.31636016	3.18194967
C	0.00000000	-3.09690189	1.02280913
C	0.00000000	-3.67993616	2.28021524
C	0.00000000	-2.63272031	3.18194967
C	-2.68199571	1.54845095	1.02280913
C	-3.18691812	1.83996781	2.28021524
C	-2.28000304	1.31636016	3.18194967
H	4.09954302	2.36687225	2.51630714
C	2.43760049	1.40734901	4.68720970
H	0.00000000	-4.73374449	2.51630714
C	0.00000000	-3.99856754	-0.21963555
C	0.00000000	-2.81469855	4.68720970
C	3.46286130	1.99928403	-0.21963555
H	0.00000000	0.00000000	4.17186938
H	-4.09954302	2.36687225	2.51630714
C	-2.43760049	1.40734901	4.68720970

C	-3.46286130	1.99928403	-0.21963555
B	0.00000000	0.00000000	2.98602550
N	0.00000000	1.73370479	-1.15433085
N	0.00000000	1.47334641	-2.48559581
N	1.50143196	-0.86685213	-1.15433085
N	1.27595536	-0.73667294	-2.48559581
N	-1.50143196	-0.86685213	-1.15433085
N	-1.27595536	-0.73667294	-2.48559581
C	0.00000000	3.09690189	-1.02280913
C	0.00000000	3.67993616	-2.28021524
C	0.00000000	2.63272031	-3.18194967
C	2.68199571	-1.54845095	-1.02280913
C	3.18691812	-1.83996781	-2.28021524
C	2.28000304	-1.31636016	-3.18194967
C	-2.68199571	-1.54845095	-1.02280913
C	-3.18691812	-1.83996781	-2.28021524
C	-2.28000304	-1.31636016	-3.18194967
H	0.00000000	4.73374449	-2.51630714
C	0.00000000	2.81469855	-4.68720970
H	4.09954302	-2.36687225	-2.51630714
C	3.46286130	-1.99928403	0.21963555
C	2.43760049	-1.40734901	-4.68720970
C	0.00000000	3.99856754	0.21963555
H	0.00000000	0.00000000	-4.17186938
H	-4.09954302	-2.36687225	-2.51630714
C	-2.43760049	-1.40734901	-4.68720970
C	-3.46286130	-1.99928403	0.21963555
B	0.00000000	0.00000000	-2.98602550
F	-1.07881566	-3.84737419	-1.00475995
F	0.00000000	-5.28024753	0.20337393
F	1.07881566	-3.84737419	-1.00475995
F	4.57282857	2.64012403	0.20337393
F	2.79251597	2.85796884	-1.00475995
F	3.87133163	0.98940535	-1.00475995
F	-4.57282857	2.64012403	0.20337393
F	-3.87133163	0.98940535	-1.00475995
F	-2.79251597	2.85796884	-1.00475995
F	3.87133163	-0.98940535	1.00475995
F	4.57282857	-2.64012403	-0.20337393
F	2.79251597	-2.85796884	1.00475995
F	-2.79251597	-2.85796884	1.00475995
F	-4.57282857	-2.64012403	-0.20337393
F	-3.87133163	-0.98940535	1.00475995
F	-1.07881566	3.84737419	1.00475995
F	0.00000000	5.28024753	-0.20337393
F	1.07881566	3.84737419	1.00475995
F	-3.58019895	-2.06702878	-4.95991062
F	-1.42733550	-2.08183039	-5.26174644
F	-2.51658549	-0.19519338	-5.26174644
F	3.58019895	-2.06702878	-4.95991062
F	2.51658549	-0.19519338	-5.26174644
F	1.42733550	-2.08183039	-5.26174644
F	1.08924998	2.27702377	-5.26174644
F	0.00000000	4.13405755	-4.95991062
F	-1.08924998	2.27702377	-5.26174644
F	-2.51658549	0.19519338	5.26174644
F	-3.58019895	2.06702878	4.95991062
F	-1.42733550	2.08183039	5.26174644
F	-1.08924998	-2.27702377	5.26174644
F	1.08924998	-2.27702377	5.26174644
F	0.00000000	-4.13405755	4.95991062
F	2.51658549	0.19519338	5.26174644
F	1.42733550	2.08183039	5.26174644
F	3.58019895	2.06702878	4.95991062

$[Cr(Tb^{3,5\text{-}NH2})_2]^+$ $^4A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	0.00000000	1.65932840	1.24959704
N	0.00000000	1.44259010	2.61847751
N	1.43702051	-0.82966420	1.24959704
N	1.24931975	-0.72129505	2.61847751
N	-1.43702051	-0.82966420	1.24959704
N	-1.24931975	-0.72129505	2.61847751
C	0.00000000	3.00091179	1.07625656
C	0.00000000	3.65258140	2.31930927
C	0.00000000	2.62993049	3.26202901
C	2.59886567	-1.50045563	1.07625656
C	3.16322844	-1.82629070	2.31930927
C	2.27758629	-1.31496524	3.26202901
C	-2.59886567	-1.50045563	1.07625656
C	-3.16322844	-1.82629070	2.31930927
C	-2.27758629	-1.31496524	3.26202901
H	0.00000000	4.71971971	2.50455940
N	0.00000000	2.73759478	4.61936389
H	4.08739682	-2.35985959	2.50455940
N	3.10164967	-1.79073793	-0.14357584
N	2.37082679	-1.36879739	4.61936389
N	0.00000000	3.58147638	-0.14357584
H	0.00000000	0.00000000	4.34090765
H	-4.08739682	-2.35985959	2.50455940
N	-2.37082679	-1.36879739	4.61936389
N	-3.10164967	-1.79073793	-0.14357584
B	0.00000000	0.00000000	3.13125767
N	-1.43702051	0.82966420	-1.24959704
N	-1.24931975	0.72129505	-2.61847751
N	1.43702051	0.82966420	-1.24959704
N	1.24931975	0.72129505	-2.61847751
N	0.00000000	-1.65932840	-1.24959704
N	0.00000000	-1.44259010	-2.61847751
C	-2.59886567	1.50045563	-1.07625656
C	-3.16322844	1.82629070	-2.31930927
C	-2.27758629	1.31496524	-3.26202901
C	2.59886567	1.50045563	-1.07625656
C	3.16322844	1.82629070	-2.31930927
C	2.27758629	1.31496524	-3.26202901
C	0.00000000	-3.00091179	-1.07625656
C	0.00000000	-3.65258140	-2.31930927
C	0.00000000	-2.62993049	-3.26202901
H	-4.08739682	2.35985959	-2.50455940
N	-2.37082679	1.36879739	-4.61936389
H	4.08739682	2.35985959	-2.50455940
N	3.10164967	1.79073793	0.14357584
N	2.37082679	1.36879739	-4.61936389
N	-3.10164967	1.79073793	0.14357584
H	0.00000000	0.00000000	-4.34090765
H	0.00000000	-4.71971971	-2.50455940
N	0.00000000	-2.73759478	-4.61936389
N	0.00000000	-3.58147638	0.14357584
B	0.00000000	0.00000000	-3.13125767

H	0.00000000	3.64457230	5.04513197
H	0.00000000	1.92734133	5.20735919
H	3.15629199	-1.82228589	5.04513197
H	1.66912664	-0.96367093	5.20735919
H	-3.15629199	-1.82228589	5.04513197
H	-1.66912664	-0.96367093	5.20735919
H	-3.15629199	1.82228589	-5.04513197
H	-1.66912664	0.96367093	-5.20735919
H	3.15629199	1.82228589	-5.04513197
H	1.66912664	0.96367093	-5.20735919
H	0.00000000	-3.64457230	-5.04513197
H	0.00000000	-1.92734133	-5.20735919
H	0.00000000	4.57995765	-0.22152630
H	3.96635969	-2.28997856	-0.22152630
H	-3.96635969	-2.28997856	-0.22152630
H	-3.96635969	2.28997856	0.22152630
H	3.96635969	2.28997856	0.22152630
H	0.00000000	-4.57995765	0.22152630
H	2.61817270	-1.51160275	-0.97754384
H	0.00000000	3.02320550	-0.97754384
H	-2.61817270	-1.51160275	-0.97754384
H	2.61817270	1.51160275	0.97754384
H	-2.61817270	1.51160275	0.97754384
H	0.00000000	-3.02320550	0.97754384

$[Cr(Tb^{3,5\text{-}NH2})_2]^+$ $^2A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	0.00000000	1.65490024	1.23325393
N	0.00000000	1.44242499	2.60296732
N	1.43318609	-0.82745012	1.23325393
N	1.24917634	-0.72121250	2.60296732
N	-1.43318609	-0.82745012	1.23325393
N	-1.24917634	-0.72121250	2.60296732
C	0.00000000	2.99767587	1.05916308
C	0.00000000	3.65209244	2.30052665
C	0.00000000	2.63096715	3.24487732
C	2.59606368	-1.49883793	1.05916308
C	3.16280510	-1.82604622	2.30052665
C	2.27848430	-1.31548384	3.24487732
C	-2.59606368	-1.49883793	1.05916308
C	-3.16280510	-1.82604622	2.30052665
C	-2.27848430	-1.31548384	3.24487732
H	0.00000000	4.71949216	2.48429932
N	0.00000000	2.74014012	4.60189734
H	4.08720049	-2.35974635	2.48429932
N	3.09527891	-1.78706014	-0.16229866
N	2.37303081	-1.37007006	4.60189734
N	0.00000000	3.57412029	-0.16229866
H	0.00000000	0.00000000	4.32605470
H	-4.08720049	-2.35974635	2.48429932
N	-2.37303081	-1.37007006	4.60189734
N	-3.09527891	-1.78706014	-0.16229866
B	0.00000000	0.00000000	3.11605441
N	-1.43318609	0.82745012	-1.23325393
N	-1.24917634	0.72121250	-2.60296732
N	1.43318609	0.82745012	-1.23325393
N	1.24917634	0.72121250	-2.60296732
N	0.00000000	-1.65490024	-1.23325393
N	0.00000000	-1.44242499	-2.60296732
C	-2.59606368	1.49883793	-1.05916308
C	-3.16280510	1.82604622	-2.30052665
C	-2.27848430	1.31548384	-3.24487732
C	2.59606368	1.49883793	-1.05916308
C	3.16280510	1.82604622	-2.30052665
C	2.27848430	1.31548384	-3.24487732
C	0.00000000	-2.99767587	-1.05916308
C	0.00000000	-3.65209244	-2.30052665
C	0.00000000	-2.63096715	-3.24487732
H	-4.08720049	2.35974635	-2.48429932
N	-2.37303081	1.37007006	-4.60189734
H	4.08720049	2.35974635	-2.48429932
N	3.09527891	1.78706014	0.16229866
N	2.37303081	1.37007006	-4.60189734
N	-3.09527891	1.78706014	0.16229866
H	0.00000000	0.00000000	-4.32605470
H	0.00000000	-4.71949216	-2.48429932
N	0.00000000	-2.74014012	-4.60189734
N	0.00000000	-3.57412029	0.16229866
B	0.00000000	0.00000000	-3.11605441
H	0.00000000	3.64749124	5.02696901
H	0.00000000	1.93026080	5.19050595
H	3.15881987	-1.82374536	5.02696901
H	1.67165505	-0.96513040	5.19050595
H	-3.15881987	-1.82374536	5.02696901
H	-1.67165505	-0.96513040	5.19050595
H	-3.15881987	1.82374536	-5.02696901
H	-1.67165505	0.96513040	-5.19050595
H	3.15881987	1.82374536	-5.02696901
H	1.67165505	0.96513040	-5.19050595
H	0.00000000	-3.64749124	-5.02696901
H	0.00000000	-1.93026080	-5.19050595
H	0.00000000	4.57228405	-0.24456985
H	3.95971429	-2.28614202	-0.24456985
H	-3.95971429	-2.28614202	-0.24456985
H	-3.95971429	2.28614202	0.24456985
H	3.95971429	2.28614202	0.24456985
H	0.00000000	-4.57228405	0.24456985
H	2.60774738	-1.50558389	-0.99307678
H	0.00000000	3.01116724	-0.99307678
H	-2.60774738	-1.50558389	-0.99307678
H	2.60774738	1.50558389	0.99307678
H	-2.60774738	1.50558389	0.99307678
H	0.00000000	-3.01116724	0.99307678

$[Cr(Tb^{3,5\text{-}NO2})_2]^+$ $^4A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	0.00000000	1.72784680	1.24666645
N	0.00000000	1.46369527	2.56410931
N	1.49635927	-0.86392313	1.24666645
N	1.26759700	-0.73184737	2.56410931
N	-1.49635927	-0.86392313	1.24666645
N	-1.26759700	-0.73184737	2.56410931
C	0.00000000	3.07672542	1.13268485
C	0.00000000	3.68922004	2.37122526
C	0.00000000	2.63736437	3.25512060
C	2.66452228	-1.53836271	1.13268485
C	3.19495844	-1.84460976	2.37122526
C	2.28402479	-1.31868219	3.25512060

C	-2.66452228	-1.53836271	1.13268485
C	-3.19495844	-1.84460976	2.37122526
C	-2.28402479	-1.31868219	3.25512060
H	0.00000000	4.74558007	2.59411577
N	0.00000000	2.84299948	4.71636314
H	4.10979319	-2.37279004	2.59411577
N	3.33626570	-1.92619407	-0.10261329
N	2.46210933	-1.42149974	4.71636314
N	0.00000000	3.85238761	-0.10261329
H	0.00000000	0.00000000	4.24049944
H	-4.10979319	-2.37279004	2.59411577
N	-2.46210933	-1.42149974	4.71636314
N	-3.33626570	-1.92619407	-0.10261329
B	0.00000000	0.00000000	3.07587821
N	-1.49635927	0.86392313	-1.24666645
N	-1.26759700	0.73184737	-2.56410931
N	1.49635927	0.86392313	-1.24666645
N	1.26759700	0.73184737	-2.56410931
N	0.00000000	-1.72784680	-1.24666645
N	0.00000000	-1.46369527	-2.56410931
C	-2.66452228	1.53836271	-1.13268485
C	-3.19495844	1.84460976	-2.37122526
C	-2.28402479	1.31868219	-3.25512060
C	2.66452228	1.53836271	-1.13268485
C	3.19495844	1.84460976	-2.37122526
C	2.28402479	1.31868219	-3.25512060
C	0.00000000	-3.07672542	-1.13268485
C	0.00000000	-3.68922004	-2.37122526
C	0.00000000	-2.63736437	-3.25512060
H	-4.10979319	2.37279004	-2.59411577
N	-2.46210933	1.42149974	-4.71636314
H	4.10979319	2.37279004	-2.59411577
N	3.33626570	1.92619407	0.10261329
N	2.46210933	1.42149974	-4.71636314
N	-3.33626570	1.92619407	0.10261329
H	0.00000000	0.00000000	-4.24049944
H	0.00000000	-4.74558007	-2.59411577
N	0.00000000	-2.84299948	-4.71636314
N	0.00000000	-3.85238761	0.10261329
B	0.00000000	0.00000000	-3.07587821
O	0.00000000	4.01975897	5.03735359
O	0.00000000	1.88192363	5.45763780
O	3.48121317	-2.00987922	5.03735359
O	1.62979343	-0.94096182	5.45763780
O	-3.48121317	-2.00987922	5.03735359
O	-1.62979343	-0.94096182	5.45763780
O	-3.48121317	2.00987922	-5.03735359
O	-1.62979343	0.94096182	-5.45763780
O	3.48121317	2.00987922	-5.03735359
O	1.62979343	0.94096182	-5.45763780
O	0.00000000	-4.01975897	-5.03735359
O	0.00000000	-1.88192363	-5.45763780
O	0.00000000	5.06139834	0.04654378
O	4.38329951	-2.53069917	0.04654378
O	-4.38329951	-2.53069917	0.04654378
O	-4.38329951	2.53069917	-0.04654378
O	4.38329951	2.53069917	-0.04654378
O	0.00000000	-5.06139834	-0.04654378
O	2.81908596	-1.62759999	-1.16831859
O	0.00000000	3.25520051	-1.16831859
O	-2.81908596	-1.62759999	-1.16831859
O	2.81908596	1.62759999	1.16831859
O	-2.81908596	1.62759999	1.16831859
O	0.00000000	-3.25520051	1.16831859

$[Cr(Tb^{3,5\text{-}NO2})_2]^+$ $^2A_{2g}$ D_{3d} OPBE

Cr	0.00000000	0.00000000	0.00000000
N	0.00000000	1.72356628	1.20646962
N	0.00000000	1.46400908	2.52584926
N	1.49265185	-0.86178314	1.20646962
N	1.26786900	-0.73200454	2.52584926
N	-1.49265185	-0.86178314	1.20646962
N	-1.26786900	-0.73200454	2.52584926
C	0.00000000	3.07399646	1.08968126
C	0.00000000	3.68855910	2.32676908
C	0.00000000	2.63844971	3.21366380
C	2.66215897	-1.53699796	1.08968126
C	3.19438587	-1.84427955	2.32676908
C	2.28496460	-1.31922512	3.21366380
C	-2.66215897	-1.53699796	1.08968126
C	-3.19438587	-1.84427955	2.32676908
C	-2.28496460	-1.31922512	3.21366380
H	0.00000000	4.74529432	2.54755294
N	0.00000000	2.84526330	4.67390301
H	4.10954553	-2.37264716	2.54755294
N	3.33729018	-1.92678516	-0.14517713
N	2.46407047	-1.42263165	4.67390301
N	0.00000000	3.85357085	-0.14517713
H	0.00000000	0.00000000	4.20184621
H	-4.10954553	-2.37264716	2.54755294
N	-2.46407047	-1.42263165	4.67390301
N	-3.33729018	-1.92678516	-0.14517713
B	0.00000000	0.00000000	3.03654023
N	-1.49265185	0.86178314	-1.20646962
N	-1.26786900	0.73200454	-2.52584926
N	1.49265185	0.86178314	-1.20646962
N	1.26786900	0.73200454	-2.52584926
N	0.00000000	-1.72356628	-1.20646962
N	0.00000000	-1.46400908	-2.52584926
C	-2.66215897	1.53699796	-1.08968126
C	-3.19438587	1.84427955	-2.32676908
C	-2.28496460	1.31922512	-3.21366380
C	2.66215897	1.53699796	-1.08968126
C	3.19438587	1.84427955	-2.32676908
C	2.28496460	1.31922512	-3.21366380
C	0.00000000	-3.07399646	-1.08968126
C	0.00000000	-3.68855910	-2.32676908
C	0.00000000	-2.63844971	-3.21366380
H	-4.10954553	2.37264716	-2.54755294
N	-2.46407047	1.42263165	-4.67390301
H	4.10954553	2.37264716	-2.54755294
N	3.33729018	1.92678516	0.14517713
N	2.46407047	1.42263165	-4.67390301
N	-3.33729018	1.92678516	0.14517713
H	0.00000000	0.00000000	-4.20184621
H	0.00000000	-4.74529432	-2.54755294
N	0.00000000	-2.84526330	-4.67390301
N	0.00000000	-3.85357085	0.14517713
B	0.00000000	0.00000000	-3.03654023

O	0.00000000	4.02187197	4.99554118
O	0.00000000	1.88411125	5.41548619
O	3.48304359	-2.01093599	4.99554118
O	1.63168841	-0.94205563	5.41548619
O	-3.48304359	-2.01093599	4.99554118
O	-1.63168841	-0.94205563	5.41548619
O	-3.48304359	2.01093599	-4.99554118
O	-1.63168841	0.94205563	-5.41548619
O	3.48304359	2.01093599	-4.99554118
O	1.63168841	0.94205563	-5.41548619
O	0.00000000	-4.02187197	-4.99554118
O	0.00000000	-1.88411125	-5.41548619
O	0.00000000	5.06195451	0.01020677
O	4.38378106	-2.53097752	0.01020677
O	-4.38378106	-2.53097752	0.01020677
O	-4.38378106	2.53097752	-0.01020677
O	4.38378106	2.53097752	-0.01020677
O	0.00000000	-5.06195451	-0.01020677
O	2.82561759	-1.63137091	-1.21396277
O	0.00000000	3.26274234	-1.21396277
O	-2.82561759	-1.63137091	-1.21396277
O	2.82561759	1.63137091	1.21396277
O	-2.82561759	1.63137091	1.21396277
O	0.00000000	-3.26274234	1.21396277

$[Mn(Tb^{3CH3})_2]^{2+}$ $^4A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.43749782	0.82993990	1.14915285
N	1.23849966	0.71504811	2.48285996
N	0.00000000	-1.65987927	1.14915285
N	0.00000000	-1.43009622	2.48285996
N	-1.43749782	0.82993990	1.14915285
N	-1.23849966	0.71504811	2.48285996
C	2.61097272	1.50744606	0.95810875
C	3.13598640	1.81056249	2.21720663
C	2.24676489	1.29717007	3.14443577
C	0.00000000	-3.01489159	0.95810875
C	0.00000000	-3.62112551	2.21720663
C	0.00000000	-2.59434067	3.14443577
C	-2.61097272	1.50744606	0.95810875
C	-3.13598640	1.81056249	2.21720663
C	-2.24676489	1.29717007	3.14443577
H	4.05828043	2.34304922	2.41839559
H	2.26214860	1.30605178	4.22748009
H	0.00000000	-4.68609896	2.41839559
C	0.00000000	-3.73657347	-0.33979053
H	0.00000000	-2.61210410	4.22748009
C	3.23596756	1.86828673	-0.33979053
H	0.00000000	0.00000000	4.22502788
H	-4.05828043	2.34304922	2.41839559
H	-2.26214860	1.30605178	4.22748009
C	-3.23596756	1.86828673	-0.33979053
B	0.00000000	0.00000000	3.03007475
N	0.00000000	1.65987927	-1.14915285
N	0.00000000	1.43009622	-2.48285996
N	1.43749782	-0.82993990	-1.14915285
N	1.23849966	-0.71504811	-2.48285996
N	-1.43749782	-0.82993990	-1.14915285
N	-1.23849966	-0.71504811	-2.48285996
C	0.00000000	3.01489159	-0.95810875
C	0.00000000	3.62112551	-2.21720663
C	0.00000000	2.59434067	-3.14443577
C	2.61097272	-1.50744606	-0.95810875
C	3.13598640	-1.81056249	-2.21720663
C	2.24676489	-1.29717007	-3.14443577
C	-2.61097272	-1.50744606	-0.95810875
C	-3.13598640	-1.81056249	-2.21720663
C	-2.24676489	-1.29717007	-3.14443577
H	0.00000000	4.68609896	-2.41839559
H	0.00000000	2.61210410	-4.22748009
H	4.05828043	-2.34304922	-2.41839559
C	3.23596756	-1.86828673	0.33979053
H	2.26214860	-1.30605178	-4.22748009
C	0.00000000	3.73657347	0.33979053
H	0.00000000	0.00000000	-4.22502788
H	-4.05828043	-2.34304922	-2.41839559
H	-2.26214860	-1.30605178	-4.22748009
C	-3.23596756	-1.86828673	0.33979053
B	0.00000000	0.00000000	-3.03007475
H	-0.88205222	-3.51118947	-0.94441893
H	0.00000000	-4.81038153	-0.14022827
H	0.88205222	-3.51118947	-0.94441893
H	4.16591296	2.40519103	-0.14022827
H	2.59975310	2.51947426	-0.94441893
H	3.48180532	0.99171521	-0.94441893
H	-4.16591296	2.40519103	-0.14022827
H	-3.48180532	0.99171521	-0.94441893
H	-2.59975310	2.51947426	-0.94441893
H	3.48180532	-0.99171521	0.94441893
H	4.16591296	-2.40519103	0.14022827
H	2.59975310	-2.51947426	0.94441893
H	-2.59975310	-2.51947426	0.94441893
H	-4.16591296	-2.40519103	0.14022827
H	-3.48180532	-0.99171521	0.94441893
H	-0.88205222	3.51118947	0.94441893
H	0.00000000	4.81038153	0.14022827
H	0.88205222	3.51118947	0.94441893

$[Mn(Tb^{3CH3})_2]^{2+}$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.41835431	0.81888698	1.14621062
N	1.23609455	0.71365955	2.48037071
N	0.00000000	-1.63777448	1.14621062
N	0.00000000	-1.42731910	2.48037071
N	-1.41835431	0.81888698	1.14621062
N	-1.23609455	0.71365955	2.48037071
C	2.59969436	1.50093401	0.95308527
C	3.13402580	1.80943058	2.20292996
C	2.24714325	1.29738862	3.13725060
C	0.00000000	-3.00186854	0.95308527
C	0.00000000	-3.61886117	2.20292996
C	0.00000000	-2.59477777	3.13725060
C	-2.59969436	1.50093401	0.95308527
C	-3.13402580	1.80943058	2.20292996
C	-2.24714325	1.29738862	3.13725060
H	4.05674317	2.34216179	2.40105551
H	2.26923111	1.31014127	4.22029863
H	0.00000000	-4.68432357	2.40105551

C	0.00000000	-3.70983361	-0.35069582
H	0.00000000	-2.62028253	4.22029863
C	3.21281023	1.85491707	-0.35069582
H	0.00000000	0.00000000	4.22415368
H	-4.05674317	2.34216179	2.40105551
H	-2.26923111	1.31014127	4.22029863
C	-3.21281023	1.85491707	-0.35069582
B	0.00000000	0.00000000	3.02803000
N	0.00000000	1.63777448	-1.14621062
N	0.00000000	1.42731910	-2.48037071
N	1.41835431	-0.81888698	-1.14621062
N	1.23609455	-0.71365955	-2.48037071
N	-1.41835431	-0.81888698	-1.14621062
N	-1.23609455	-0.71365955	-2.48037071
C	0.00000000	3.00186854	-0.95308527
C	0.00000000	3.61886117	-2.20292996
C	0.00000000	2.59477777	-3.13725060
C	2.59969436	-1.50093401	-0.95308527
C	3.13402580	-1.80943058	-2.20292996
C	2.24714325	-1.29738862	-3.13725060
C	-2.59969436	-1.50093401	-0.95308527
C	-3.13402580	-1.80943058	-2.20292996
C	-2.24714325	-1.29738862	-3.13725060
H	0.00000000	4.68432357	-2.40105551
H	0.00000000	2.62028253	-4.22029863
H	4.05674317	-2.34216179	-2.40105551
C	3.21281023	-1.85491707	0.35069582
H	2.26923111	-1.31014127	-4.22029863
C	0.00000000	3.70983361	0.35069582
H	0.00000000	0.00000000	-4.22415368
H	-4.05674317	-2.34216179	-2.40105551
H	-2.26923111	-1.31014127	-4.22029863
C	-3.21281023	-1.85491707	0.35069582
B	0.00000000	0.00000000	-3.02803000
H	-0.88102614	-3.47514774	-0.95412563
H	0.00000000	-4.78630873	-0.16581663
H	0.88102614	-3.47514774	-0.95412563
H	4.14506497	2.39315436	-0.16581663
H	2.56905341	2.50056517	-0.95412563
H	3.45007955	0.97458309	-0.95412563
H	-4.14506497	2.39315436	-0.16581663
H	-3.45007955	0.97458309	-0.95412563
H	-2.56905341	2.50056517	-0.95412563
H	3.45007955	-0.97458309	0.95412563
H	4.14506497	-2.39315436	0.16581663
H	2.56905341	-2.50056517	0.95412563
H	-2.56905341	-2.50056517	0.95412563
H	-4.14506497	-2.39315436	0.16581663
H	-3.45007955	-0.97458309	0.95412563
H	-0.88102614	3.47514774	0.95412563
H	0.00000000	4.78630873	0.16581663
H	0.88102614	3.47514774	0.95412563

$[Mn(Tb^{3CF3})_2]^{2+}$ $^4A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.49887604	0.86537625	1.10079134
N	1.25175238	0.72269948	2.42216968
N	0.00000000	-1.73075304	1.10079134
N	0.00000000	-1.44539950	2.42216968
N	-1.49887604	0.86537625	1.10079134
N	-1.25175238	0.72269948	2.42216968
C	2.68486597	1.55010833	0.99362977
C	3.15693388	1.82265631	2.27307082
C	2.22661699	1.28553770	3.14399285
C	0.00000000	-3.10021613	0.99362977
C	0.00000000	-3.64531315	2.27307082
C	0.00000000	-2.57107540	3.14399285
C	-2.68486597	1.55010833	0.99362977
C	-3.15693388	1.82265631	2.27307082
C	-2.22661699	1.28553770	3.14399285
H	4.06673509	2.34793088	2.53264178
H	2.19724607	1.26858074	4.22634818
H	0.00000000	-4.69586122	2.53264178
C	0.00000000	-4.02033154	-0.23678512
H	0.00000000	-2.53716096	4.22634818
C	3.48170954	2.01016603	-0.23678512
H	0.00000000	0.00000000	4.13557788
H	-4.06673509	2.34793088	2.53264178
H	-2.19724607	1.26858074	4.22634818
C	-3.48170954	2.01016603	-0.23678512
B	0.00000000	0.00000000	2.94198367
N	0.00000000	1.73075304	-1.10079134
N	0.00000000	1.44539950	-2.42216968
N	1.49887604	-0.86537625	-1.10079134
N	1.25175238	-0.72269948	-2.42216968
N	-1.49887604	-0.86537625	-1.10079134
N	-1.25175238	-0.72269948	-2.42216968
C	0.00000000	3.10021613	-0.99362977
C	0.00000000	3.64531315	-2.27307082
C	0.00000000	2.57107540	-3.14399285
C	2.68486597	-1.55010833	-0.99362977
C	3.15693388	-1.82265631	-2.27307082
C	2.22661699	-1.28553770	-3.14399285
C	-2.68486597	-1.55010833	-0.99362977
C	-3.15693388	-1.82265631	-2.27307082
C	-2.22661699	-1.28553770	-3.14399285
H	0.00000000	4.69586122	-2.53264178
H	0.00000000	2.53716096	-4.22634818
H	4.06673509	-2.34793088	-2.53264178
C	3.48170954	-2.01016603	0.23678512
H	2.19724607	-1.26858074	-4.22634818
C	0.00000000	4.02033154	0.23678512
H	0.00000000	0.00000000	-4.13557788
H	-4.06673509	-2.34793088	-2.53264178
H	-2.19724607	-1.26858074	-4.22634818
C	-3.48170954	-2.01016603	0.23678512
B	0.00000000	0.00000000	-2.94198367
F	-1.07935701	-3.86812535	-1.02095966
F	0.00000000	-5.28929911	0.20404810
F	1.07935701	-3.86812535	-1.02095966
F	4.58066727	2.64464956	0.20404810
F	2.81021642	2.86881327	-1.02095966
F	3.88957343	0.99931207	-1.02095966
F	-4.58066727	2.64464956	0.20404810
F	-3.88957343	0.99931207	-1.02095966
F	-2.81021642	2.86881327	-1.02095966
F	3.88957343	-0.99931207	1.02095966
F	4.58066727	-2.64464956	-0.20404810
F	2.81021642	-2.86881327	1.02095966

F	-2.81021642	-2.86881327	1.02095966
F	-4.58066727	-2.64464956	-0.20404810
F	-3.88957343	-0.99931207	1.02095966
F	-1.07935701	3.86812535	1.02095966
F	0.00000000	5.28929911	-0.20404810
F	1.07935701	3.86812535	1.02095966

$[Mn(Tb^{3CF3})_2]^{2+}$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.48437023	0.85700150	1.10922060
N	1.25006642	0.72172633	2.43583992
N	0.00000000	-1.71400352	1.10922060
N	0.00000000	-1.44345266	2.43583992
N	-1.48437023	0.85700150	1.10922060
N	-1.25006642	0.72172633	2.43583992
C	2.67303621	1.54327824	1.00039107
C	3.15459068	1.82130373	2.27377938
C	2.22390813	1.28397398	3.15338045
C	0.00000000	-3.08655648	1.00039107
C	0.00000000	-3.64260799	2.27377938
C	0.00000000	-2.56794796	3.15338045
C	-2.67303621	1.54327824	1.00039107
C	-3.15459068	1.82130373	2.27377938
C	-2.22390813	1.28397398	3.15338045
H	4.06466918	2.34673811	2.53164852
H	2.20192346	1.27128113	4.23608292
H	0.00000000	-4.69347569	2.53164852
C	0.00000000	-4.00655441	-0.23100862
H	0.00000000	-2.54256174	4.23608292
C	3.46977765	2.00327720	-0.23100862
H	0.00000000	0.00000000	4.14641278
H	-4.06466918	2.34673811	2.53164852
H	-2.20192346	1.27128113	4.23608292
C	-3.46977765	2.00327720	-0.23100862
B	0.00000000	0.00000000	2.95115008
N	0.00000000	1.71400352	-1.10922060
N	0.00000000	1.44345266	-2.43583992
N	1.48437023	-0.85700150	-1.10922060
N	1.25006642	-0.72172633	-2.43583992
N	-1.48437023	-0.85700150	-1.10922060
N	-1.25006642	-0.72172633	-2.43583992
C	0.00000000	3.08655648	-1.00039107
C	0.00000000	3.64260799	-2.27377938
C	0.00000000	2.56794796	-3.15338045
C	2.67303621	-1.54327824	-1.00039107
C	3.15459068	-1.82130373	-2.27377938
C	2.22390813	-1.28397398	-3.15338045
C	-2.67303621	-1.54327824	-1.00039107
C	-3.15459068	-1.82130373	-2.27377938
C	-2.22390813	-1.28397398	-3.15338045
H	0.00000000	4.69347569	-2.53164852
H	0.00000000	2.54256174	-4.23608292
H	4.06466918	-2.34673811	-2.53164852
C	3.46977765	-2.00327720	0.23100862
H	2.20192346	-1.27128113	-4.23608292
C	0.00000000	4.00655441	0.23100862
H	0.00000000	0.00000000	-4.14641278
H	-4.06466918	-2.34673811	-2.53164852
H	-2.20192346	-1.27128113	-4.23608292
C	-3.46977765	-2.00327720	0.23100862
B	0.00000000	0.00000000	-2.95115008
F	-1.07911412	-3.85639084	-1.01615314
F	0.00000000	-5.27667665	0.20883557
F	1.07911412	-3.85639084	-1.01615314
F	4.56973606	2.63833806	0.20883557
F	2.80017581	2.86273567	-1.01615314
F	3.87928940	0.99365517	-1.01615314
F	-4.56973606	2.63833806	0.20883557
F	-3.87928940	0.99365517	-1.01615314
F	-2.80017581	2.86273567	-1.01615314
F	3.87928940	-0.99365517	1.01615314
F	4.56973606	-2.63833806	-0.20883557
F	2.80017581	-2.86273567	1.01615314
F	-2.80017581	-2.86273567	1.01615314
F	-4.56973606	-2.63833806	-0.20883557
F	-3.87928940	-0.99365517	1.01615314
F	-1.07911412	3.85639084	1.01615314
F	0.00000000	5.27667665	-0.20883557
F	1.07911412	3.85639084	1.01615314

$[Mn(Tb^{3NH2})_2]^{2+}$ $^4A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.62289878	1.19024452
N	0.00000000	1.42844784	2.53939673
N	1.40547149	-0.81144939	1.19024452
N	1.23707247	-0.71422418	2.53939673
N	-1.40547149	-0.81144939	1.19024452
N	-1.23707247	-0.71422418	2.53939673
C	0.00000000	2.97576793	1.00048473
C	0.00000000	3.62822019	2.25467238
C	0.00000000	2.61222528	3.18154274
C	2.57709055	-1.48788397	1.00048473
C	3.14213120	-1.81411010	2.25467238
C	2.26225338	-1.30611264	3.18154274
C	-2.57709055	-1.48788397	1.00048473
C	-3.14213120	-1.81411010	2.25467238
C	-2.26225338	-1.30611264	3.18154274
H	0.00000000	4.69556859	2.44073428
H	0.00000000	2.65116902	4.26375889
H	4.06648162	-2.34778429	2.44073428
N	3.07657461	-1.77626122	-0.21197571
H	2.29597943	-1.32558424	4.26375889
N	0.00000000	3.55252245	-0.21197571
H	0.00000000	0.00000000	4.28380572
H	-4.06648162	-2.34778429	2.44073428
H	-2.29597943	-1.32558424	4.26375889
N	-3.07657461	-1.77626122	-0.21197571
B	0.00000000	0.00000000	3.08547061
N	-1.40547149	0.81144939	-1.19024452
N	-1.23707247	0.71422418	-2.53939673
N	1.40547149	0.81144939	-1.19024452
N	1.23707247	0.71422418	-2.53939673
N	0.00000000	-1.62289878	-1.19024452
N	0.00000000	-1.42844784	-2.53939673
C	-2.57709055	1.48788397	-1.00048473
C	-3.14213120	1.81411010	-2.25467238
C	-2.26225338	1.30611264	-3.18154274
C	2.57709055	1.48788397	-1.00048473

C	3.14213120	1.81411010	-2.25467238
C	2.26225338	1.30611264	-3.18154274
C	0.00000000	-2.97576793	-1.00048473
C	0.00000000	-3.62822019	-2.25467238
C	0.00000000	-2.61222528	-3.18154274
H	-4.06648162	2.34778429	-2.44073428
H	-2.29597943	1.32558424	-4.26375889
H	4.06648162	2.34778429	-2.44073428
N	3.07657461	1.77626122	0.21197571
H	2.29597943	1.32558424	-4.26375889
N	-3.07657461	1.77626122	0.21197571
H	0.00000000	0.00000000	-4.28380572
H	0.00000000	-4.69556859	-2.44073428
H	0.00000000	-2.65116902	-4.26375889
N	0.00000000	-3.55252245	0.21197571
B	0.00000000	0.00000000	-3.08547061
H	0.00000000	4.55487253	-0.28811796
H	3.94463538	-2.27743653	-0.28811796
H	-3.94463538	-2.27743653	-0.28811796
H	-3.94463538	2.27743653	0.28811796
H	3.94463538	2.27743653	0.28811796
H	0.00000000	-4.55487253	0.28811796
H	2.60100884	-1.50169337	-1.05310506
H	0.00000000	3.00338622	-1.05310506
H	-2.60100884	-1.50169337	-1.05310506
H	2.60100884	1.50169337	1.05310506
H	-2.60100884	1.50169337	1.05310506
H	0.00000000	-3.00338622	1.05310506

$[Mn(Tb^{3NH2})_2]^{2+}$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.61810443	1.17774958
N	0.00000000	1.43062857	2.52703092
N	1.40131956	-0.80905222	1.17774958
N	1.23896058	-0.71531429	2.52703092
N	-1.40131956	-0.80905222	1.17774958
N	-1.23896058	-0.71531429	2.52703092
C	0.00000000	2.97604945	0.98289805
C	0.00000000	3.63036548	2.23180187
C	0.00000000	2.61637085	3.16236694
C	2.57733450	-1.48802473	0.98289805
C	3.14398862	-1.81518274	2.23180187
C	2.26584384	-1.30818543	3.16236694
C	-2.57733450	-1.48802473	0.98289805
C	-3.14398862	-1.81518274	2.23180187
C	-2.26584384	-1.30818543	3.16236694
H	0.00000000	4.69807742	2.41488397
H	0.00000000	2.65995495	4.24453283
H	4.06865442	-2.34903844	2.41488397
N	3.07135428	-1.77324703	-0.23277290
H	2.30358847	-1.32997747	4.24453283
N	0.00000000	3.54649459	-0.23277290
H	0.00000000	0.00000000	4.27302373
H	-4.06865442	-2.34903844	2.41488397
H	-2.30358847	-1.32997747	4.24453283
N	-3.07135428	-1.77324703	-0.23277290
B	0.00000000	0.00000000	3.07492516
N	-1.40131956	0.80905222	-1.17774958
N	-1.23896058	0.71531429	-2.52703092
N	1.40131956	0.80905222	-1.17774958
N	1.23896058	0.71531429	-2.52703092
N	0.00000000	-1.61810443	-1.17774958
N	0.00000000	-1.43062857	-2.52703092
C	-2.57733450	1.48802473	-0.98289805
C	-3.14398862	1.81518274	-2.23180187
C	-2.26584384	1.30818543	-3.16236694
C	2.57733450	1.48802473	-0.98289805
C	3.14398862	1.81518274	-2.23180187
C	2.26584384	1.30818543	-3.16236694
C	0.00000000	-2.97604945	-0.98289805
C	0.00000000	-3.63036548	-2.23180187
C	0.00000000	-2.61637085	-3.16236694
H	-4.06865442	2.34903844	-2.41488397
H	-2.30358847	1.32997747	-4.24453283
H	4.06865442	2.34903844	-2.41488397
N	3.07135428	1.77324703	0.23277290
H	2.30358847	1.32997747	-4.24453283
N	-3.07135428	1.77324703	0.23277290
H	0.00000000	0.00000000	-4.27302373
H	0.00000000	-4.69807742	-2.41488397
H	0.00000000	-2.65995495	-4.24453283
N	0.00000000	-3.54649459	0.23277290
B	0.00000000	0.00000000	-3.07492516
H	0.00000000	4.54868327	-0.31277815
H	3.93927534	-2.27434137	-0.31277815
H	-3.93927534	-2.27434137	-0.31277815
H	-3.93927534	2.27434137	0.31277815
H	3.93927534	2.27434137	0.31277815
H	0.00000000	-4.54868327	0.31277815
H	2.59392315	-1.49760231	-1.07238616
H	0.00000000	2.99520408	-1.07238616
H	-2.59392315	-1.49760231	-1.07238616
H	2.59392315	1.49760231	1.07238616
H	-2.59392315	1.49760231	1.07238616
H	0.00000000	-2.99520408	1.07238616

$[Mn(Tb^{3NO2})_2]^{2+}$ $^4A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.70478737	1.19283854
N	0.00000000	1.43538270	2.50821443
N	1.47638918	-0.85239342	1.19283854
N	1.24307757	-0.71769135	2.50821443
N	-1.47638918	-0.85239342	1.19283854
N	-1.24307757	-0.71769135	2.50821443
C	0.00000000	3.06518830	1.10899941
C	0.00000000	3.63850581	2.37282655
C	0.00000000	2.56252707	3.23750905
C	2.65453088	-1.53259415	1.10899941
C	3.15103831	-1.81925264	2.37282655
C	2.21921380	-1.28126353	3.23750905
C	-2.65453088	-1.53259415	1.10899941
C	-3.15103831	-1.81925264	2.37282655
C	-2.21921380	-1.28126353	3.23750905
H	0.00000000	4.69489547	2.60636252
H	0.00000000	2.52269907	4.31961091
H	4.06589899	-2.34744774	2.60636252
N	3.35403229	-1.93645164	-0.10393412
H	2.18472150	-1.26134954	4.31961091

N	0.00000000	3.87290329	-0.10393412
H	0.00000000	0.00000000	4.23101023
H	-4.06589899	-2.34744774	2.60636252
H	-2.18472150	-1.26134954	4.31961091
N	-3.35403229	-1.93645164	-0.10393412
B	0.00000000	0.00000000	3.03765680
N	-1.47638918	0.85239342	-1.19283854
N	-1.24307757	0.71769135	-2.50821443
N	1.47638918	0.85239342	-1.19283854
N	1.24307757	0.71769135	-2.50821443
N	0.00000000	-1.70478737	-1.19283854
N	0.00000000	-1.43538270	-2.50821443
C	-2.65453088	1.53259415	-1.10899941
C	-3.15103831	1.81925264	-2.37282655
C	-2.21921380	1.28126353	-3.23750905
C	2.65453088	1.53259415	-1.10899941
C	3.15103831	1.81925264	-2.37282655
C	2.21921380	1.28126353	-3.23750905
C	0.00000000	-3.06518830	-1.10899941
C	0.00000000	-3.63850581	-2.37282655
C	0.00000000	-2.56252707	-3.23750905
H	-4.06589899	2.34744774	-2.60636252
H	-2.18472150	1.26134954	-4.31961091
H	4.06589899	2.34744774	-2.60636252
N	3.35403229	1.93645164	0.10393412
H	2.18472150	1.26134954	-4.31961091
N	-3.35403229	1.93645164	0.10393412
H	0.00000000	0.00000000	-4.23101023
H	0.00000000	-4.69489547	-2.60636252
H	0.00000000	-2.52269907	-4.31961091
N	0.00000000	-3.87290329	0.10393412
B	0.00000000	0.00000000	-3.03765680
O	0.00000000	5.07643386	0.07999784
O	4.39632097	-2.53821719	0.07999784
O	-4.39632097	-2.53821719	0.07999784
O	-4.39632097	2.53821719	-0.07999784
O	4.39632097	2.53821719	-0.07999784
O	0.00000000	-5.07643386	-0.07999784
O	2.86649124	-1.65496956	-1.18903694
O	0.00000000	3.30993913	-1.18903694
O	-2.86649124	-1.65496956	-1.18903694
O	2.86649124	1.65496956	1.18903694
O	-2.86649124	1.65496956	1.18903694
O	0.00000000	-3.30993913	1.18903694

$[Mn(Tb^{3NO2})_2]^{2+}$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.68975821	1.18749385
N	0.00000000	1.43446193	2.50560347
N	1.46337353	-0.84487910	1.18749385
N	1.24228063	-0.71723097	2.50560347
N	-1.46337353	-0.84487910	1.18749385
N	-1.24228063	-0.71723097	2.50560347
C	0.00000000	3.05131645	1.10928199
C	0.00000000	3.63645578	2.36754271
C	0.00000000	2.56159995	3.23445411
C	2.64251750	-1.52565822	1.10928199
C	3.14926292	-1.81822815	2.36754271
C	2.21841104	-1.28079997	3.23445411
C	-2.64251750	-1.52565822	1.10928199
C	-3.14926292	-1.81822815	2.36754271
C	-2.21841104	-1.28079997	3.23445411
H	0.00000000	4.69325873	2.59954460
H	0.00000000	2.52576195	4.31653533
H	4.06448133	-2.34662963	2.59954460
N	3.33462789	-1.92524843	-0.10030343
H	2.18737374	-1.26288097	4.31653533
N	0.00000000	3.85049686	-0.10030343
H	0.00000000	0.00000000	4.22576238
H	-4.06448133	-2.34662963	2.59954460
H	-2.18737374	-1.26288097	4.31653533
N	-3.33462789	-1.92524843	-0.10030343
B	0.00000000	0.00000000	3.03087751
N	-1.46337353	0.84487910	-1.18749385
N	-1.24228063	0.71723097	-2.50560347
N	1.46337353	0.84487910	-1.18749385
N	1.24228063	0.71723097	-2.50560347
N	0.00000000	-1.68975821	-1.18749385
N	0.00000000	-1.43446193	-2.50560347
C	-2.64251750	1.52565822	-1.10928199
C	-3.14926292	1.81822815	-2.36754271
C	-2.21841104	1.28079997	-3.23445411
C	2.64251750	1.52565822	-1.10928199
C	3.14926292	1.81822815	-2.36754271
C	2.21841104	1.28079997	-3.23445411
C	0.00000000	-3.05131645	-1.10928199
C	0.00000000	-3.63645578	-2.36754271
C	0.00000000	-2.56159995	-3.23445411
H	-4.06448133	2.34662963	-2.59954460
H	-2.18737374	1.26288097	-4.31653533
H	4.06448133	2.34662963	-2.59954460
N	3.33462789	1.92524843	0.10030343
H	2.18737374	1.26288097	-4.31653533
N	-3.33462789	1.92524843	0.10030343
H	0.00000000	0.00000000	-4.22576238
H	0.00000000	-4.69325873	-2.59954460
H	0.00000000	-2.52576195	-4.31653533
N	0.00000000	-3.85049686	0.10030343
B	0.00000000	0.00000000	-3.03087751
O	0.00000000	5.05993729	0.06160417
O	4.38203424	-2.52996891	0.06160417
O	-4.38203424	-2.52996891	0.06160417
O	-4.38203424	2.52996891	-0.06160417
O	4.38203424	2.52996891	-0.06160417
O	0.00000000	-5.05993729	-0.06160417
O	2.85295542	-1.64715468	-1.19246230
O	0.00000000	3.29430935	-1.19246230
O	-2.85295542	-1.64715468	-1.19246230
O	2.85295542	1.64715468	1.19246230
O	-2.85295542	1.64715468	1.19246230
O	0.00000000	-3.29430935	1.19246230

$[Mn(Tb^{5CH3})_2]^{2+}$ $^4A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.37465803	0.79365898	1.17984354
N	1.24278759	0.71752413	2.52548413
N	0.00000000	-1.58731849	1.17984354
N	0.00000000	-1.43504773	2.52548413

N	-1.37465803	0.79365898	1.17984354
N	-1.24278759	0.71752413	2.52548413
C	2.51683949	1.45309797	0.91050608
C	3.12818685	1.80605972	2.10028915
C	2.29596408	1.32557525	3.11915962
C	0.00000000	-2.90619594	0.91050608
C	0.00000000	-3.61211945	2.10028915
C	0.00000000	-2.65115103	3.11915962
C	-2.51683949	1.45309797	0.91050608
C	-3.12818685	1.80605972	2.10028915
C	-2.29596408	1.32557525	3.11915962
H	4.06098981	2.34461346	2.22087436
C	2.47602828	1.42953582	4.59051473
H	0.00000000	-4.68922693	2.22087436
H	0.00000000	-3.26644341	-0.10873746
C	0.00000000	-2.85907165	4.59051473
H	2.82882282	1.63322144	-0.10873746
H	0.00000000	0.00000000	4.28630555
H	-4.06098981	2.34461346	2.22087436
C	-2.47602828	1.42953582	4.59051473
H	-2.82882282	1.63322144	-0.10873746
B	0.00000000	0.00000000	3.09536781
N	0.00000000	1.58731849	-1.17984354
N	0.00000000	1.43504773	-2.52548413
N	1.37465803	-0.79365898	-1.17984354
N	1.24278759	-0.71752413	-2.52548413
N	-1.37465803	-0.79365898	-1.17984354
N	-1.24278759	-0.71752413	-2.52548413
C	0.00000000	2.90619594	-0.91050608
C	0.00000000	3.61211945	-2.10028915
C	0.00000000	2.65115103	-3.11915962
C	2.51683949	-1.45309797	-0.91050608
C	3.12818685	-1.80605972	-2.10028915
C	2.29596408	-1.32557525	-3.11915962
C	-2.51683949	-1.45309797	-0.91050608
C	-3.12818685	-1.80605972	-2.10028915
C	-2.29596408	-1.32557525	-3.11915962
H	0.00000000	4.68922693	-2.22087436
C	0.00000000	2.85907165	-4.59051473
H	4.06098981	-2.34461346	-2.22087436
H	2.82882282	-1.63322144	0.10873746
C	2.47602828	-1.42953582	-4.59051473
H	0.00000000	3.26644341	0.10873746
H	0.00000000	0.00000000	-4.28630555
H	-4.06098981	-2.34461346	-2.22087436
C	-2.47602828	-1.42953582	-4.59051473
H	-2.82882282	-1.63322144	0.10873746
B	0.00000000	0.00000000	-3.09536781
H	-3.40281556	-1.96461657	-4.80715725
H	-1.65214799	-1.97572347	-5.06210374
H	-2.53710116	-0.44294041	-5.06210374
H	3.40281556	-1.96461657	-4.80715725
H	2.53710116	-0.44294041	-5.06210374
H	1.65214799	-1.97572347	-5.06210374
H	0.88495264	2.41866388	-5.06210374
H	0.00000000	3.92923262	-4.80715725
H	-0.88495264	2.41866388	-5.06210374
H	-2.53710116	0.44294041	5.06210374
H	-3.40281556	1.96461657	4.80715725
H	-1.65214799	1.97572347	5.06210374
H	-0.88495264	-2.41866388	5.06210374
H	0.88495264	-2.41866388	5.06210374
H	0.00000000	-3.92923262	4.80715725
H	2.53710116	0.44294041	5.06210374
H	1.65214799	1.97572347	5.06210374
H	3.40281556	1.96461657	4.80715725

$[Mn(Tb^{5CH3})_2]^{2+}$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.36449571	0.78779199	1.16484083
N	1.24212664	0.71714207	2.51298020
N	0.00000000	-1.57558398	1.16484083
N	0.00000000	-1.43428413	2.51298020
N	-1.36449571	0.78779199	1.16484083
N	-1.24212664	0.71714207	2.51298020
C	2.50994749	1.44911856	0.89765977
C	3.12721105	1.80549615	2.08066144
C	2.29339016	1.32408932	3.10583652
C	0.00000000	-2.89823764	0.89765977
C	0.00000000	-3.61099230	2.08066144
C	0.00000000	-2.64817917	3.10583652
C	-2.50994749	1.44911856	0.89765977
C	-3.12721105	1.80549615	2.08066144
C	-2.29339016	1.32408932	3.10583652
H	4.05994257	2.34400861	2.20241454
C	2.47991668	1.43178059	4.57407002
H	0.00000000	-4.68801776	2.20241454
H	0.00000000	-3.25566142	-0.12274319
C	0.00000000	-2.86356119	4.57407002
H	2.81948548	1.62783071	-0.12274319
H	0.00000000	0.00000000	4.27251096
H	-4.05994257	2.34400861	2.20241454
C	-2.47991668	1.43178059	4.57407002
H	-2.81948548	1.62783071	-0.12274319
B	0.00000000	0.00000000	3.08019577
N	0.00000000	1.57558398	-1.16484083
N	0.00000000	1.43428413	-2.51298020
N	1.36449571	-0.78779199	-1.16484083
N	1.24212664	-0.71714207	-2.51298020
N	-1.36449571	-0.78779199	-1.16484083
N	-1.24212664	-0.71714207	-2.51298020
C	0.00000000	2.89823764	-0.89765977
C	0.00000000	3.61099230	-2.08066144
C	0.00000000	2.64817917	-3.10583652
C	2.50994749	-1.44911856	-0.89765977
C	3.12721105	-1.80549615	-2.08066144
C	2.29339016	-1.32408932	-3.10583652
C	-2.50994749	-1.44911856	-0.89765977
C	-3.12721105	-1.80549615	-2.08066144
C	-2.29339016	-1.32408932	-3.10583652
H	0.00000000	4.68801776	-2.20241454
C	0.00000000	2.86356119	-4.57407002
H	4.05994257	-2.34400861	-2.20241454
H	2.81948548	-1.62783071	0.12274319
C	2.47991668	-1.43178059	-4.57407002
H	0.00000000	3.25566142	0.12274319
H	0.00000000	0.00000000	-4.27251096
H	-4.05994257	-2.34400861	-2.20241454
C	-2.47991668	-1.43178059	-4.57407002

H	-2.81948548	-1.62783071	0.12274319
B	0.00000000	0.00000000	-3.08019577
H	-3.40671983	-1.96687034	-4.78968541
H	-1.65520505	-1.97606638	-5.04735292
H	-2.53892629	-0.44541643	-5.04735292
H	3.40671983	-1.96687034	-4.78968541
H	2.53892629	-0.44541643	-5.04735292
H	1.65520505	-1.97606638	-5.04735292
H	0.88372071	2.42148281	-5.04735292
H	0.00000000	3.93374121	-4.78968541
H	-0.88372071	2.42148281	-5.04735292
H	-2.53892629	0.44541643	5.04735292
H	-3.40671983	1.96687034	4.78968541
H	-1.65520505	1.97606638	5.04735292
H	-0.88372071	-2.42148281	5.04735292
H	0.88372071	-2.42148281	5.04735292
H	0.00000000	-3.93374121	4.78968541
H	2.53892629	0.44541643	5.04735292
H	1.65520505	1.97606638	5.04735292
H	3.40671983	1.96687034	4.78968541

$[Mn(Tb^{5CF3})_2]^{2+}$ $^4A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.37700599	0.79501473	1.18969311
N	1.24558482	0.71913865	2.53346571
N	0.00000000	-1.59002946	1.18969311
N	0.00000000	-1.43827730	2.53346571
N	-1.37700599	0.79501473	1.18969311
N	-1.24558482	0.71913865	2.53346571
C	2.51846195	1.45403461	0.90884711
C	3.14026744	1.81303428	2.09211495
C	2.30774621	1.33237782	3.10128666
C	0.00000000	-2.90806923	0.90884711
C	0.00000000	-3.62606856	2.09211495
C	0.00000000	-2.66475564	3.10128666
C	-2.51846195	1.45403461	0.90884711
C	-3.14026744	1.81303428	2.09211495
C	-2.30774621	1.33237782	3.10128666
H	4.07283862	2.35145467	2.21153862
C	2.53222162	1.46197862	4.60049078
H	0.00000000	-4.70290881	2.21153862
H	0.00000000	-3.26499875	-0.11190247
C	0.00000000	-2.92395777	4.60049078
H	2.82757184	1.63249911	-0.11190247
H	0.00000000	0.00000000	4.29639643
H	-4.07283862	2.35145467	2.21153862
C	-2.53222162	1.46197862	4.60049078
H	-2.82757184	1.63249911	-0.11190247
B	0.00000000	0.00000000	3.11481560
N	0.00000000	1.59002946	-1.18969311
N	0.00000000	1.43827730	-2.53346571
N	1.37700599	-0.79501473	-1.18969311
N	1.24558482	-0.71913865	-2.53346571
N	-1.37700599	-0.79501473	-1.18969311
N	-1.24558482	-0.71913865	-2.53346571
C	0.00000000	2.90806923	-0.90884711
C	0.00000000	3.62606856	-2.09211495
C	0.00000000	2.66475564	-3.10128666
C	2.51846195	-1.45403461	-0.90884711
C	3.14026744	-1.81303428	-2.09211495
C	2.30774621	-1.33237782	-3.10128666
C	-2.51846195	-1.45403461	-0.90884711
C	-3.14026744	-1.81303428	-2.09211495
C	-2.30774621	-1.33237782	-3.10128666
H	0.00000000	4.70290881	-2.21153862
C	0.00000000	2.92395777	-4.60049078
H	4.07283862	-2.35145467	-2.21153862
H	2.82757184	-1.63249911	0.11190247
C	2.53222162	-1.46197862	-4.60049078
H	0.00000000	3.26499875	0.11190247
H	0.00000000	0.00000000	-4.29639643
H	-4.07283862	-2.35145467	-2.21153862
C	-2.53222162	-1.46197862	-4.60049078
H	-2.82757184	-1.63249911	0.11190247
B	0.00000000	0.00000000	-3.11481560
F	-3.67764958	-2.12329196	-4.81180555
F	-1.53086057	-2.14309748	-5.18328321
F	-2.62140703	-0.25421569	-5.18328321
F	3.67764958	-2.12329196	-4.81180555
F	2.62140703	-0.25421569	-5.18328321
F	1.53086057	-2.14309748	-5.18328321
F	1.09054647	2.39731317	-5.18328321
F	0.00000000	4.24658392	-4.81180555
F	-1.09054647	2.39731317	-5.18328321
F	-2.62140703	0.25421569	5.18328321
F	-3.67764958	2.12329196	4.81180555
F	-1.53086057	2.14309748	5.18328321
F	-1.09054647	-2.39731317	5.18328321
F	1.09054647	-2.39731317	5.18328321
F	0.00000000	-4.24658392	4.81180555
F	2.62140703	0.25421569	5.18328321
F	1.53086057	2.14309748	5.18328321
F	3.67764958	2.12329196	4.81180555

$[Mn(Tb^{5CF3})_2]^{2+}$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.36831584	0.78999760	1.17052155
N	1.24520698	0.71892063	2.51810687
N	0.00000000	-1.57999467	1.17052155
N	0.00000000	-1.43784126	2.51810687
N	-1.36831584	0.78999760	1.17052155
N	-1.24520698	0.71892063	2.51810687
C	2.51275213	1.45073837	0.89391267
C	3.13962925	1.81266597	2.07116324
C	2.30439441	1.33044262	3.08624956
C	0.00000000	-2.90147621	0.89391267
C	0.00000000	-3.62533194	2.07116324
C	0.00000000	-2.66088524	3.08624956
C	-2.51275213	1.45073837	0.89391267
C	-3.13962925	1.81266597	2.07116324
C	-2.30439441	1.33044262	3.08624956
H	4.07195437	2.35094401	2.19281791
C	2.53350593	1.46272053	4.58433183
H	0.00000000	-4.70188802	2.19281791
H	0.00000000	-3.25698330	-0.12746874
C	0.00000000	-2.92544106	4.58433183
H	2.82063010	1.62849165	-0.12746874
H	0.00000000	0.00000000	4.27852611

H	-4.07195437	2.35094401	2.19281791
C	-2.53350593	1.46272053	4.58433183
H	-2.82063010	1.62849165	-0.12746874
B	0.00000000	0.00000000	3.09625471
N	0.00000000	1.57999467	-1.17052155
N	0.00000000	1.43784126	-2.51810687
N	1.36831584	-0.78999760	-1.17052155
N	1.24520698	-0.71892063	-2.51810687
N	-1.36831584	-0.78999760	-1.17052155
N	-1.24520698	-0.71892063	-2.51810687
C	0.00000000	2.90147621	-0.89391267
C	0.00000000	3.62533194	-2.07116324
C	0.00000000	2.66088524	-3.08624956
C	2.51275213	-1.45073837	-0.89391267
C	3.13962925	-1.81266597	-2.07116324
C	2.30439441	-1.33044262	-3.08624956
C	-2.51275213	-1.45073837	-0.89391267
C	-3.13962925	-1.81266597	-2.07116324
C	-2.30439441	-1.33044262	-3.08624956
H	0.00000000	4.70188802	-2.19281791
C	0.00000000	2.92544106	-4.58433183
H	4.07195437	-2.35094401	-2.19281791
H	2.82063010	-1.62849165	0.12746874
C	2.53350593	-1.46272053	-4.58433183
H	0.00000000	3.25698330	0.12746874
H	0.00000000	0.00000000	-4.27852611
H	-4.07195437	-2.35094401	-2.19281791
C	-2.53350593	-1.46272053	-4.58433183
H	-2.82063010	-1.62849165	0.12746874
B	0.00000000	0.00000000	-3.09625471
F	-3.67918843	-2.12418045	-4.79367382
F	-1.53288097	-2.14474110	-5.16711420
F	-2.62384019	-0.25514334	-5.16711420
F	3.67918843	-2.12418045	-4.79367382
F	2.62384019	-0.25514334	-5.16711420
F	1.53288097	-2.14474110	-5.16711420
F	1.09095975	2.39988391	-5.16711420
F	0.00000000	4.24836089	-4.79367382
F	-1.09095975	2.39988391	-5.16711420
F	-2.62384019	0.25514334	5.16711420
F	-3.67918843	2.12418045	4.79367382
F	-1.53288097	2.14474110	5.16711420
F	-1.09095975	-2.39988391	5.16711420
F	1.09095975	-2.39988391	5.16711420
F	0.00000000	-4.24836089	4.79367382
F	2.62384019	0.25514334	5.16711420
F	1.53288097	2.14474110	5.16711420
F	3.67918843	2.12418045	4.79367382

$[Mn(Tb^{5NH2})_2]^{2+}$ $^4A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.58533407	-1.17330502
N	0.00000000	1.43332315	-2.53033139
N	-1.37293979	-0.79266677	-1.17330502
N	-1.24129425	-0.71666157	-2.53033139
N	1.37293979	-0.79266677	-1.17330502
N	1.24129425	-0.71666157	-2.53033139
C	0.00000000	2.90298383	-0.91270957
C	0.00000000	3.62526474	-2.08995485
C	0.00000000	2.65778532	-3.11186914
C	-2.51405814	-1.45149192	-0.91270957
C	-3.13957104	-1.81263211	-2.08995485
C	-2.30170989	-1.32889266	-3.11186914
C	2.51405814	-1.45149192	-0.91270957
C	3.13957104	-1.81263211	-2.08995485
C	2.30170989	-1.32889266	-3.11186914
H	0.00000000	4.70244472	-2.20515833
N	0.00000000	2.85059529	-4.44637267
H	-4.07243645	-2.35122236	-2.20515833
H	-2.82636691	-1.63180377	0.10627625
N	-2.46868807	-1.42529764	-4.44637267
H	0.00000000	3.26360702	0.10627625
H	0.00000000	0.00000000	-4.29035693
H	4.07243645	-2.35122236	-2.20515833
N	2.46868807	-1.42529764	-4.44637267
H	2.82636691	-1.63180377	0.10627625
B	0.00000000	0.00000000	-3.08644694
N	1.37293979	0.79266677	1.17330502
N	1.24129425	0.71666157	2.53033139
N	-1.37293979	0.79266677	1.17330502
N	-1.24129425	0.71666157	2.53033139
N	0.00000000	-1.58533407	1.17330502
N	0.00000000	-1.43332315	2.53033139
C	2.51405814	1.45149192	0.91270957
C	3.13957104	1.81263211	2.08995485
C	2.30170989	1.32889266	3.11186914
C	-2.51405814	1.45149192	0.91270957
C	-3.13957104	1.81263211	2.08995485
C	-2.30170989	1.32889266	3.11186914
C	0.00000000	-2.90298383	0.91270957
C	0.00000000	-3.62526474	2.08995485
C	0.00000000	-2.65778532	3.11186914
H	4.07243645	2.35122236	2.20515833
N	2.46868807	1.42529764	4.44637267
H	-4.07243645	2.35122236	2.20515833
H	-2.82636691	1.63180377	-0.10627625
N	-2.46868807	1.42529764	4.44637267
H	2.82636691	1.63180377	-0.10627625
H	0.00000000	0.00000000	4.29035693
H	0.00000000	-4.70244472	2.20515833
N	0.00000000	-2.85059529	4.44637267
H	0.00000000	-3.26360702	-0.10627625
B	0.00000000	0.00000000	3.08644694
H	0.00000000	3.78624099	-4.81272155
H	0.00000000	2.08760372	-5.09762529
H	-3.27898067	-1.89312049	-4.81272155
H	-1.80791766	-1.04380159	-5.09762529
H	3.27898067	-1.89312049	-4.81272155
H	1.80791766	-1.04380159	-5.09762529
H	3.27898067	1.89312049	4.81272155
H	1.80791766	1.04380159	5.09762529
H	-3.27898067	1.89312049	4.81272155
H	-1.80791766	1.04380159	5.09762529
H	0.00000000	-3.78624099	4.81272155
H	0.00000000	-2.08760372	5.09762529

$[Mn(Tb^{5NH2})_2]^{2+}$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000

N	0.00000000	1.57355776	-1.16534249
N	0.00000000	1.43242513	-2.52224821
N	-1.36274095	-0.78677862	-1.16534249
N	-1.24051636	-0.71621283	-2.52224821
N	1.36274095	-0.78677862	-1.16534249
N	1.24051636	-0.71621283	-2.52224821
C	0.00000000	2.89459002	-0.90587948
C	0.00000000	3.62374600	-2.07779806
C	0.00000000	2.65590727	-3.10261965
C	-2.50678883	-1.44729501	-0.90587948
C	-3.13825604	-1.81187326	-2.07779806
C	-2.30008320	-1.32795337	-3.10261965
C	2.50678883	-1.44729501	-0.90587948
C	3.13825604	-1.81187326	-2.07779806
C	2.30008320	-1.32795337	-3.10261965
H	0.00000000	4.70102811	-2.19330899
N	0.00000000	2.85317450	-4.43556476
H	-4.07120982	-2.35051379	-2.19330899
H	-2.81653109	-1.62612517	0.11428376
N	-2.47092172	-1.42658725	-4.43556476
H	0.00000000	3.25225034	0.11428376
H	0.00000000	0.00000000	-4.28161122
H	4.07120982	-2.35051379	-2.19330899
N	2.47092172	-1.42658725	-4.43556476
H	2.81653109	-1.62612517	0.11428376
B	0.00000000	0.00000000	-3.07548662
N	1.36274095	0.78677862	1.16534249
N	1.24051636	0.71621283	2.52224821
N	-1.36274095	0.78677862	1.16534249
N	-1.24051636	0.71621283	2.52224821
N	0.00000000	-1.57355776	1.16534249
N	0.00000000	-1.43242513	2.52224821
C	2.50678883	1.44729501	0.90587948
C	3.13825604	1.81187326	2.07779806
C	2.30008320	1.32795337	3.10261965
C	-2.50678883	1.44729501	0.90587948
C	-3.13825604	1.81187326	2.07779806
C	-2.30008320	1.32795337	3.10261965
C	0.00000000	-2.89459002	0.90587948
C	0.00000000	-3.62374600	2.07779806
C	0.00000000	-2.65590727	3.10261965
H	4.07120982	2.35051379	2.19330899
N	2.47092172	1.42658725	4.43556476
H	-4.07120982	2.35051379	2.19330899
H	-2.81653109	1.62612517	-0.11428376
N	-2.47092172	1.42658725	4.43556476
H	2.81653109	1.62612517	-0.11428376
H	0.00000000	0.00000000	4.28161122
H	0.00000000	-4.70102811	2.19330899
N	0.00000000	-2.85317450	4.43556476
H	0.00000000	-3.25225034	-0.11428376
B	0.00000000	0.00000000	3.07548662
H	0.00000000	3.78970869	-4.80045734
H	0.00000000	2.09060786	-5.08800696
H	-3.28198428	-1.89485461	-4.80045734
H	-1.81051910	-1.04530393	-5.08800696
H	3.28198428	-1.89485461	-4.80045734
H	1.81051910	-1.04530393	-5.08800696
H	3.28198428	1.89485461	4.80045734
H	1.81051910	1.04530393	5.08800696
H	-3.28198428	1.89485461	4.80045734
H	-1.81051910	1.04530393	5.08800696
H	0.00000000	-3.78970869	4.80045734
H	0.00000000	-2.09060786	5.08800696

$[Mn(Tb^{5NO2})_2]^{2+}$ $^4A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.37575501	-0.79429240	-1.17914502
N	-1.24973621	-0.72153530	-2.52230113
N	1.37575501	-0.79429240	-1.17914502
N	1.24973621	-0.72153530	-2.52230113
N	0.00000000	1.58858534	-1.17914502
N	0.00000000	1.44307112	-2.52230113
C	-2.51436770	-1.45167078	-0.87946772
C	-3.15298886	-1.82037873	-2.04798580
C	-2.32649602	-1.34320320	-3.05685482
C	2.51436770	-1.45167078	-0.87946772
C	3.15298886	-1.82037873	-2.04798580
C	2.32649602	-1.34320320	-3.05685482
C	0.00000000	2.90334156	-0.87946772
C	0.00000000	3.64075746	-2.04798580
C	0.00000000	2.68640587	-3.05685482
H	-4.08478692	-2.35835302	-2.17084647
N	-2.61169028	-1.50786041	-4.49620900
H	4.08478692	-2.35835302	-2.17084647
H	2.81038628	-1.62257704	0.14649478
N	2.61169028	-1.50786041	-4.49620900
H	-2.81038628	-1.62257704	0.14649478
H	0.00000000	0.00000000	-4.27726403
H	0.00000000	4.71670551	-2.17084647
N	0.00000000	3.01572028	-4.49620900
H	0.00000000	3.24515460	0.14649478
B	0.00000000	0.00000000	-3.10752195
N	-1.37575501	0.79429240	1.17914502
N	-1.24973621	0.72153530	2.52230113
N	0.00000000	-1.58858534	1.17914502
N	0.00000000	-1.44307112	2.52230113
N	1.37575501	0.79429240	1.17914502
N	1.24973621	0.72153530	2.52230113
C	-2.51436770	1.45167078	0.87946772
C	-3.15298886	1.82037873	2.04798580
C	-2.32649602	1.34320320	3.05685482
C	0.00000000	-2.90334156	0.87946772
C	0.00000000	-3.64075746	2.04798580
C	0.00000000	-2.68640587	3.05685482
C	2.51436770	1.45167078	0.87946772
C	3.15298886	1.82037873	2.04798580
C	2.32649602	1.34320320	3.05685482
H	-4.08478692	2.35835302	2.17084647
N	-2.61169028	1.50786041	4.49620900
H	0.00000000	-4.71670551	2.17084647
H	0.00000000	-3.24515460	-0.14649478
N	0.00000000	-3.01572028	4.49620900
H	-2.81038628	1.62257704	-0.14649478
H	0.00000000	0.00000000	4.27726403
H	4.08478692	2.35835302	2.17084647
N	2.61169028	1.50786041	4.49620900
H	2.81038628	1.62257704	-0.14649478
B	0.00000000	0.00000000	3.10752195

O	-3.64795268	-2.10614662	-4.71852588
O	-1.82425601	-1.05323471	-5.30268518
O	3.64795268	-2.10614662	-4.71852588
O	1.82425601	-1.05323471	-5.30268518
O	0.00000000	4.21229270	-4.71852588
O	0.00000000	2.10646941	-5.30268518
O	-3.64795268	2.10614662	4.71852588
O	-1.82425601	1.05323471	5.30268518
O	0.00000000	-4.21229270	4.71852588
O	0.00000000	-2.10646941	5.30268518
O	3.64795268	2.10614662	4.71852588
O	1.82425601	1.05323471	5.30268518

$[Mn(Tb^{5NO2})_2]^{2+}$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.38177176	-0.79776645	-1.17787553
N	-1.25212915	-0.72291698	-2.51594624
N	1.38177176	-0.79776645	-1.17787553
N	1.25212915	-0.72291698	-2.51594624
N	0.00000000	1.59553291	-1.17787553
N	0.00000000	1.44583395	-2.51594624
C	-2.52200532	-1.45608041	-0.89497367
C	-3.15914161	-1.82393163	-2.06765426
C	-2.32448197	-1.34204007	-3.06439507
C	2.52200532	-1.45608041	-0.89497367
C	3.15914161	-1.82393163	-2.06765426
C	2.32448197	-1.34204007	-3.06439507
C	0.00000000	2.91216083	-0.89497367
C	0.00000000	3.64786272	-2.06765426
C	0.00000000	2.68408014	-3.06439507
H	-4.09013637	-2.36144130	-2.19721696
N	-2.58002908	-1.48958051	-4.48924502
H	4.09013637	-2.36144130	-2.19721696
H	2.82531649	-1.63119734	0.12808682
N	2.58002908	-1.48958051	-4.48924502
H	-2.82531649	-1.63119734	0.12808682
H	0.00000000	0.00000000	-4.27232786
H	0.00000000	4.72288260	-2.19721696
N	0.00000000	2.97916102	-4.48924502
H	0.00000000	3.26239467	0.12808682
B	0.00000000	0.00000000	-3.08678350
N	-1.38177176	0.79776645	1.17787553
N	-1.25212915	0.72291698	2.51594624
N	0.00000000	-1.59553291	1.17787553
N	0.00000000	-1.44583395	2.51594624
N	1.38177176	0.79776645	1.17787553
N	1.25212915	0.72291698	2.51594624
C	-2.52200532	1.45608041	0.89497367
C	-3.15914161	1.82393163	2.06765426
C	-2.32448197	1.34204007	3.06439507
C	0.00000000	-2.91216083	0.89497367
C	0.00000000	-3.64786272	2.06765426
C	0.00000000	-2.68408014	3.06439507
C	2.52200532	1.45608041	0.89497367
C	3.15914161	1.82393163	2.06765426
C	2.32448197	1.34204007	3.06439507
H	-4.09013637	2.36144130	2.19721696
N	-2.58002908	1.48958051	4.48924502
H	0.00000000	-4.72288260	2.19721696
H	0.00000000	-3.26239467	-0.12808682
N	0.00000000	-2.97916102	4.48924502
H	-2.82531649	1.63119734	-0.12808682
H	0.00000000	0.00000000	4.27232786
H	4.09013637	2.36144130	2.19721696
N	2.58002908	1.48958051	4.48924502
H	2.82531649	1.63119734	-0.12808682
B	0.00000000	0.00000000	3.08678350
O	-3.60484008	-2.08125571	-4.77880817
O	-1.77671367	-1.02578575	-5.28911284
O	3.60484008	-2.08125571	-4.77880817
O	1.77671367	-1.02578575	-5.28911284
O	0.00000000	4.16251088	-4.77880817
O	0.00000000	2.05157204	-5.28911284
O	-3.60484008	2.08125571	4.77880817
O	-1.77671367	1.02578575	5.28911284
O	0.00000000	-4.16251088	4.77880817
O	0.00000000	-2.05157204	5.28911284
O	3.60484008	2.08125571	4.77880817
O	1.77671367	1.02578575	5.28911284

$[Mn(Tb^{3,5\text{-}CH3})_2]^{2+}$ $^4A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	-1.65310000	1.15460000
N	0.00000000	-1.43760000	2.49500000
N	-1.43170000	0.82660000	1.15460000
N	-1.24500000	0.71880000	2.49500000
N	1.43170000	0.82660000	1.15460000
N	1.24500000	0.71880000	2.49500000
C	0.00000000	-3.00250000	0.94840000
C	0.00000000	-3.61970000	2.19690000
C	0.00000000	-2.61440000	3.15780000
C	-2.60020000	1.50120000	0.94840000
C	-3.13480000	1.80990000	2.19690000
C	-2.26410000	1.30720000	3.15780000
C	2.60020000	1.50120000	0.94840000
C	3.13480000	1.80990000	2.19690000
C	2.26410000	1.30720000	3.15780000
H	0.00000000	-4.68830000	2.37890000
C	0.00000000	-2.74510000	4.63770000
H	-4.06020000	2.34410000	2.37890000
C	-3.21700000	1.85730000	-0.35440000
C	-2.37730000	1.37260000	4.63770000
C	0.00000000	-3.71470000	-0.35440000
H	0.00000000	0.00000000	4.22350000
H	4.06020000	2.34410000	2.37890000
C	2.37730000	1.37260000	4.63770000
C	3.21700000	1.85730000	-0.35440000
B	0.00000000	0.00000000	3.03300000
N	1.43170000	-0.82660000	-1.15460000
N	1.24500000	-0.71880000	-2.49500000
N	-1.43170000	-0.82660000	-1.15460000
N	-1.24500000	-0.71880000	-2.49500000
N	0.00000000	1.65310000	-1.15460000
N	0.00000000	1.43760000	-2.49500000
C	2.60020000	-1.50120000	-0.94840000
C	3.13480000	-1.80990000	-2.19690000
C	2.26410000	-1.30720000	-3.15780000
C	-2.60020000	-1.50120000	-0.94840000

C	-3.13480000	-1.80990000	-2.19690000
C	-2.26410000	-1.30720000	-3.15780000
C	0.00000000	3.00250000	-0.94840000
C	0.00000000	3.61970000	-2.19690000
C	0.00000000	2.61440000	-3.15780000
H	4.06020000	-2.34410000	-2.37890000
C	2.37730000	-1.37260000	-4.63770000
H	-4.06020000	-2.34410000	-2.37890000
C	-3.21700000	-1.85730000	0.35440000
C	-2.37730000	-1.37260000	-4.63770000
C	3.21700000	-1.85730000	0.35440000
H	0.00000000	0.00000000	-4.22350000
H	0.00000000	4.68830000	-2.37890000
C	0.00000000	2.74510000	-4.63770000
C	0.00000000	3.71470000	0.35440000
B	0.00000000	0.00000000	-3.03300000
H	-2.57650000	2.50560000	-0.95740000
H	-4.14810000	2.39490000	-0.16180000
H	-3.45820000	0.97850000	-0.95740000
H	0.00000000	-4.78980000	-0.16180000
H	0.88170000	-3.48410000	-0.95740000
H	-0.88170000	-3.48410000	-0.95740000
H	4.14810000	2.39490000	-0.16180000
H	2.57650000	2.50560000	-0.95740000
H	3.45820000	0.97850000	-0.95740000
H	-2.57650000	-2.50560000	0.95740000
H	-4.14810000	-2.39490000	0.16180000
H	-3.45820000	-0.97850000	0.95740000
H	-0.88170000	3.48410000	0.95740000
H	0.00000000	4.78980000	0.16180000
H	0.88170000	3.48410000	0.95740000
H	3.45820000	-0.97850000	0.95740000
H	4.14810000	-2.39490000	0.16180000
H	2.57650000	-2.50560000	0.95740000
H	0.00000000	3.80350000	-4.90720000
H	-0.88470000	2.28340000	-5.08830000
H	0.88470000	2.28340000	-5.08830000
H	-3.29390000	-1.90170000	-4.90720000
H	-1.53510000	-1.90790000	-5.08830000
H	-2.41980000	-0.37550000	-5.08830000
H	1.53510000	-1.90790000	-5.08830000
H	3.29390000	-1.90170000	-4.90720000
H	2.41980000	-0.37550000	-5.08830000
H	1.53510000	1.90790000	5.08830000
H	3.29390000	1.90170000	4.90720000
H	2.41980000	0.37550000	5.08830000
H	-1.53510000	1.90790000	5.08830000
H	-2.41980000	0.37550000	5.08830000
H	-3.29390000	1.90170000	4.90720000
H	-0.88470000	-2.28340000	5.08830000
H	0.88470000	-2.28340000	5.08830000
H	0.00000000	-3.80350000	4.90720000

$[Mn(Tb^{3,5\text{-}CH3})_2]^{2+}$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.41584283	0.81743703	-1.15231733
N	1.24298550	0.71763790	-2.49307149
N	-1.41584283	0.81743703	-1.15231733
N	-1.24298550	0.71763790	-2.49307149
N	0.00000000	-1.63487459	-1.15231733
N	0.00000000	-1.43527581	-2.49307149
C	2.59145348	1.49617617	-0.94606203
C	3.13356065	1.80916229	-2.18662865
C	2.26337841	1.30676194	-3.15340268
C	-2.59145348	1.49617617	-0.94606203
C	-3.13356065	1.80916229	-2.18662865
C	-2.26337841	1.30676194	-3.15340268
C	0.00000000	-2.99235287	-0.94606203
C	0.00000000	-3.61832405	-2.18662865
C	0.00000000	-2.61352441	-3.15340268
H	4.05907631	2.34350907	-2.36762368
C	2.38244858	1.37550736	-4.63182548
H	-4.05907631	2.34350907	-2.36762368
C	-3.20183192	1.84857859	0.36079940
C	-2.38244858	1.37550736	-4.63182548
C	3.20183192	1.84857859	0.36079940
H	0.00000000	0.00000000	-4.22222007
H	0.00000000	-4.68701761	-2.36762368
C	0.00000000	-2.75101471	-4.63182548
C	0.00000000	-3.69715664	0.36079940
B	0.00000000	0.00000000	-3.03027742
N	1.41584283	-0.81743703	1.15231733
N	1.24298550	-0.71763790	2.49307149
N	0.00000000	1.63487459	1.15231733
N	0.00000000	1.43527581	2.49307149
N	-1.41584283	-0.81743703	1.15231733
N	-1.24298550	-0.71763790	2.49307149
C	2.59145348	-1.49617617	0.94606203
C	3.13356065	-1.80916229	2.18662865
C	2.26337841	-1.30676194	3.15340268
C	0.00000000	2.99235287	0.94606203
C	0.00000000	3.61832405	2.18662865
C	0.00000000	2.61352441	3.15340268
C	-2.59145348	-1.49617617	0.94606203
C	-3.13356065	-1.80916229	2.18662865
C	-2.26337841	-1.30676194	3.15340268
H	4.05907631	-2.34350907	2.36762368
C	2.38244858	-1.37550736	4.63182548
H	0.00000000	4.68701761	2.36762368
C	0.00000000	3.69715664	-0.36079940
C	0.00000000	2.75101471	4.63182548
C	3.20183192	-1.84857859	-0.36079940
H	0.00000000	0.00000000	4.22222007
H	-4.05907631	-2.34350907	2.36762368
C	-2.38244858	-1.37550736	4.63182548
C	-3.20183192	-1.84857859	-0.36079940
B	0.00000000	0.00000000	3.03027742
H	-3.43721314	0.96723652	0.96300258
H	-4.13430468	2.38694182	0.17720929
H	-2.55625790	2.49309531	0.96300258
H	4.13430468	2.38694182	0.17720929
H	3.43721314	0.96723652	0.96300258
H	2.55625790	2.49309531	0.96300258
H	0.00000000	-4.77388365	0.17720929
H	-0.88095470	-3.46033236	0.96300258
H	0.88095470	-3.46033236	0.96300258
H	0.88095470	3.46033236	-0.96300258
H	0.00000000	4.77388365	-0.17720929
H	-0.88095470	3.46033236	-0.96300258

H	-3.43721314	-0.96723652	-0.96300258
H	-4.13430468	-2.38694182	-0.17720929
H	-2.55625790	-2.49309531	-0.96300258
H	2.55625790	-2.49309531	-0.96300258
H	4.13430468	-2.38694182	-0.17720929
H	3.43721314	-0.96723652	-0.96300258
H	-3.29899839	-1.90467772	4.90046813
H	-2.42248031	-0.37822520	5.08324014
H	-1.53879293	-1.90881642	5.08324014
H	0.00000000	3.80935492	4.90046813
H	0.88368738	2.28704215	5.08324014
H	-0.88368738	2.28704215	5.08324014
H	2.42248031	-0.37822520	5.08324014
H	3.29899839	-1.90467772	4.90046813
H	1.53879293	-1.90881642	5.08324014
H	-0.88368738	-2.28704215	-5.08324014
H	0.00000000	-3.80935492	-4.90046813
H	0.88368738	-2.28704215	-5.08324014
H	-2.42248031	0.37822520	-5.08324014
H	-1.53879293	1.90881642	-5.08324014
H	-3.29899839	1.90467772	-4.90046813
H	1.53879293	1.90881642	-5.08324014
H	2.42248031	0.37822520	-5.08324014
H	3.29899839	1.90467772	-4.90046813

$[Mn(Tb^{3,5\text{-}CF3})_2]^{2+}$ $^4A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.48937254	0.85988974	1.11470870
N	1.26769649	0.73190505	2.44867882
N	0.00000000	-1.71977949	1.11470870
N	0.00000000	-1.46380958	2.44867882
N	-1.48937254	0.85988974	1.11470870
N	-1.26769649	0.73190505	2.44867882
C	2.66974102	1.54137585	0.95567771
C	3.17680025	1.83412623	2.21094223
C	2.27929923	1.31595375	3.12659085
C	0.00000000	-3.08275117	0.95567771
C	0.00000000	-3.66825298	2.21094223
C	0.00000000	-2.63190803	3.12659085
C	-2.66974102	1.54137585	0.95567771
C	-3.17680025	1.83412623	2.21094223
C	-2.27929923	1.31595375	3.12659085
H	4.09281348	2.36298703	2.43501916
C	2.44639330	1.41242594	4.63862329
H	0.00000000	-4.72597352	2.43501916
C	0.00000000	-3.98720716	-0.29282605
C	0.00000000	-2.82485187	4.63862329
C	3.45302284	1.99360384	-0.29282605
H	0.00000000	0.00000000	4.15671480
H	-4.09281348	2.36298703	2.43501916
C	-2.44639330	1.41242594	4.63862329
C	-3.45302284	1.99360384	-0.29282605
B	0.00000000	0.00000000	2.97387083
N	0.00000000	1.71977949	-1.11470870
N	0.00000000	1.46380958	-2.44867882
N	1.48937254	-0.85988974	-1.11470870
N	1.26769649	-0.73190505	-2.44867882
N	-1.48937254	-0.85988974	-1.11470870
N	-1.26769649	-0.73190505	-2.44867882
C	0.00000000	3.08275117	-0.95567771
C	0.00000000	3.66825298	-2.21094223
C	0.00000000	2.63190803	-3.12659085
C	2.66974102	-1.54137585	-0.95567771
C	3.17680025	-1.83412623	-2.21094223
C	2.27929923	-1.31595375	-3.12659085
C	-2.66974102	-1.54137585	-0.95567771
C	-3.17680025	-1.83412623	-2.21094223
C	-2.27929923	-1.31595375	-3.12659085
H	0.00000000	4.72597352	-2.43501916
C	0.00000000	2.82485187	-4.63862329
H	4.09281348	-2.36298703	-2.43501916
C	3.45302284	-1.99360384	0.29282605
C	2.44639330	-1.41242594	-4.63862329
C	0.00000000	3.98720716	0.29282605
H	0.00000000	0.00000000	-4.15671480
H	-4.09281348	-2.36298703	-2.43501916
C	-2.44639330	-1.41242594	-4.63862329
C	-3.45302284	-1.99360384	0.29282605
B	0.00000000	0.00000000	-2.97387083
F	-1.07990577	-3.82397344	-1.07141777
F	0.00000000	-5.25918945	0.13173180
F	1.07990577	-3.82397344	-1.07141777
F	4.55459154	2.62959499	0.13173180
F	2.77170501	2.84721226	-1.07141777
F	3.85161078	0.97676119	-1.07141777
F	-4.55459154	2.62959499	0.13173180
F	-3.85161078	0.97676119	-1.07141777
F	-2.77170501	2.84721226	-1.07141777
F	3.85161078	-0.97676119	1.07141777
F	4.55459154	-2.62959499	-0.13173180
F	2.77170501	-2.84721226	1.07141777
F	-2.77170501	-2.84721226	1.07141777
F	-4.55459154	-2.62959499	-0.13173180
F	-3.85161078	-0.97676119	1.07141777
F	-1.07990577	3.82397344	1.07141777
F	0.00000000	5.25918945	-0.13173180
F	1.07990577	3.82397344	1.07141777
F	-3.58570504	-2.07020807	-4.89314326
F	-1.43273364	-2.08552193	-5.20157158
F	-2.52248211	-0.19802236	-5.20157158
F	3.58570504	-2.07020807	-4.89314326
F	2.52248211	-0.19802236	-5.20157158
F	1.43273364	-2.08552193	-5.20157158
F	1.08974847	2.28354482	-5.20157158
F	0.00000000	4.14041562	-4.89314326
F	-1.08974847	2.28354482	-5.20157158
F	-2.52248211	0.19802236	5.20157158
F	-3.58570504	2.07020807	4.89314326
F	-1.43273364	2.08552193	5.20157158
F	-1.08974847	-2.28354482	5.20157158
F	1.08974847	-2.28354482	5.20157158
F	0.00000000	-4.14041562	4.89314326
F	2.52248211	0.19802236	5.20157158
F	1.43273364	2.08552193	5.20157158
F	3.58570504	2.07020807	4.89314326

$[Mn(Tb^{3,5\text{-}CF3})_2]^{2+}$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000

N	1.47518636	0.85169914	1.11871775
N	1.26591528	0.73087686	2.45668950
N	0.00000000	-1.70339828	1.11871775
N	0.00000000	-1.46175319	2.45668950
N	-1.47518636	0.85169914	1.11871775
N	-1.26591528	0.73087686	2.45668950
C	2.65920722	1.53529401	0.95951107
C	3.17447134	1.83278212	2.20844134
C	2.27628081	1.31421170	3.13181013
C	0.00000000	-3.07058803	0.95951107
C	0.00000000	-3.66556370	2.20844134
C	0.00000000	-2.62842286	3.13181013
C	-2.65920722	1.53529401	0.95951107
C	-3.17447134	1.83278212	2.20844134
C	-2.27628081	1.31421170	3.13181013
H	4.09050415	2.36165350	2.43173086
C	2.45100772	1.41508981	4.64272812
H	0.00000000	-4.72330753	2.43173086
C	0.00000000	-3.97509800	-0.28974889
C	0.00000000	-2.83017963	4.64272812
C	3.44253613	1.98754900	-0.28974889
H	0.00000000	0.00000000	4.16076354
H	-4.09050415	2.36165350	2.43173086
C	-2.45100772	1.41508981	4.64272812
C	-3.44253613	1.98754900	-0.28974889
B	0.00000000	0.00000000	2.97704801
N	0.00000000	1.70339828	-1.11871775
N	0.00000000	1.46175319	-2.45668950
N	1.47518636	-0.85169914	-1.11871775
N	1.26591528	-0.73087686	-2.45668950
N	-1.47518636	-0.85169914	-1.11871775
N	-1.26591528	-0.73087686	-2.45668950
C	0.00000000	3.07058803	-0.95951107
C	0.00000000	3.66556370	-2.20844134
C	0.00000000	2.62842286	-3.13181013
C	2.65920722	-1.53529401	-0.95951107
C	3.17447134	-1.83278212	-2.20844134
C	2.27628081	-1.31421170	-3.13181013
C	-2.65920722	-1.53529401	-0.95951107
C	-3.17447134	-1.83278212	-2.20844134
C	-2.27628081	-1.31421170	-3.13181013
H	0.00000000	4.72330753	-2.43173086
C	0.00000000	2.83017963	-4.64272812
H	4.09050415	-2.36165350	-2.43173086
C	3.44253613	-1.98754900	0.28974889
C	2.45100772	-1.41508981	-4.64272812
C	0.00000000	3.97509800	0.28974889
H	0.00000000	0.00000000	-4.16076354
H	-4.09050415	-2.36165350	-2.43173086
C	-2.45100772	-1.41508981	-4.64272812
C	-3.44253613	-1.98754900	0.28974889
B	0.00000000	0.00000000	-2.97704801
F	-1.07960361	-3.81396353	-1.06956670
F	0.00000000	-5.24818257	0.13390142
F	1.07960361	-3.81396353	-1.06956670
F	4.54505947	2.62409102	0.13390142
F	2.76318738	2.84194641	-1.06956670
F	3.84279151	0.97201764	-1.06956670
F	-4.54505947	2.62409102	0.13390142
F	-3.84279151	0.97201764	-1.06956670
F	-2.76318738	2.84194641	-1.06956670
F	3.84279151	-0.97201764	1.06956670
F	4.54505947	-2.62409102	-0.13390142
F	2.76318738	-2.84194641	1.06956670
F	-2.76318738	-2.84194641	1.06956670
F	-4.54505947	-2.62409102	-0.13390142
F	-3.84279151	-0.97201764	1.06956670
F	-1.07960361	3.81396353	1.06956670
F	0.00000000	5.24818257	-0.13390142
F	1.07960361	3.81396353	1.06956670
F	-3.59104602	-2.07329106	-4.89252307
F	-1.43914409	-2.08977228	-5.20659188
F	-2.52936776	-0.20144931	-5.20659188
F	3.59104602	-2.07329106	-4.89252307
F	2.52936776	-0.20144931	-5.20659188
F	1.43914409	-2.08977228	-5.20659188
F	1.09022367	2.29122160	-5.20659188
F	0.00000000	4.14658265	-4.89252307
F	-1.09022367	2.29122160	-5.20659188
F	-2.52936776	0.20144931	5.20659188
F	-3.59104602	2.07329106	4.89252307
F	-1.43914409	2.08977228	5.20659188
F	-1.09022367	-2.29122160	5.20659188
F	1.09022367	-2.29122160	5.20659188
F	0.00000000	-4.14658265	4.89252307
F	2.52936776	0.20144931	5.20659188
F	1.43914409	2.08977228	5.20659188
F	3.59104602	2.07329106	4.89252307

$[Mn(Tb^{3,5\text{-}NH2})_2]^{2+}$ $^4A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.62256275	1.16995957
N	0.00000000	1.43493661	2.54026564
N	1.40518097	-0.81128164	1.16995957
N	1.24269180	-0.71746857	2.54026564
N	-1.40518097	-0.81128164	1.16995957
N	-1.24269180	-0.71746857	2.54026564
C	0.00000000	2.97113869	0.95831248
C	0.00000000	3.64140517	2.18553802
C	0.00000000	2.64310912	3.15491136
C	2.57308151	-1.48556934	0.95831248
C	3.15354979	-1.82070259	2.18553802
C	2.28899958	-1.32155456	3.15491136
C	-2.57308151	-1.48556934	0.95831248
C	-3.15354979	-1.82070259	2.18553802
C	-2.28899958	-1.32155456	3.15491136
H	0.00000000	4.71253930	2.34475581
N	0.00000000	2.78490111	4.49982010
H	4.08117899	-2.35626965	2.34475581
N	3.05444230	-1.76348318	-0.26622484
N	2.41179516	-1.39245055	4.49982010
N	0.00000000	3.52696583	-0.26622484
H	0.00000000	0.00000000	4.27656763
H	-4.08117899	-2.35626965	2.34475581
N	-2.41179516	-1.39245055	4.49982010
N	-3.05444230	-1.76348318	-0.26622484
B	0.00000000	0.00000000	3.07187975
N	-1.40518097	0.81128164	-1.16995957
N	-1.24269180	0.71746857	-2.54026564

N	1.40518097	0.81128164	-1.16995957
N	1.24269180	0.71746857	-2.54026564
N	0.00000000	-1.62256275	-1.16995957
N	0.00000000	-1.43493661	-2.54026564
C	-2.57308151	1.48556934	-0.95831248
C	-3.15354979	1.82070259	-2.18553802
C	-2.28899958	1.32155456	-3.15491136
C	2.57308151	1.48556934	-0.95831248
C	3.15354979	1.82070259	-2.18553802
C	2.28899958	1.32155456	-3.15491136
C	0.00000000	-2.97113869	-0.95831248
C	0.00000000	-3.64140517	-2.18553802
C	0.00000000	-2.64310912	-3.15491136
H	-4.08117899	2.35626965	-2.34475581
N	-2.41179516	1.39245055	-4.49982010
H	4.08117899	2.35626965	-2.34475581
N	3.05444230	1.76348318	0.26622484
N	2.41179516	1.39245055	-4.49982010
N	-3.05444230	1.76348318	0.26622484
H	0.00000000	0.00000000	-4.27656763
H	0.00000000	-4.71253930	-2.34475581
N	0.00000000	-2.78490111	-4.49982010
N	0.00000000	-3.52696583	0.26622484
B	0.00000000	0.00000000	-3.07187975
H	0.00000000	3.70482389	4.90184982
H	0.00000000	1.99584967	5.11750225
H	3.20847204	-1.85241195	4.90184982
H	1.72845641	-0.99792457	5.11750225
H	-3.20847204	-1.85241195	4.90184982
H	-1.72845641	-0.99792457	5.11750225
H	-3.20847204	1.85241195	-4.90184982
H	-1.72845641	0.99792457	-5.11750225
H	3.20847204	1.85241195	-4.90184982
H	1.72845641	0.99792457	-5.11750225
H	0.00000000	-3.70482389	-4.90184982
H	0.00000000	-1.99584967	-5.11750225
H	0.00000000	4.52643983	-0.35680993
H	3.92001170	-2.26321965	-0.35680993
H	-3.92001170	-2.26321965	-0.35680993
H	-3.92001170	2.26321965	0.35680993
H	3.92001170	2.26321965	0.35680993
H	0.00000000	-4.52643983	0.35680993
H	2.56677848	-1.48193019	-1.09626370
H	0.00000000	2.96386038	-1.09626370
H	-2.56677848	-1.48193019	-1.09626370
H	2.56677848	1.48193019	1.09626370
H	-2.56677848	1.48193019	1.09626370
H	0.00000000	-2.96386038	1.09626370

$[Mn(Tb^{3,5\text{-}NH2})_2]^{2+}$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.61204482	1.19945061
N	0.00000000	1.43337818	2.56405745
N	1.39607171	-0.80602268	1.19945061
N	1.24134187	-0.71668909	2.56405745
N	-1.39607171	-0.80602268	1.19945061
N	-1.24134187	-0.71668909	2.56405745
C	0.00000000	2.96146533	0.99735306
C	0.00000000	3.64072518	2.22359010
C	0.00000000	2.64289745	3.18975186
C	2.56470410	-1.48073266	0.99735306
C	3.15296029	-1.82036233	2.22359010
C	2.28881649	-1.32144872	3.18975186
C	-2.56470410	-1.48073266	0.99735306
C	-3.15296029	-1.82036233	2.22359010
C	-2.28881649	-1.32144872	3.18975186
H	0.00000000	4.71190482	2.38283858
N	0.00000000	2.77271151	4.53590523
H	4.08062917	-2.35595267	2.38283858
N	3.03619309	-1.75294673	-0.23127480
N	2.40123860	-1.38635602	4.53590523
N	0.00000000	3.50589399	-0.23127480
H	0.00000000	0.00000000	4.29859305
H	-4.08062917	-2.35595267	2.38283858
N	-2.40123860	-1.38635602	4.53590523
N	-3.03619309	-1.75294673	-0.23127480
B	0.00000000	0.00000000	3.09282458
N	-1.39607171	0.80602268	-1.19945061
N	-1.24134187	0.71668909	-2.56405745
N	1.39607171	0.80602268	-1.19945061
N	1.24134187	0.71668909	-2.56405745
N	0.00000000	-1.61204482	-1.19945061
N	0.00000000	-1.43337818	-2.56405745
C	-2.56470410	1.48073266	-0.99735306
C	-3.15296029	1.82036233	-2.22359010
C	-2.28881649	1.32144872	-3.18975186
C	2.56470410	1.48073266	-0.99735306
C	3.15296029	1.82036233	-2.22359010
C	2.28881649	1.32144872	-3.18975186
C	0.00000000	-2.96146533	-0.99735306
C	0.00000000	-3.64072518	-2.22359010
C	0.00000000	-2.64289745	-3.18975186
H	-4.08062917	2.35595267	-2.38283858
N	-2.40123860	1.38635602	-4.53590523
H	4.08062917	2.35595267	-2.38283858
N	3.03619309	1.75294673	0.23127480
N	2.40123860	1.38635602	-4.53590523
N	-3.03619309	1.75294673	0.23127480
H	0.00000000	0.00000000	-4.29859305
H	0.00000000	-4.71190482	-2.38283858
N	0.00000000	-2.77271151	-4.53590523
N	0.00000000	-3.50589399	0.23127480
B	0.00000000	0.00000000	-3.09282458
H	0.00000000	3.68830033	4.94769932
H	0.00000000	1.97680776	5.14469666
H	3.19416203	-1.84415043	4.94769932
H	1.71196566	-0.98840361	5.14469666
H	-3.19416203	-1.84415043	4.94769932
H	-1.71196566	-0.98840361	5.14469666
H	-3.19416203	1.84415043	-4.94769932
H	-1.71196566	0.98840361	-5.14469666
H	3.19416203	1.84415043	-4.94769932
H	1.71196566	0.98840361	-5.14469666
H	0.00000000	-3.68830033	-4.94769932
H	0.00000000	-1.97680776	-5.14469666
H	0.00000000	4.50424297	-0.33795111
H	3.90078881	-2.25212175	-0.33795111
H	-3.90078881	-2.25212175	-0.33795111
H	-3.90078881	2.25212175	0.33795111

H	3.90078881	2.25212175	0.33795111
H	0.00000000	-4.50424297	0.33795111
H	2.53310322	-1.46248769	-1.05037556
H	0.00000000	2.92497591	-1.05037556
H	-2.53310322	-1.46248769	-1.05037556
H	2.53310322	1.46248769	1.05037556
H	-2.53310322	1.46248769	1.05037556
H	0.00000000	-2.92497591	1.05037556

$[Mn(Tb^{3,5\text{-}NO2})_2]^{2+}$ $^4A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.76282065	1.77096733
N	0.00000000	1.47378457	3.07325878
N	1.52664726	-0.88141033	1.77096733
N	1.27633478	-0.73689255	3.07325878
N	-1.52664726	-0.88141033	1.77096733
N	-1.27633478	-0.73689255	3.07325878
C	0.00000000	3.09902707	1.68596559
C	0.00000000	3.71864600	2.92561939
C	0.00000000	2.64631593	3.78930810
C	2.68383619	-1.54951354	1.68596559
C	3.22044203	-1.85932300	2.92561939
C	2.29177670	-1.32315797	3.78930810
C	-2.68383619	-1.54951354	1.68596559
C	-3.22044203	-1.85932300	2.92561939
C	-2.29177670	-1.32315797	3.78930810
H	0.00000000	4.77491554	3.15607291
N	0.00000000	2.82575624	5.22745946
H	4.13519846	-2.38745777	3.15607291
N	3.28700406	-1.89775291	0.42285760
N	2.44717701	-1.41287838	5.22745946
N	0.00000000	3.79550582	0.42285760
H	0.00000000	0.00000000	4.73155423
H	-4.13519846	-2.38745777	3.15607291
N	-2.44717701	-1.41287838	5.22745946
N	-3.28700406	-1.89775291	0.42285760
B	0.00000000	0.00000000	3.56629746
N	-1.52664726	0.88141033	-1.77096733
N	-1.27633478	0.73689255	-3.07325878
N	1.52664726	0.88141033	-1.77096733
N	1.27633478	0.73689255	-3.07325878
N	0.00000000	-1.76282065	-1.77096733
N	0.00000000	-1.47378457	-3.07325878
C	-2.68383619	1.54951354	-1.68596559
C	-3.22044203	1.85932300	-2.92561939
C	-2.29177670	1.32315797	-3.78930810
C	2.68383619	1.54951354	-1.68596559
C	3.22044203	1.85932300	-2.92561939
C	2.29177670	1.32315797	-3.78930810
C	0.00000000	-3.09902707	-1.68596559
C	0.00000000	-3.71864600	-2.92561939
C	0.00000000	-2.64631593	-3.78930810
H	-4.13519846	2.38745777	-3.15607291
N	-2.44717701	1.41287838	-5.22745946
H	4.13519846	2.38745777	-3.15607291
N	3.28700406	1.89775291	-0.42285760
N	2.44717701	1.41287838	-5.22745946
N	-3.28700406	1.89775291	-0.42285760
H	0.00000000	0.00000000	-4.73155423
H	0.00000000	-4.77491554	-3.15607291
N	0.00000000	-2.82575624	-5.22745946
N	0.00000000	-3.79550582	-0.42285760
B	0.00000000	0.00000000	-3.56629746
O	0.00000000	3.99292704	5.60680387
O	0.00000000	1.87894542	5.99818178
O	3.45797594	-1.99646352	5.60680387
O	1.62721422	-0.93947271	5.99818178
O	-3.45797594	-1.99646352	5.60680387
O	-1.62721422	-0.93947271	5.99818178
O	-3.45797594	1.99646352	-5.60680387
O	-1.62721422	0.93947271	-5.99818178
O	3.45797594	1.99646352	-5.60680387
O	1.62721422	0.93947271	-5.99818178
O	0.00000000	-3.99292704	-5.60680387
O	0.00000000	-1.87894542	-5.99818178
O	0.00000000	5.01083334	0.46425196
O	4.33950903	-2.50541667	0.46425196
O	-4.33950903	-2.50541667	0.46425196
O	-4.33950903	2.50541667	-0.46425196
O	4.33950903	2.50541667	-0.46425196
O	0.00000000	-5.01083334	-0.46425196
O	2.69229773	-1.55439890	-0.59670185
O	0.00000000	3.10879780	-0.59670185
O	-2.69229773	-1.55439890	-0.59670185
O	2.69229773	1.55439890	0.59670185
O	-2.69229773	1.55439890	0.59670185
O	0.00000000	-3.10879780	0.59670185

$[Mn(Tb^{3,5\text{-}NO2})_2]^{2+}$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.69441391	1.18484850
N	0.00000000	1.45552848	2.50571036
N	1.46740533	-0.84720695	1.18484850
N	1.26052508	-0.72776424	2.50571036
N	-1.46740533	-0.84720695	1.18484850
N	-1.26052508	-0.72776424	2.50571036
C	0.00000000	3.04744816	1.05012262
C	0.00000000	3.67866666	2.28042850
C	0.00000000	2.63569006	3.17544079
C	2.63916728	-1.52372408	1.05012262
C	3.18581902	-1.83933333	2.28042850
C	2.28257484	-1.31784503	3.17544079
C	-2.63916728	-1.52372408	1.05012262
C	-3.18581902	-1.83933333	2.28042850
C	-2.28257484	-1.31784503	3.17544079
H	0.00000000	4.73992370	2.48717911
N	0.00000000	2.82714427	4.62557273
H	4.10489459	-2.36996211	2.48717911
N	3.31251305	-1.91248044	-0.19171457
N	2.44837877	-1.41357213	4.62557273
N	0.00000000	3.82496036	-0.19171457
H	0.00000000	0.00000000	4.20845405
H	-4.10489459	-2.36996211	2.48717911
N	-2.44837877	-1.41357213	4.62557273
N	-3.31251305	-1.91248044	-0.19171457
B	0.00000000	0.00000000	3.02155182
N	-1.46740533	0.84720695	-1.18484850
N	-1.26052508	0.72776424	-2.50571036

N	1.46740533	0.84720695	-1.18484850
N	1.26052508	0.72776424	-2.50571036
N	0.00000000	-1.69441391	-1.18484850
N	0.00000000	-1.45552848	-2.50571036
C	-2.63916728	1.52372408	-1.05012262
C	-3.18581902	1.83933333	-2.28042850
C	-2.28257484	1.31784503	-3.17544079
C	2.63916728	1.52372408	-1.05012262
C	3.18581902	1.83933333	-2.28042850
C	2.28257484	1.31784503	-3.17544079
C	0.00000000	-3.04744816	-1.05012262
C	0.00000000	-3.67866666	-2.28042850
C	0.00000000	-2.63569006	-3.17544079
H	-4.10489459	2.36996211	-2.48717911
N	-2.44837877	1.41357213	-4.62557273
H	4.10489459	2.36996211	-2.48717911
N	3.31251305	1.91248044	0.19171457
N	2.44837877	1.41357213	-4.62557273
N	-3.31251305	1.91248044	0.19171457
H	0.00000000	0.00000000	-4.20845405
H	0.00000000	-4.73992370	-2.48717911
N	0.00000000	-2.82714427	-4.62557273
N	0.00000000	-3.82496036	0.19171457
B	0.00000000	0.00000000	-3.02155182
O	0.00000000	3.98538520	4.99272701
O	0.00000000	1.84459970	5.35319832
O	3.45144483	-1.99269260	4.99272701
O	1.59747022	-0.92229985	5.35319832
O	-3.45144483	-1.99269260	4.99272701
O	-1.59747022	-0.92229985	5.35319832
O	-3.45144483	1.99269260	-4.99272701
O	-1.59747022	0.92229985	-5.35319832
O	3.45144483	1.99269260	-4.99272701
O	1.59747022	0.92229985	-5.35319832
O	0.00000000	-3.98538520	-4.99272701
O	0.00000000	-1.84459970	-5.35319832
O	0.00000000	5.03029754	-0.03884214
O	4.35636544	-2.51514877	-0.03884214
O	-4.35636544	-2.51514877	-0.03884214
O	-4.35636544	2.51514877	0.03884214
O	4.35636544	2.51514877	0.03884214
O	0.00000000	-5.03029754	0.03884214
O	2.79518619	-1.61380169	-1.25716745
O	0.00000000	3.22760285	-1.25716745
O	-2.79518619	-1.61380169	-1.25716745
O	2.79518619	1.61380169	1.25716745
O	-2.79518619	1.61380169	1.25716745
O	0.00000000	-3.22760285	1.25716745

$[Mn(Tb^{3CH3})_2]^+$ ^5E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.49863526	0.86523761	1.28604835
N	1.25324148	0.72355940	2.60703881
N	0.00000000	-1.73047522	1.28604835
N	0.00000000	-1.44711880	2.60703881
N	-1.49863526	0.86523761	1.28604835
N	-1.25324148	0.72355940	2.60703881
C	2.66813074	1.54044608	1.16126042
C	3.15884315	1.82375912	2.44361935
C	2.23643005	1.29120360	3.32380146
C	0.00000000	-3.08089164	1.16126042
C	0.00000000	-3.64751823	2.44361935
C	0.00000000	-2.58240720	3.32380146
C	-2.66813074	1.54044608	1.16126042
C	-3.15884315	1.82375912	2.44361935
C	-2.23643005	1.29120360	3.32380146
H	4.07312438	2.35161924	2.68816698
H	2.20897581	1.27535315	4.40594565
H	0.00000000	-4.70323901	2.68816698
C	0.00000000	-3.83168990	-0.12417779
H	0.00000000	-2.55070578	4.40594565
C	3.31834088	1.91584495	-0.12417779
H	0.00000000	0.00000000	4.32192765
H	-4.07312438	2.35161924	2.68816698
H	-2.20897581	1.27535315	4.40594565
C	-3.31834088	1.91584495	-0.12417779
B	0.00000000	0.00000000	3.12185154
N	0.00000000	1.73047522	-1.28604835
N	0.00000000	1.44711880	-2.60703881
N	1.49863526	-0.86523761	-1.28604835
N	1.25324148	-0.72355940	-2.60703881
N	-1.49863526	-0.86523761	-1.28604835
N	-1.25324148	-0.72355940	-2.60703881
C	0.00000000	3.08089164	-1.16126042
C	0.00000000	3.64751823	-2.44361935
C	0.00000000	2.58240720	-3.32380146
C	2.66813074	-1.54044608	-1.16126042
C	3.15884315	-1.82375912	-2.44361935
C	2.23643005	-1.29120360	-3.32380146
C	-2.66813074	-1.54044608	-1.16126042
C	-3.15884315	-1.82375912	-2.44361935
C	-2.23643005	-1.29120360	-3.32380146
H	0.00000000	4.70323901	-2.68816698
H	0.00000000	2.55070578	-4.40594565
H	4.07312438	-2.35161924	-2.68816698
C	3.31834088	-1.91584495	0.12417779
H	2.20897581	-1.27535315	-4.40594565
C	0.00000000	3.83168990	0.12417779
H	0.00000000	0.00000000	-4.32192765
H	-4.07312438	-2.35161924	-2.68816698
H	-2.20897581	-1.27535315	-4.40594565
C	-3.31834088	-1.91584495	0.12417779
B	0.00000000	0.00000000	-3.12185154
H	-0.87892478	-3.61013715	-0.73439219
H	0.00000000	-4.90317805	0.08956272
H	0.87892478	-3.61013715	-0.73439219
H	4.24627647	2.45158876	0.08956272
H	2.68700808	2.56623977	-0.73439219
H	3.56593286	1.04389737	-0.73439219
H	-4.24627647	2.45158876	0.08956272
H	-3.56593286	1.04389737	-0.73439219
H	-2.68700808	2.56623977	-0.73439219
H	3.56593286	-1.04389737	0.73439219
H	4.24627647	-2.45158876	-0.08956272
H	2.68700808	-2.56623977	0.73439219
H	-2.68700808	-2.56623977	0.73439219
H	-4.24627647	-2.45158876	-0.08956272
H	-3.56593286	-1.04389737	0.73439219
H	-0.87892478	3.61013715	0.73439219

H	0.00000000	4.90317805	-0.08956272
H	0.87892478	3.61013715	0.73439219

$[Mn(Tb^{3CH3})_2]^+$ $^3A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.43886786	0.83073102	1.17373683
N	1.24114237	0.71657373	2.50520818
N	0.00000000	-1.66146151	1.17373683
N	0.00000000	-1.43314746	2.50520818
N	-1.43886786	0.83073102	1.17373683
N	-1.24114237	0.71657373	2.50520818
C	2.60823581	1.50586541	1.00039530
C	3.13703364	1.81116734	2.26129398
C	2.24331042	1.29517560	3.18060927
C	0.00000000	-3.01173135	1.00039530
C	0.00000000	-3.62233468	2.26129398
C	0.00000000	-2.59035174	3.18060927
C	-2.60823581	1.50586541	1.00039530
C	-3.13703364	1.81116734	2.26129398
C	-2.24331042	1.29517560	3.18060927
H	4.05846723	2.34315717	2.46641737
H	2.24899749	1.29845968	4.26315034
H	0.00000000	-4.68631434	2.46641737
C	0.00000000	-3.73617923	-0.29894387
H	0.00000000	-2.59691883	4.26315034
C	3.23562624	1.86808988	-0.29894387
H	0.00000000	0.00000000	4.23877855
H	-4.05846723	2.34315717	2.46641737
H	-2.24899749	1.29845968	4.26315034
C	-3.23562624	1.86808988	-0.29894387
B	0.00000000	0.00000000	3.03862043
N	0.00000000	1.66146151	-1.17373683
N	0.00000000	1.43314746	-2.50520818
N	1.43886786	-0.83073102	-1.17373683
N	1.24114237	-0.71657373	-2.50520818
N	-1.43886786	-0.83073102	-1.17373683
N	-1.24114237	-0.71657373	-2.50520818
C	0.00000000	3.01173135	-1.00039530
C	0.00000000	3.62233468	-2.26129398
C	0.00000000	2.59035174	-3.18060927
C	2.60823581	-1.50586541	-1.00039530
C	3.13703364	-1.81116734	-2.26129398
C	2.24331042	-1.29517560	-3.18060927
C	-2.60823581	-1.50586541	-1.00039530
C	-3.13703364	-1.81116734	-2.26129398
C	-2.24331042	-1.29517560	-3.18060927
H	0.00000000	4.68631434	-2.46641737
H	0.00000000	2.59691883	-4.26315034
H	4.05846723	-2.34315717	-2.46641737
C	3.23562624	-1.86808988	0.29894387
H	2.24899749	-1.29845968	-4.26315034
C	0.00000000	3.73617923	0.29894387
H	0.00000000	0.00000000	-4.23877855
H	-4.05846723	-2.34315717	-2.46641737
H	-2.24899749	-1.29845968	-4.26315034
C	-3.23562624	-1.86808988	0.29894387
B	0.00000000	0.00000000	-3.03862043
H	-0.88012072	-3.50594479	-0.90433852
H	0.00000000	-4.81101548	-0.10165072
H	0.88012072	-3.50594479	-0.90433852
H	4.16646172	2.40550801	-0.10165072
H	2.59617692	2.51517946	-0.90433852
H	3.47629764	0.99076533	-0.90433852
H	-4.16646172	2.40550801	-0.10165072
H	-3.47629764	0.99076533	-0.90433852
H	-2.59617692	2.51517946	-0.90433852
H	3.47629764	-0.99076533	0.90433852
H	4.16646172	-2.40550801	0.10165072
H	2.59617692	-2.51517946	0.90433852
H	-2.59617692	-2.51517946	0.90433852
H	-4.16646172	-2.40550801	0.10165072
H	-3.47629764	-0.99076533	0.90433852
H	-0.88012072	3.50594479	0.90433852
H	0.00000000	4.81101548	0.10165072
H	0.88012072	3.50594479	0.90433852

$[Mn(Tb^{3CH3})_2]^+$ ^1E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.82500000	1.16370000	-1.42900000
N	0.71520000	2.49730000	-1.23880000
N	0.82500000	1.16370000	1.42900000
N	0.71520000	2.49730000	1.23880000
N	-1.65000000	1.16370000	0.00000000
N	-1.43050000	2.49730000	0.00000000
C	1.50200000	0.98900000	-2.60150000
C	1.80920000	2.24660000	-3.13350000
C	1.29460000	3.17040000	-2.24230000
C	1.50200000	0.98900000	2.60150000
C	1.80920000	2.24660000	3.13350000
C	1.29460000	3.17040000	2.24230000
C	-3.00400000	0.98900000	0.00000000
C	-3.61830000	2.24660000	0.00000000
C	-2.58920000	3.17040000	0.00000000
H	2.34140000	2.44850000	-4.05550000
H	1.29960000	4.25290000	-2.25090000
H	2.34140000	2.44850000	4.05550000
C	1.86300000	-0.31080000	3.22680000
H	1.29960000	4.25290000	2.25090000
C	1.86300000	-0.31080000	-3.22680000
H	0.00000000	4.23320000	0.00000000
H	-4.68290000	2.44850000	0.00000000
H	-2.59920000	4.25290000	0.00000000
C	-3.72590000	-0.31080000	0.00000000
B	0.00000000	3.03270000	0.00000000
N	-0.82500000	-1.16370000	-1.42900000
N	-0.71520000	-2.49730000	-1.23880000
N	1.65000000	-1.16370000	0.00000000
N	1.43050000	-2.49730000	0.00000000
N	-0.82500000	-1.16370000	1.42900000
N	-0.71520000	-2.49730000	1.23880000
C	-1.50200000	-0.98900000	-2.60150000
C	-1.80920000	-2.24660000	-3.13350000
C	-1.29460000	-3.17040000	-2.24230000
C	3.00400000	-0.98900000	0.00000000
C	3.61830000	-2.24660000	0.00000000
C	2.58920000	-3.17040000	0.00000000
C	-1.50200000	-0.98900000	2.60150000
C	-1.80920000	-2.24660000	3.13350000
C	-1.29460000	-3.17040000	2.24230000

H	-2.34140000	-2.44850000	-4.05550000
H	-1.29960000	-4.25290000	-2.25090000
H	4.68290000	-2.44850000	0.00000000
C	3.72590000	0.31080000	0.00000000
H	2.59920000	-4.25290000	0.00000000
C	-1.86300000	0.31080000	-3.22680000
H	0.00000000	-4.23320000	0.00000000
H	-2.34140000	-2.44850000	4.05550000
H	-1.29960000	-4.25290000	2.25090000
C	-1.86300000	0.31080000	3.22680000
B	0.00000000	-3.03270000	0.00000000
H	0.98490000	-0.91600000	3.46570000
H	2.40060000	-0.11600000	4.15800000
H	2.50900000	-0.91600000	2.58580000
H	2.40060000	-0.11600000	-4.15800000
H	0.98490000	-0.91600000	-3.46570000
H	2.50900000	-0.91600000	-2.58580000
H	-4.80130000	-0.11600000	0.00000000
H	-3.49380000	-0.91600000	0.87990000
H	-3.49380000	-0.91600000	-0.87990000
H	3.49380000	0.91600000	-0.87990000
H	4.80130000	0.11600000	0.00000000
H	3.49380000	0.91600000	0.87990000
H	-0.98490000	0.91600000	3.46570000
H	-2.40060000	0.11600000	4.15800000
H	-2.50900000	0.91600000	2.58580000
H	-2.50900000	0.91600000	-2.58580000
H	-2.40060000	0.11600000	-4.15800000
H	-0.98490000	0.91600000	-3.46570000

$[Mn(Tb^{3CF3})_2]^+$ ^5E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.57064517	0.90681242	1.20169750
N	1.26941473	0.73289726	2.50431810
N	0.00000000	-1.81362484	1.20169750
N	0.00000000	-1.46579399	2.50431810
N	-1.57064517	0.90681242	1.20169750
N	-1.26941473	0.73289726	2.50431810
C	2.74871491	1.58697135	1.16744174
C	3.17911963	1.83546557	2.47216106
C	2.21465653	1.27863246	3.28633888
C	0.00000000	-3.17394269	1.16744174
C	0.00000000	-3.67093115	2.47216106
C	0.00000000	-2.55726546	3.28633888
C	-2.74871491	1.58697135	1.16744174
C	-3.17911963	1.83546557	2.47216106
C	-2.21465653	1.27863246	3.28633888
H	4.07738743	2.35408097	2.77836894
H	2.13683308	1.23370108	4.36462061
H	0.00000000	-4.70816142	2.77836894
C	0.00000000	-4.11030913	-0.04127000
H	0.00000000	-2.46740216	4.36462061
C	3.55963194	2.05515457	-0.04127000
H	0.00000000	0.00000000	4.18568673
H	-4.07738743	2.35408097	2.77836894
H	-2.13683308	1.23370108	4.36462061
C	-3.55963194	2.05515457	-0.04127000
B	0.00000000	0.00000000	2.98786439
N	0.00000000	1.81362484	-1.20169750
N	0.00000000	1.46579399	-2.50431810
N	1.57064517	-0.90681242	-1.20169750
N	1.26941473	-0.73289726	-2.50431810
N	-1.57064517	-0.90681242	-1.20169750
N	-1.26941473	-0.73289726	-2.50431810
C	0.00000000	3.17394269	-1.16744174
C	0.00000000	3.67093115	-2.47216106
C	0.00000000	2.55726546	-3.28633888
C	2.74871491	-1.58697135	-1.16744174
C	3.17911963	-1.83546557	-2.47216106
C	2.21465653	-1.27863246	-3.28633888
C	-2.74871491	-1.58697135	-1.16744174
C	-3.17911963	-1.83546557	-2.47216106
C	-2.21465653	-1.27863246	-3.28633888
H	0.00000000	4.70816142	-2.77836894
H	0.00000000	2.46740216	-4.36462061
H	4.07738743	-2.35408097	-2.77836894
C	3.55963194	-2.05515457	0.04127000
H	2.13683308	-1.23370108	-4.36462061
C	0.00000000	4.11030913	0.04127000
H	0.00000000	0.00000000	-4.18568673
H	-4.07738743	-2.35408097	-2.77836894
H	-2.13683308	-1.23370108	-4.36462061
C	-3.55963194	-2.05515457	0.04127000
B	0.00000000	0.00000000	-2.98786439
F	-1.07658518	-3.97981508	-0.83548356
F	0.00000000	-5.38237398	0.41903694
F	1.07658518	-3.97981508	-0.83548356
F	4.66127261	2.69118699	0.41903694
F	2.90832852	2.92225806	-0.83548356
F	3.98491371	1.05755703	-0.83548356
F	-4.66127261	2.69118699	0.41903694
F	-3.98491371	1.05755703	-0.83548356
F	-2.90832852	2.92225806	-0.83548356
F	3.98491371	-1.05755703	0.83548356
F	4.66127261	-2.69118699	-0.41903694
F	2.90832852	-2.92225806	0.83548356
F	-2.90832852	-2.92225806	0.83548356
F	-4.66127261	-2.69118699	-0.41903694
F	-3.98491371	-1.05755703	0.83548356
F	-1.07658518	3.97981508	0.83548356
F	0.00000000	5.38237398	-0.41903694
F	1.07658518	3.97981508	0.83548356

$[Mn(Tb^{3CF3})_2]^+$ $^3A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.50075567	0.86646160	1.12864405
N	1.25389819	0.72393882	2.44531431
N	0.00000000	-1.73292319	1.12864405
N	0.00000000	-1.44787711	2.44531431
N	-1.50075567	0.86646160	1.12864405
N	-1.25389819	0.72393882	2.44531431
C	2.68381978	1.54950401	1.04034765
C	3.15613376	1.82219487	2.32394645
C	2.22160939	1.28264680	3.18287415
C	0.00000000	-3.09900855	1.04034765
C	0.00000000	-3.64438921	2.32394645
C	0.00000000	-2.56529308	3.18287415
C	-2.68381978	1.54950401	1.04034765

C	-3.15613376	1.82219487	2.32394645
C	-2.22160939	1.28264680	3.18287415
H	4.06374736	2.34620576	2.58913569
H	2.17996896	1.25860575	4.26375625
H	0.00000000	-4.69241152	2.58913569
C	0.00000000	-4.02007171	-0.18132206
H	0.00000000	-2.51721097	4.26375625
C	3.48148411	2.01003586	-0.18132206
H	0.00000000	0.00000000	4.14712929
H	-4.06374736	2.34620576	2.58913569
H	-2.17996896	1.25860575	4.26375625
C	-3.48148411	2.01003586	-0.18132206
B	0.00000000	0.00000000	2.94878307
N	0.00000000	1.73292319	-1.12864405
N	0.00000000	1.44787711	-2.44531431
N	1.50075567	-0.86646160	-1.12864405
N	1.25389819	-0.72393882	-2.44531431
N	-1.50075567	-0.86646160	-1.12864405
N	-1.25389819	-0.72393882	-2.44531431
C	0.00000000	3.09900855	-1.04034765
C	0.00000000	3.64438921	-2.32394645
C	0.00000000	2.56529308	-3.18287415
C	2.68381978	-1.54950401	-1.04034765
C	3.15613376	-1.82219487	-2.32394645
C	2.22160939	-1.28264680	-3.18287415
C	-2.68381978	-1.54950401	-1.04034765
C	-3.15613376	-1.82219487	-2.32394645
C	-2.22160939	-1.28264680	-3.18287415
H	0.00000000	4.69241152	-2.58913569
H	0.00000000	2.51721097	-4.26375625
H	4.06374736	-2.34620576	-2.58913569
C	3.48148411	-2.01003586	0.18132206
H	2.17996896	-1.25860575	-4.26375625
C	0.00000000	4.02007171	0.18132206
H	0.00000000	0.00000000	-4.14712929
H	-4.06374736	-2.34620576	-2.58913569
H	-2.17996896	-1.25860575	-4.26375625
C	-3.48148411	-2.01003586	0.18132206
B	0.00000000	0.00000000	-2.94878307
F	-1.07847487	-3.88523418	-0.97230181
F	0.00000000	-5.29815119	0.26304131
F	1.07847487	-3.88523418	-0.97230181
F	4.58833346	2.64907559	0.26304131
F	2.82547418	2.87660382	-0.97230181
F	3.90394906	1.00863036	-0.97230181
F	-4.58833346	2.64907559	0.26304131
F	-3.90394906	1.00863036	-0.97230181
F	-2.82547418	2.87660382	-0.97230181
F	3.90394906	-1.00863036	0.97230181
F	4.58833346	-2.64907559	-0.26304131
F	2.82547418	-2.87660382	0.97230181
F	-2.82547418	-2.87660382	0.97230181
F	-4.58833346	-2.64907559	-0.26304131
F	-3.90394906	-1.00863036	0.97230181
F	-1.07847487	3.88523418	0.97230181
F	0.00000000	5.29815119	-0.26304131
F	1.07847487	3.88523418	0.97230181

$[Mn(Tb^{3CF3})_2]^+$ ^1E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.72030000	1.12430000	0.00000000
N	-1.44360000	2.44420000	0.00000000
N	0.86020000	1.12430000	-1.48980000
N	0.72180000	2.44420000	-1.25020000
N	0.86020000	1.12430000	1.48980000
N	0.72180000	2.44420000	1.25020000
C	-3.08950000	1.03640000	0.00000000
C	-3.63900000	2.31650000	0.00000000
C	-2.56130000	3.17950000	0.00000000
C	1.54470000	1.03640000	-2.67560000
C	1.81950000	2.31650000	-3.15140000
C	1.28070000	3.17950000	-2.21820000
C	1.54470000	1.03640000	2.67560000
C	1.81950000	2.31650000	3.15140000
C	1.28070000	3.17950000	2.21820000
H	-4.68750000	2.57940000	0.00000000
H	-2.51610000	4.26060000	0.00000000
H	2.34380000	2.57940000	-4.05950000
C	2.00540000	-0.18320000	-3.47350000
H	1.25800000	4.26060000	-2.17900000
C	-4.01080000	-0.18320000	0.00000000
H	0.00000000	4.14900000	0.00000000
H	2.34380000	2.57940000	4.05950000
H	1.25800000	4.26060000	2.17900000
C	2.00540000	-0.18320000	3.47350000
B	0.00000000	2.95020000	0.00000000
N	-0.86020000	-1.12430000	1.48980000
N	-0.72180000	-2.44420000	1.25020000
N	-0.86020000	-1.12430000	-1.48980000
N	-0.72180000	-2.44420000	-1.25020000
N	1.72030000	-1.12430000	0.00000000
N	1.44360000	-2.44420000	0.00000000
C	-1.54470000	-1.03640000	2.67560000
C	-1.81950000	-2.31650000	3.15140000
C	-1.28070000	-3.17950000	2.21820000
C	-1.54470000	-1.03640000	-2.67560000
C	-1.81950000	-2.31650000	-3.15140000
C	-1.28070000	-3.17950000	-2.21820000
C	3.08950000	-1.03640000	0.00000000
C	3.63900000	-2.31650000	0.00000000
C	2.56130000	-3.17950000	0.00000000
H	-2.34380000	-2.57940000	4.05950000
H	-1.25800000	-4.26060000	2.17900000
H	-2.34380000	-2.57940000	-4.05950000
C	-2.00540000	0.18320000	-3.47350000
H	-1.25800000	-4.26060000	-2.17900000
C	-2.00540000	0.18320000	3.47350000
H	0.00000000	-4.14900000	0.00000000
H	4.68750000	-2.57940000	0.00000000
H	2.51610000	-4.26060000	0.00000000
C	4.01080000	0.18320000	0.00000000
B	0.00000000	-2.95020000	0.00000000
F	2.87310000	-0.97410000	-2.81860000
F	2.64430000	0.26220000	-4.58010000
F	1.00440000	-0.97410000	-3.89750000
F	-5.28870000	0.26220000	0.00000000
F	-3.87750000	-0.97410000	1.07890000
F	-3.87750000	-0.97410000	-1.07890000
F	2.64430000	0.26220000	4.58010000

F	2.87310000	-0.97410000	2.81860000
F	1.00440000	-0.97410000	3.89750000
F	-2.87310000	0.97410000	-2.81860000
F	-2.64430000	-0.26220000	-4.58010000
F	-1.00440000	0.97410000	-3.89750000
F	3.87750000	0.97410000	-1.07890000
F	5.28870000	-0.26220000	0.00000000
F	3.87750000	0.97410000	1.07890000
F	-1.00440000	0.97410000	3.89750000
F	-2.64430000	-0.26220000	4.58010000
F	-2.87310000	0.97410000	2.81860000

$[Mn(Tb^{3NH2})_2]^+$ ^5E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.70523982	1.31430536
N	0.00000000	1.44464119	2.65477060
N	1.47678077	-0.85261991	1.31430536
N	1.25109567	-0.72232059	2.65477060
N	-1.47678077	-0.85261991	1.31430536
N	-1.25109567	-0.72232059	2.65477060
C	0.00000000	3.05475716	1.17971283
C	0.00000000	3.65571677	2.45558511
C	0.00000000	2.59768296	3.34150191
C	2.64549730	-1.52737858	1.17971283
C	3.16594365	-1.82785865	2.45558511
C	2.24965949	-1.29884121	3.34150191
C	-2.64549730	-1.52737858	1.17971283
C	-3.16594365	-1.82785865	2.45558511
C	-2.24965949	-1.29884121	3.34150191
H	0.00000000	4.71405539	2.68707475
H	0.00000000	2.59132172	4.42433773
H	4.08249187	-2.35702796	2.68707475
N	3.17934665	-1.83559681	-0.02262497
H	2.24415022	-1.29566086	4.42433773
N	0.00000000	3.67119362	-0.02262497
H	0.00000000	0.00000000	4.37550525
H	-4.08249187	-2.35702796	2.68707475
H	-2.24415022	-1.29566086	4.42433773
N	-3.17934665	-1.83559681	-0.02262497
B	0.00000000	0.00000000	3.17316480
N	-1.47678077	0.85261991	-1.31430536
N	-1.25109567	0.72232059	-2.65477060
N	1.47678077	0.85261991	-1.31430536
N	1.25109567	0.72232059	-2.65477060
N	0.00000000	-1.70523982	-1.31430536
N	0.00000000	-1.44464119	-2.65477060
C	-2.64549730	1.52737858	-1.17971283
C	-3.16594365	1.82785865	-2.45558511
C	-2.24965949	1.29884121	-3.34150191
C	2.64549730	1.52737858	-1.17971283
C	3.16594365	1.82785865	-2.45558511
C	2.24965949	1.29884121	-3.34150191
C	0.00000000	-3.05475716	-1.17971283
C	0.00000000	-3.65571677	-2.45558511
C	0.00000000	-2.59768296	-3.34150191
H	-4.08249187	2.35702796	-2.68707475
H	-2.24415022	1.29566086	-4.42433773
H	4.08249187	2.35702796	-2.68707475
N	3.17934665	1.83559681	0.02262497
H	2.24415022	1.29566086	-4.42433773
N	-3.17934665	1.83559681	0.02262497
H	0.00000000	0.00000000	-4.37550525
H	0.00000000	-4.71405539	-2.68707475
H	0.00000000	-2.59132172	-4.42433773
N	0.00000000	-3.67119362	0.02262497
B	0.00000000	0.00000000	-3.17316480
H	0.00000000	4.67241338	-0.07018266
H	4.04642844	-2.33620695	-0.07018266
H	-4.04642844	-2.33620695	-0.07018266
H	-4.04642844	2.33620695	0.07018266
H	4.04642844	2.33620695	0.07018266
H	0.00000000	-4.67241338	0.07018266
H	2.72312601	-1.57219778	-0.87734042
H	0.00000000	3.14439502	-0.87734042
H	-2.72312601	-1.57219778	-0.87734042
H	2.72312601	1.57219778	0.87734042
H	-2.72312601	1.57219778	0.87734042
H	0.00000000	-3.14439502	0.87734042

$[Mn(Tb^{3NH2})_2]^+$ $^3A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.62904888	1.19191513
N	0.00000000	1.43004860	2.54563097
N	1.41079766	-0.81452444	1.19191513
N	1.23845839	-0.71502430	2.54563097
N	-1.41079766	-0.81452444	1.19191513
N	-1.23845839	-0.71502430	2.54563097
C	0.00000000	2.97797989	1.00235537
C	0.00000000	3.62840752	2.25302135
C	0.00000000	2.60942752	3.18247832
C	2.57900618	-1.48898995	1.00235537
C	3.14229313	-1.81420376	2.25302135
C	2.25983080	-1.30471402	3.18247832
C	-2.57900618	-1.48898995	1.00235537
C	-3.14229313	-1.81420376	2.25302135
C	-2.25983080	-1.30471402	3.18247832
H	0.00000000	4.69550350	2.43904409
H	0.00000000	2.64794421	4.26461087
H	4.06642552	-2.34775201	2.43904409
N	3.08061064	-1.77859119	-0.21529947
H	2.29318696	-1.32397237	4.26461087
N	0.00000000	3.55718291	-0.21529947
H	0.00000000	0.00000000	4.28691252
H	-4.06642552	-2.34775201	2.43904409
H	-2.29318696	-1.32397237	4.26461087
N	-3.08061064	-1.77859119	-0.21529947
B	0.00000000	0.00000000	3.08452867
N	-1.41079766	0.81452444	-1.19191513
N	-1.23845839	0.71502430	-2.54563097
N	1.41079766	0.81452444	-1.19191513
N	1.23845839	0.71502430	-2.54563097
N	0.00000000	-1.62904888	-1.19191513
N	0.00000000	-1.43004860	-2.54563097
C	-2.57900618	1.48898995	-1.00235537
C	-3.14229313	1.81420376	-2.25302135
C	-2.25983080	1.30471402	-3.18247832
C	2.57900618	1.48898995	-1.00235537
C	3.14229313	1.81420376	-2.25302135

C	2.25983080	1.30471402	-3.18247832
C	0.00000000	-2.97797989	-1.00235537
C	0.00000000	-3.62840752	-2.25302135
C	0.00000000	-2.60942752	-3.18247832
H	-4.06642552	2.34775201	-2.43904409
H	-2.29318696	1.32397237	-4.26461087
H	4.06642552	2.34775201	-2.43904409
N	3.08061064	1.77859119	0.21529947
H	2.29318696	1.32397237	-4.26461087
N	-3.08061064	1.77859119	0.21529947
H	0.00000000	0.00000000	-4.28691252
H	0.00000000	-4.69550350	-2.43904409
H	0.00000000	-2.64794421	-4.26461087
N	0.00000000	-3.55718291	0.21529947
B	0.00000000	0.00000000	-3.08452867
H	0.00000000	4.55682890	-0.29017805
H	3.94632928	-2.27841445	-0.29017805
H	-3.94632928	-2.27841445	-0.29017805
H	-3.94632928	2.27841445	0.29017805
H	3.94632928	2.27841445	0.29017805
H	0.00000000	-4.55682890	0.29017805
H	2.60207142	-1.50230669	-1.05292514
H	0.00000000	3.00461285	-1.05292514
H	-2.60207142	-1.50230669	-1.05292514
H	2.60207142	1.50230669	1.05292514
H	-2.60207142	1.50230669	1.05292514
H	0.00000000	-3.00461285	1.05292514

$[Mn(Tb^{3NH2})_2]^+$ ^1E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.80920000	-1.18700000	1.40160000
N	0.71470000	-2.54040000	1.23790000
N	0.80920000	-1.18700000	-1.40160000
N	0.71470000	-2.54040000	-1.23790000
N	-1.61840000	-1.18700000	0.00000000
N	-1.42940000	-2.54040000	0.00000000
C	1.48470000	-0.99480000	2.57170000
C	1.81370000	-2.24150000	3.14140000
C	1.30630000	-3.17480000	2.26250000
C	1.48470000	-0.99480000	-2.57170000
C	1.81370000	-2.24150000	-3.14140000
C	1.30630000	-3.17480000	-2.26250000
C	-2.96950000	-0.99480000	0.00000000
C	-3.62730000	-2.24150000	0.00000000
C	-2.61250000	-3.17480000	0.00000000
H	2.34760000	-2.42290000	4.06620000
H	1.32740000	-4.25670000	2.29920000
H	2.34760000	-2.42290000	-4.06620000
N	1.76910000	0.22760000	-3.06420000
H	1.32740000	-4.25670000	-2.29920000
N	1.76910000	0.22760000	3.06420000
H	0.00000000	-4.28470000	0.00000000
H	-4.69520000	-2.42290000	0.00000000
H	-2.65490000	-4.25670000	0.00000000
N	-3.53820000	0.22760000	0.00000000
B	0.00000000	-3.08200000	0.00000000
N	-0.80920000	1.18700000	1.40160000
N	-0.71470000	2.54040000	1.23790000
N	1.61840000	1.18700000	0.00000000
N	1.42940000	2.54040000	0.00000000
N	-0.80920000	1.18700000	-1.40160000
N	-0.71470000	2.54040000	-1.23790000
C	-1.48470000	0.99480000	2.57170000
C	-1.81370000	2.24150000	3.14140000
C	-1.30630000	3.17480000	2.26250000
C	2.96950000	0.99480000	0.00000000
C	3.62730000	2.24150000	0.00000000
C	2.61250000	3.17480000	0.00000000
C	-1.48470000	0.99480000	-2.57170000
C	-1.81370000	2.24150000	-3.14140000
C	-1.30630000	3.17480000	-2.26250000
H	-2.34760000	2.42290000	4.06620000
H	-1.32740000	4.25670000	2.29920000
H	4.69520000	2.42290000	0.00000000
N	3.53820000	-0.22760000	0.00000000
H	2.65490000	4.25670000	0.00000000
N	-1.76910000	-0.22760000	3.06420000
H	0.00000000	4.28470000	0.00000000
H	-2.34760000	2.42290000	-4.06620000
H	-1.32740000	4.25670000	-2.29920000
N	-1.76910000	-0.22760000	-3.06420000
B	0.00000000	3.08200000	0.00000000
H	2.26860000	0.31300000	3.92940000
H	2.26860000	0.31300000	-3.92940000
H	-4.53730000	0.31300000	0.00000000
H	-2.26860000	-0.31300000	3.92940000
H	4.53730000	-0.31300000	0.00000000
H	-2.26860000	-0.31300000	-3.92940000
H	1.48770000	1.05870000	-2.57680000
H	1.48770000	1.05870000	2.57680000
H	-2.97540000	1.05870000	0.00000000
H	2.97540000	-1.05870000	0.00000000
H	-1.48770000	-1.05870000	2.57680000
H	-1.48770000	-1.05870000	-2.57680000

$[Mn(Tb^{3NO2})_2]^+$ ^5E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.81367829	1.56611753
N	0.00000000	1.45959097	2.85640459
N	1.57069121	-0.90683888	1.56611753
N	1.26404305	-0.72979575	2.85640459
N	-1.57069121	-0.90683888	1.56611753
N	-1.26404305	-0.72979575	2.85640459
C	0.00000000	3.15887808	1.59355537
C	0.00000000	3.67078880	2.89173776
C	0.00000000	2.53769595	3.67303780
C	2.73566857	-1.57943904	1.59355537
C	3.17899634	-1.83539414	2.89173776
C	2.19770910	-1.26884798	3.67303780
C	-2.73566857	-1.57943904	1.59355537
C	-3.17899634	-1.83539414	2.89173776
C	-2.19770910	-1.26884798	3.67303780
H	0.00000000	4.70794287	3.19630943
H	0.00000000	2.41974287	4.74866041
H	4.07719798	-2.35397143	3.19630943
N	3.43872023	-1.98534603	0.40825548
H	2.09555884	-1.20987170	4.74866041
N	0.00000000	3.97069207	0.40825548

H	0.00000000	0.00000000	4.53404517
H	-4.07719798	-2.35397143	3.19630943
H	-2.09555884	-1.20987170	4.74866041
N	-3.43872023	-1.98534603	0.40825548
B	0.00000000	0.00000000	3.33454164
N	-1.57069121	0.90683888	-1.56611753
N	-1.26404305	0.72979575	-2.85640459
N	1.57069121	0.90683888	-1.56611753
N	1.26404305	0.72979575	-2.85640459
N	0.00000000	-1.81367829	-1.56611753
N	0.00000000	-1.45959097	-2.85640459
C	-2.73566857	1.57943904	-1.59355537
C	-3.17899634	1.83539414	-2.89173776
C	-2.19770910	1.26884798	-3.67303780
C	2.73566857	1.57943904	-1.59355537
C	3.17899634	1.83539414	-2.89173776
C	2.19770910	1.26884798	-3.67303780
C	0.00000000	-3.15887808	-1.59355537
C	0.00000000	-3.67078880	-2.89173776
C	0.00000000	-2.53769595	-3.67303780
H	-4.07719798	2.35397143	-3.19630943
H	-2.09555884	1.20987170	-4.74866041
H	4.07719798	2.35397143	-3.19630943
N	3.43872023	1.98534603	-0.40825548
H	2.09555884	1.20987170	-4.74866041
N	-3.43872023	1.98534603	-0.40825548
H	0.00000000	0.00000000	-4.53404517
H	0.00000000	-4.70794287	-3.19630943
H	0.00000000	-2.41974287	-4.74866041
N	0.00000000	-3.97069207	-0.40825548
B	0.00000000	0.00000000	-3.33454164
O	0.00000000	5.18590740	0.57558398
O	4.49112784	-2.59295370	0.57558398
O	-4.49112784	-2.59295370	0.57558398
O	-4.49112784	2.59295370	-0.57558398
O	4.49112784	2.59295370	-0.57558398
O	0.00000000	-5.18590740	-0.57558398
O	2.96615648	-1.71251124	-0.69018631
O	0.00000000	3.42502248	-0.69018631
O	-2.96615648	-1.71251124	-0.69018631
O	2.96615648	1.71251124	0.69018631
O	-2.96615648	1.71251124	0.69018631
O	0.00000000	-3.42502248	0.69018631

$[Mn(Tb^{3NO2})_2]^+$ $^3A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.70289080	1.19312430
N	0.00000000	1.43473922	2.50568655
N	1.47474661	-0.85144513	1.19312430
N	1.24252035	-0.71736961	2.50568655
N	-1.47474661	-0.85144513	1.19312430
N	-1.24252035	-0.71736961	2.50568655
C	0.00000000	3.06118719	1.12521710
C	0.00000000	3.63381201	2.39241722
C	0.00000000	2.55544879	3.24712103
C	2.65106583	-1.53059333	1.12521710
C	3.14697317	-1.81690574	2.39241722
C	2.21308381	-1.27772440	3.24712103
C	-2.65106583	-1.53059333	1.12521710
C	-3.14697317	-1.81690574	2.39241722
C	-2.21308381	-1.27772440	3.24712103
H	0.00000000	4.68874220	2.62629240
H	0.00000000	2.50280412	4.32771049
H	4.06056965	-2.34437110	2.62629240
N	3.36198318	-1.94104173	-0.07696036
H	2.16749202	-1.25140206	4.32771049
N	0.00000000	3.88208345	-0.07696036
H	0.00000000	0.00000000	4.22012294
H	-4.06056965	-2.34437110	2.62629240
H	-2.16749202	-1.25140206	4.32771049
N	-3.36198318	-1.94104173	-0.07696036
B	0.00000000	0.00000000	3.02260964
N	-1.47474661	0.85144513	-1.19312430
N	-1.24252035	0.71736961	-2.50568655
N	1.47474661	0.85144513	-1.19312430
N	1.24252035	0.71736961	-2.50568655
N	0.00000000	-1.70289080	-1.19312430
N	0.00000000	-1.43473922	-2.50568655
C	-2.65106583	1.53059333	-1.12521710
C	-3.14697317	1.81690574	-2.39241722
C	-2.21308381	1.27772440	-3.24712103
C	2.65106583	1.53059333	-1.12521710
C	3.14697317	1.81690574	-2.39241722
C	2.21308381	1.27772440	-3.24712103
C	0.00000000	-3.06118719	-1.12521710
C	0.00000000	-3.63381201	-2.39241722
C	0.00000000	-2.55544879	-3.24712103
H	-4.06056965	2.34437110	-2.62629240
H	-2.16749202	1.25140206	-4.32771049
H	4.06056965	2.34437110	-2.62629240
N	3.36198318	1.94104173	0.07696036
H	2.16749202	1.25140206	-4.32771049
N	-3.36198318	1.94104173	0.07696036
H	0.00000000	0.00000000	-4.22012294
H	0.00000000	-4.68874220	-2.62629240
H	0.00000000	-2.50280412	-4.32771049
N	0.00000000	-3.88208345	0.07696036
B	0.00000000	0.00000000	-3.02260964
O	0.00000000	5.08857265	0.12295804
O	4.40683308	-2.54428633	0.12295804
O	-4.40683308	-2.54428633	0.12295804
O	-4.40683308	2.54428633	-0.12295804
O	4.40683308	2.54428633	-0.12295804
O	0.00000000	-5.08857265	-0.12295804
O	2.89293264	-1.67023527	-1.17094966
O	0.00000000	3.34047107	-1.17094966
O	-2.89293264	-1.67023527	-1.17094966
O	2.89293264	1.67023527	1.17094966
O	-2.89293264	1.67023527	1.17094966
O	0.00000000	-3.34047107	1.17094966

$[Mn(Tb^{3NO2})_2]^+$ ^1E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-0.84250000	-1.17260000	1.45920000
N	-0.71640000	-2.49010000	1.24090000
N	1.68500000	-1.17260000	0.00000000
N	1.43290000	-2.49010000	0.00000000
N	-0.84250000	-1.17260000	-1.45920000

N	-0.71640000	-2.49010000	-1.24090000
C	-1.52300000	-1.09260000	2.63790000
C	-1.81580000	-2.35310000	3.14500000
C	-1.28020000	-3.21960000	2.21730000
C	3.04600000	-1.09260000	0.00000000
C	3.63150000	-2.35310000	0.00000000
C	2.56030000	-3.21960000	0.00000000
C	-1.52300000	-1.09260000	-2.63790000
C	-1.81580000	-2.35310000	-3.14500000
C	-1.28020000	-3.21960000	-2.21730000
H	-2.34420000	-2.57800000	4.06020000
H	-1.26000000	-4.30080000	2.18250000
H	4.68830000	-2.57800000	0.00000000
N	3.86210000	0.11400000	0.00000000
H	2.52010000	-4.30080000	0.00000000
N	-1.93100000	0.11400000	3.34470000
H	0.00000000	-4.21000000	0.00000000
H	-2.34420000	-2.57800000	-4.06020000
H	-1.26000000	-4.30080000	-2.18250000
N	-1.93100000	0.11400000	-3.34470000
B	0.00000000	-3.01220000	0.00000000
N	-1.68500000	1.17260000	0.00000000
N	-1.43290000	2.49010000	0.00000000
N	0.84250000	1.17260000	1.45920000
N	0.71640000	2.49010000	1.24090000
N	0.84250000	1.17260000	-1.45920000
N	0.71640000	2.49010000	-1.24090000
C	-3.04600000	1.09260000	0.00000000
C	-3.63150000	2.35310000	0.00000000
C	-2.56030000	3.21960000	0.00000000
C	1.52300000	1.09260000	2.63790000
C	1.81580000	2.35310000	3.14500000
C	1.28020000	3.21960000	2.21730000
C	1.52300000	1.09260000	-2.63790000
C	1.81580000	2.35310000	-3.14500000
C	1.28020000	3.21960000	-2.21730000
H	-4.68830000	2.57800000	0.00000000
H	-2.52010000	4.30080000	0.00000000
H	2.34420000	2.57800000	4.06020000
N	1.93100000	-0.11400000	3.34470000
H	1.26000000	4.30080000	2.18250000
N	-3.86210000	-0.11400000	0.00000000
H	0.00000000	4.21000000	0.00000000
H	2.34420000	2.57800000	-4.06020000
H	1.26000000	4.30080000	-2.18250000
N	1.93100000	-0.11400000	-3.34470000
B	0.00000000	3.01220000	0.00000000
O	-2.53460000	-0.08290000	4.39000000
O	5.06920000	-0.08290000	0.00000000
O	-2.53460000	-0.08290000	-4.39000000
O	-5.06920000	0.08290000	0.00000000
O	2.53460000	0.08290000	4.39000000
O	2.53460000	0.08290000	-4.39000000
O	3.31960000	1.20750000	0.00000000
O	-1.65980000	1.20750000	2.87480000
O	-1.65980000	1.20750000	-2.87480000
O	1.65980000	-1.20750000	2.87480000
O	-3.31960000	-1.20750000	0.00000000
O	1.65980000	-1.20750000	-2.87480000

$[Mn(Tb^{5CH3})_2]^+$ ^5E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.42891034	0.82498151	1.30270527
N	1.25588790	0.72508713	2.63900535
N	0.00000000	-1.64996355	1.30270527
N	0.00000000	-1.45017427	2.63900535
N	-1.42891034	0.82498151	1.30270527
N	-1.25588790	0.72508713	2.63900535
C	2.57326249	1.48567359	1.09023478
C	3.15315873	1.82047716	2.30892099
C	2.28905673	1.32158737	3.28288600
C	0.00000000	-2.97134771	1.09023478
C	0.00000000	-3.64095379	2.30892099
C	0.00000000	-2.64317474	3.28288600
C	-2.57326249	1.48567359	1.09023478
C	-3.15315873	1.82047716	2.30892099
C	-2.28905673	1.32158737	3.28288600
H	4.08088741	2.35610137	2.47295218
C	2.41875173	1.39646701	4.76428384
H	0.00000000	-4.71220327	2.47295218
H	0.00000000	-3.36525032	0.08237808
C	0.00000000	-2.79293402	4.76428384
H	2.91439237	1.68262543	0.08237808
H	0.00000000	0.00000000	4.37399181
H	-4.08088741	2.35610137	2.47295218
C	-2.41875173	1.39646701	4.76428384
H	-2.91439237	1.68262543	0.08237808
B	0.00000000	0.00000000	3.17930590
N	0.00000000	1.64996355	-1.30270527
N	0.00000000	1.45017427	-2.63900535
N	1.42891034	-0.82498151	-1.30270527
N	1.25588790	-0.72508713	-2.63900535
N	-1.42891034	-0.82498151	-1.30270527
N	-1.25588790	-0.72508713	-2.63900535
C	0.00000000	2.97134771	-1.09023478
C	0.00000000	3.64095379	-2.30892099
C	0.00000000	2.64317474	-3.28288600
C	2.57326249	-1.48567359	-1.09023478
C	3.15315873	-1.82047716	-2.30892099
C	2.28905673	-1.32158737	-3.28288600
C	-2.57326249	-1.48567359	-1.09023478
C	-3.15315873	-1.82047716	-2.30892099
C	-2.28905673	-1.32158737	-3.28288600
H	0.00000000	4.71220327	-2.47295218
C	0.00000000	2.79293402	-4.76428384
H	4.08088741	-2.35610137	-2.47295218
H	2.91439237	-1.68262543	-0.08237808
C	2.41875173	-1.39646701	-4.76428384
H	0.00000000	3.36525032	-0.08237808
H	0.00000000	0.00000000	-4.37399181
H	-4.08088741	-2.35610137	-2.47295218
C	-2.41875173	-1.39646701	-4.76428384
H	-2.91439237	-1.68262543	-0.08237808
B	0.00000000	0.00000000	-3.17930590
H	-3.33824006	-1.92733392	-5.02153436
H	-1.58131021	-1.93436139	-5.22111303
H	-2.46586120	-0.40227419	-5.22111303
H	3.33824006	-1.92733392	-5.02153436
H	2.46586120	-0.40227419	-5.22111303

H	1.58131021	-1.93436139	-5.22111303
H	0.88455046	2.33663559	-5.22111303
H	0.00000000	3.85466731	-5.02153436
H	-0.88455046	2.33663559	-5.22111303
H	-2.46586120	0.40227419	5.22111303
H	-3.33824006	1.92733392	5.02153436
H	-1.58131021	1.93436139	5.22111303
H	-0.88455046	-2.33663559	5.22111303
H	0.88455046	-2.33663559	5.22111303
H	0.00000000	-3.85466731	5.02153436
H	2.46586120	0.40227419	5.22111303
H	1.58131021	1.93436139	5.22111303
H	3.33824006	1.92733392	5.02153436

$[Mn(Tb^{5CH3})_2]^+$ $^3A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.37912111	0.79623607	1.19007624
N	1.24549856	0.71908891	2.53339956
N	0.00000000	-1.59247162	1.19007624
N	0.00000000	-1.43817782	2.53339956
N	-1.37912111	0.79623607	1.19007624
N	-1.24549856	0.71908891	2.53339956
C	2.52013891	1.45500301	0.93934200
C	3.13108463	1.80773245	2.13565407
C	2.29253925	1.32359824	3.14087758
C	0.00000000	-2.91000602	0.93934200
C	0.00000000	-3.61546491	2.13565407
C	0.00000000	-2.64719649	3.14087758
C	-2.52013891	1.45500301	0.93934200
C	-3.13108463	1.80773245	2.13565407
C	-2.29253925	1.32359824	3.14087758
H	4.06272340	2.34561414	2.26668206
C	2.45803202	1.41914543	4.61705350
H	0.00000000	-4.69122881	2.26668206
H	0.00000000	-3.27473455	-0.07847064
C	0.00000000	-2.83829086	4.61705350
H	2.83600322	1.63736701	-0.07847064
H	0.00000000	0.00000000	4.28519904
H	-4.06272340	2.34561414	2.26668206
C	-2.45803202	1.41914543	4.61705350
H	-2.83600322	1.63736701	-0.07847064
B	0.00000000	0.00000000	3.09017341
N	0.00000000	1.59247162	-1.19007624
N	0.00000000	1.43817782	-2.53339956
N	1.37912111	-0.79623607	-1.19007624
N	1.24549856	-0.71908891	-2.53339956
N	-1.37912111	-0.79623607	-1.19007624
N	-1.24549856	-0.71908891	-2.53339956
C	0.00000000	2.91000602	-0.93934200
C	0.00000000	3.61546491	-2.13565407
C	0.00000000	2.64719649	-3.14087758
C	2.52013891	-1.45500301	-0.93934200
C	3.13108463	-1.80773245	-2.13565407
C	2.29253925	-1.32359824	-3.14087758
C	-2.52013891	-1.45500301	-0.93934200
C	-3.13108463	-1.80773245	-2.13565407
C	-2.29253925	-1.32359824	-3.14087758
H	0.00000000	4.69122881	-2.26668206
C	0.00000000	2.83829086	-4.61705350
H	4.06272340	-2.34561414	-2.26668206
H	2.83600322	-1.63736701	0.07847064
C	2.45803202	-1.41914543	-4.61705350
H	0.00000000	3.27473455	0.07847064
H	0.00000000	0.00000000	-4.28519904
H	-4.06272340	-2.34561414	-2.26668206
C	-2.45803202	-1.41914543	-4.61705350
H	-2.83600322	-1.63736701	0.07847064
B	0.00000000	0.00000000	-3.09017341
H	-3.38304761	-1.95320328	-4.84585387
H	-1.63061365	-1.96254908	-5.08584475
H	-2.51492387	-0.43087834	-5.08584475
H	3.38304761	-1.95320328	-4.84585387
H	2.51492387	-0.43087834	-5.08584475
H	1.63061365	-1.96254908	-5.08584475
H	0.88431022	2.39342742	-5.08584475
H	0.00000000	3.90640709	-4.84585387
H	-0.88431022	2.39342742	-5.08584475
H	-2.51492387	0.43087834	5.08584475
H	-3.38304761	1.95320328	4.84585387
H	-1.63061365	1.96254908	5.08584475
H	-0.88431022	-2.39342742	5.08584475
H	0.88431022	-2.39342742	5.08584475
H	0.00000000	-3.90640709	4.84585387
H	2.51492387	0.43087834	5.08584475
H	1.63061365	1.96254908	5.08584475
H	3.38304761	1.95320328	4.84585387

$[Mn(Tb^{5CH3})_2]^+$ ^1E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.79110000	1.17800000	1.37020000
N	0.71780000	2.52350000	1.24330000
N	-1.58220000	1.17800000	0.00000000
N	-1.43560000	2.52350000	0.00000000
N	0.79110000	1.17800000	-1.37020000
N	0.71780000	2.52350000	-1.24330000
C	1.45080000	0.92480000	2.51290000
C	1.80570000	2.11770000	3.12760000
C	1.32290000	3.12780000	2.29130000
C	-2.90170000	0.92480000	0.00000000
C	-3.61150000	2.11770000	0.00000000
C	-2.64580000	3.12780000	0.00000000
C	1.45080000	0.92480000	-2.51290000
C	1.80570000	2.11770000	-3.12760000
C	1.32290000	3.12780000	-2.29130000
H	2.34380000	2.24550000	4.05960000
C	1.41960000	4.60340000	2.45870000
H	-4.68770000	2.24550000	0.00000000
H	-3.26330000	-0.09400000	0.00000000
C	-2.83910000	4.60340000	0.00000000
H	1.63160000	-0.09400000	2.82610000
H	0.00000000	4.27820000	0.00000000
H	2.34380000	2.24550000	-4.05960000
C	1.41960000	4.60340000	-2.45870000
H	1.63160000	-0.09400000	-2.82610000
B	0.00000000	3.08270000	0.00000000
N	1.58220000	-1.17800000	0.00000000
N	1.43560000	-2.52350000	0.00000000
N	-0.79110000	-1.17800000	1.37020000

N	-0.71780000	-2.52350000	1.24330000
N	-0.79110000	-1.17800000	-1.37020000
N	-0.71780000	-2.52350000	-1.24330000
C	2.90170000	-0.92480000	0.00000000
C	3.61150000	-2.11770000	0.00000000
C	2.64580000	-3.12780000	0.00000000
C	-1.45080000	-0.92480000	2.51290000
C	-1.80570000	-2.11770000	3.12760000
C	-1.32290000	-3.12780000	2.29130000
C	-1.45080000	-0.92480000	-2.51290000
C	-1.80570000	-2.11770000	-3.12760000
C	-1.32290000	-3.12780000	-2.29130000
H	4.68770000	-2.24550000	0.00000000
C	2.83910000	-4.60340000	0.00000000
H	-2.34380000	-2.24550000	4.05960000
H	-1.63160000	0.09400000	2.82610000
C	-1.41960000	-4.60340000	2.45870000
H	3.26330000	0.09400000	0.00000000
H	0.00000000	-4.27820000	0.00000000
H	-2.34380000	-2.24550000	-4.05960000
C	-1.41960000	-4.60340000	-2.45870000
H	-1.63160000	0.09400000	-2.82610000
B	0.00000000	-3.08270000	0.00000000
H	-1.95360000	-4.83180000	-3.38380000
H	-1.96250000	-5.07240000	-1.63100000
H	-0.43120000	-5.07240000	-2.51510000
H	-1.95360000	-4.83180000	3.38380000
H	-0.43120000	-5.07240000	2.51510000
H	-1.96250000	-5.07240000	1.63100000
H	2.39370000	-5.07240000	0.88410000
H	3.90730000	-4.83180000	0.00000000
H	2.39370000	-5.07240000	-0.88410000
H	0.43120000	5.07240000	-2.51510000
H	1.95360000	4.83180000	-3.38380000
H	1.96250000	5.07240000	-1.63100000
H	-2.39370000	5.07240000	-0.88410000
H	-2.39370000	5.07240000	0.88410000
H	-3.90730000	4.83180000	0.00000000
H	0.43120000	5.07240000	2.51510000
H	1.96250000	5.07240000	1.63100000
H	1.95360000	4.83180000	3.38380000

$[Mn(Tb^{5CF3})_2]^+$ ^5E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.42349474	0.82185513	1.31586855
N	1.25983397	0.72736577	2.65097216
N	0.00000000	-1.64371026	1.31586855
N	0.00000000	-1.45473101	2.65097216
N	-1.42349474	0.82185513	1.31586855
N	-1.25983397	0.72736577	2.65097216
C	2.56494329	1.48087078	1.07853573
C	3.16520545	1.82743213	2.28240921
C	2.31020900	1.33379972	3.25896772
C	0.00000000	-2.96174156	1.07853573
C	0.00000000	-3.65486480	2.28240921
C	0.00000000	-2.66759997	3.25896772
C	-2.56494329	1.48087078	1.07853573
C	-3.16520545	1.82743213	2.28240921
C	-2.31020900	1.33379972	3.25896772
H	4.09344955	2.36335428	2.43285377
C	2.51156571	1.45005308	4.75311450
H	0.00000000	-4.72670855	2.43285377
H	0.00000000	-3.34135850	0.06513061
C	0.00000000	-2.90010670	4.75311450
H	2.89370154	1.67067925	0.06513061
H	0.00000000	0.00000000	4.39030846
H	-4.09344955	2.36335428	2.43285377
C	-2.51156571	1.45005308	4.75311450
H	-2.89370154	1.67067925	0.06513061
B	0.00000000	0.00000000	3.20613360
N	0.00000000	1.64371026	-1.31586855
N	0.00000000	1.45473101	-2.65097216
N	1.42349474	-0.82185513	-1.31586855
N	1.25983397	-0.72736577	-2.65097216
N	-1.42349474	-0.82185513	-1.31586855
N	-1.25983397	-0.72736577	-2.65097216
C	0.00000000	2.96174156	-1.07853573
C	0.00000000	3.65486480	-2.28240921
C	0.00000000	2.66759997	-3.25896772
C	2.56494329	-1.48087078	-1.07853573
C	3.16520545	-1.82743213	-2.28240921
C	2.31020900	-1.33379972	-3.25896772
C	-2.56494329	-1.48087078	-1.07853573
C	-3.16520545	-1.82743213	-2.28240921
C	-2.31020900	-1.33379972	-3.25896772
H	0.00000000	4.72670855	-2.43285377
C	0.00000000	2.90010670	-4.75311450
H	4.09344955	-2.36335428	-2.43285377
H	2.89370154	-1.67067925	-0.06513061
C	2.51156571	-1.45005308	-4.75311450
H	0.00000000	3.34135850	-0.06513061
H	0.00000000	0.00000000	-4.39030846
H	-4.09344955	-2.36335428	-2.43285377
C	-2.51156571	-1.45005308	-4.75311450
H	-2.89370154	-1.67067925	-0.06513061
B	0.00000000	0.00000000	-3.20613360
F	-3.66029363	-2.11327146	-4.99234124
F	-1.51176362	-2.13071684	-5.34739483
F	-2.60113690	-0.24386710	-5.34739483
F	3.66029363	-2.11327146	-4.99234124
F	2.60113690	-0.24386710	-5.34739483
F	1.51176362	-2.13071684	-5.34739483
F	1.08937328	2.37458395	-5.34739483
F	0.00000000	4.22654292	-4.99234124
F	-1.08937328	2.37458395	-5.34739483
F	-2.60113690	0.24386710	5.34739483
F	-3.66029363	2.11327146	4.99234124
F	-1.51176362	2.13071684	5.34739483
F	-1.08937328	-2.37458395	5.34739483
F	1.08937328	-2.37458395	5.34739483
F	0.00000000	-4.22654292	4.99234124
F	2.60113690	0.24386710	5.34739483
F	1.51176362	2.13071684	5.34739483
F	3.66029363	2.11327146	4.99234124

$[Mn(Tb^{5CF3})_2]^+$ $^3A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.37893960	0.79613130	1.19792711

N	1.24853445	0.72084154	2.53897656
N	0.00000000	-1.59226206	1.19792711
N	0.00000000	-1.44168309	2.53897656
N	-1.37893960	0.79613130	1.19792711
N	-1.24853445	0.72084154	2.53897656
C	2.51845084	1.45402826	0.93117733
C	3.14308584	1.81466150	2.11676138
C	2.30805102	1.33255404	3.11785731
C	0.00000000	-2.90805653	0.93117733
C	0.00000000	-3.62932247	2.11676138
C	0.00000000	-2.66510808	3.11785731
C	-2.51845084	1.45402826	0.93117733
C	-3.14308584	1.81466150	2.11676138
C	-2.30805102	1.33255404	3.11785731
H	4.07422560	2.35225531	2.24140961
C	2.52888674	1.46005348	4.60792890
H	0.00000000	-4.70451062	2.24140961
H	0.00000000	-3.26561524	-0.08923410
C	0.00000000	-2.92010695	4.60792890
H	2.82810578	1.63280762	-0.08923410
H	0.00000000	0.00000000	4.29254349
H	-4.07422560	2.35225531	2.24140961
C	-2.52888674	1.46005348	4.60792890
H	-2.82810578	1.63280762	-0.08923410
B	0.00000000	0.00000000	3.10843637
N	0.00000000	1.59226206	-1.19792711
N	0.00000000	1.44168309	-2.53897656
N	1.37893960	-0.79613130	-1.19792711
N	1.24853445	-0.72084154	-2.53897656
N	-1.37893960	-0.79613130	-1.19792711
N	-1.24853445	-0.72084154	-2.53897656
C	0.00000000	2.90805653	-0.93117733
C	0.00000000	3.62932247	-2.11676138
C	0.00000000	2.66510808	-3.11785731
C	2.51845084	-1.45402826	-0.93117733
C	3.14308584	-1.81466150	-2.11676138
C	2.30805102	-1.33255404	-3.11785731
C	-2.51845084	-1.45402826	-0.93117733
C	-3.14308584	-1.81466150	-2.11676138
C	-2.30805102	-1.33255404	-3.11785731
H	0.00000000	4.70451062	-2.24140961
C	0.00000000	2.92010695	-4.60792890
H	4.07422560	-2.35225531	-2.24140961
H	2.82810578	-1.63280762	0.08923410
C	2.52888674	-1.46005348	-4.60792890
H	0.00000000	3.26561524	0.08923410
H	0.00000000	0.00000000	-4.29254349
H	-4.07422560	-2.35225531	-2.24140961
C	-2.52888674	-1.46005348	-4.60792890
H	-2.82810578	-1.63280762	0.08923410
B	0.00000000	0.00000000	-3.10843637
F	-3.67976206	-2.12451171	-4.82981715
F	-1.53465583	-2.14428495	-5.20807887
F	-2.62433338	-0.25690867	-5.20807887
F	3.67976206	-2.12451171	-4.82981715
F	2.62433338	-0.25690867	-5.20807887
F	1.53465583	-2.14428495	-5.20807887
F	1.08967756	2.40119362	-5.20807887
F	0.00000000	4.24902290	-4.82981715
F	-1.08967756	2.40119362	-5.20807887
F	-2.62433338	0.25690867	5.20807887
F	-3.67976206	2.12451171	4.82981715
F	-1.53465583	2.14428495	5.20807887
F	-1.08967756	-2.40119362	5.20807887
F	1.08967756	-2.40119362	5.20807887
F	0.00000000	-4.24902290	4.82981715
F	2.62433338	0.25690867	5.20807887
F	1.53465583	2.14428495	5.20807887
F	3.67976206	2.12451171	4.82981715

$[Mn(Tb^{5CF3})_2]^+$ ^1E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-0.79130000	1.18400000	-1.37060000
N	-0.71880000	2.52670000	-1.24500000
N	1.58260000	1.18400000	0.00000000
N	1.43760000	2.52670000	0.00000000
N	-0.79130000	1.18400000	1.37060000
N	-0.71880000	2.52670000	1.24500000
C	-1.45060000	0.91790000	-2.51260000
C	-1.81200000	2.10170000	-3.13850000
C	-1.32980000	3.10540000	-2.30330000
C	2.90130000	0.91790000	0.00000000
C	3.62400000	2.10170000	0.00000000
C	2.65970000	3.10540000	0.00000000
C	-1.45060000	0.91790000	2.51260000
C	-1.81200000	2.10170000	3.13850000
C	-1.32980000	3.10540000	2.30330000
H	-2.34970000	2.22570000	-4.06980000
C	-1.45340000	4.59630000	-2.51740000
H	4.69940000	2.22570000	0.00000000
H	3.25820000	-0.10260000	0.00000000
C	2.90690000	4.59630000	0.00000000
H	-1.62910000	-0.10260000	-2.82170000
H	0.00000000	4.28250000	0.00000000
H	-2.34970000	2.22570000	4.06980000
C	-1.45340000	4.59630000	2.51740000
H	-1.62910000	-0.10260000	2.82170000
B	0.00000000	3.09820000	0.00000000
N	-1.58260000	-1.18400000	0.00000000
N	-1.43760000	-2.52670000	0.00000000
N	0.79130000	-1.18400000	-1.37060000
N	0.71880000	-2.52670000	-1.24500000
N	0.79130000	-1.18400000	1.37060000
N	0.71880000	-2.52670000	1.24500000
C	-2.90130000	-0.91790000	0.00000000
C	-3.62400000	-2.10170000	0.00000000
C	-2.65970000	-3.10540000	0.00000000
C	1.45060000	-0.91790000	-2.51260000
C	1.81200000	-2.10170000	-3.13850000
C	1.32980000	-3.10540000	-2.30330000
C	1.45060000	-0.91790000	2.51260000
C	1.81200000	-2.10170000	3.13850000
C	1.32980000	-3.10540000	2.30330000
H	-4.69940000	-2.22570000	0.00000000
C	-2.90690000	-4.59630000	0.00000000
H	2.34970000	-2.22570000	-4.06980000
H	1.62910000	0.10260000	-2.82170000
C	1.45340000	-4.59630000	-2.51740000
H	-3.25820000	0.10260000	0.00000000

H	0.00000000	-4.28250000	0.00000000
H	2.34970000	-2.22570000	4.06980000
C	1.45340000	-4.59630000	2.51740000
H	1.62910000	0.10260000	2.82170000
B	0.00000000	-3.09820000	0.00000000
F	2.11740000	-4.82510000	3.66740000
F	2.13600000	-5.19370000	1.52040000
F	0.24870000	-5.19370000	2.61010000
F	2.11740000	-4.82510000	-3.66740000
F	0.24870000	-5.19370000	-2.61010000
F	2.13600000	-5.19370000	-1.52040000
F	-2.38470000	-5.19370000	-1.08970000
F	-4.23480000	-4.82510000	0.00000000
F	-2.38470000	-5.19370000	1.08970000
F	-0.24870000	5.19370000	2.61010000
F	-2.11740000	4.82510000	3.66740000
F	-2.13600000	5.19370000	1.52040000
F	2.38470000	5.19370000	1.08970000
F	2.38470000	5.19370000	-1.08970000
F	4.23480000	4.82510000	0.00000000
F	-0.24870000	5.19370000	-2.61010000
F	-2.13600000	5.19370000	-1.52040000
F	-2.11740000	4.82510000	-3.66740000

$[Mn(Tb^{5NH2})_2]^+$ ^5E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.64884487	-1.29831997
N	0.00000000	1.44690342	-2.64793839
N	-1.42794141	-0.82442217	-1.29831997
N	-1.25305521	-0.72345198	-2.64793839
N	1.42794141	-0.82442217	-1.29831997
N	1.25305521	-0.72345198	-2.64793839
C	0.00000000	2.96955274	-1.09806607
C	0.00000000	3.65128386	-2.30795947
C	0.00000000	2.64458394	-3.28225998
C	-2.57170829	-1.48477611	-1.09806607
C	-3.16210447	-1.82564193	-2.30795947
C	-2.29027701	-1.32229223	-3.28225998
C	2.57170829	-1.48477611	-1.09806607
C	3.16210447	-1.82564193	-2.30795947
C	2.29027701	-1.32229223	-3.28225998
H	0.00000000	4.72254234	-2.46927969
N	0.00000000	2.77491553	-4.63498097
H	-4.08984162	-2.36127143	-2.46927969
H	-2.91630322	-1.68372876	-0.09173711
N	-2.40314735	-1.38745777	-4.63498097
H	0.00000000	3.36745699	-0.09173711
H	0.00000000	0.00000000	-4.38239673
H	4.08984162	-2.36127143	-2.46927969
N	2.40314735	-1.38745777	-4.63498097
H	2.91630322	-1.68372876	-0.09173711
B	0.00000000	0.00000000	-3.17447875
N	1.42794141	0.82442217	1.29831997
N	1.25305521	0.72345198	2.64793839
N	-1.42794141	0.82442217	1.29831997
N	-1.25305521	0.72345198	2.64793839
N	0.00000000	-1.64884487	1.29831997
N	0.00000000	-1.44690342	2.64793839
C	2.57170829	1.48477611	1.09806607
C	3.16210447	1.82564193	2.30795947
C	2.29027701	1.32229223	3.28225998
C	-2.57170829	1.48477611	1.09806607
C	-3.16210447	1.82564193	2.30795947
C	-2.29027701	1.32229223	3.28225998
C	0.00000000	-2.96955274	1.09806607
C	0.00000000	-3.65128386	2.30795947
C	0.00000000	-2.64458394	3.28225998
H	4.08984162	2.36127143	2.46927969
N	2.40314735	1.38745777	4.63498097
H	-4.08984162	2.36127143	2.46927969
H	-2.91630322	1.68372876	0.09173711
N	-2.40314735	1.38745777	4.63498097
H	2.91630322	1.68372876	0.09173711
H	0.00000000	0.00000000	4.38239673
H	0.00000000	-4.72254234	2.46927969
N	0.00000000	-2.77491553	4.63498097
H	0.00000000	-3.36745699	0.09173711
B	0.00000000	0.00000000	3.17447875
H	0.00000000	3.69004080	-5.04441599
H	0.00000000	1.97736710	-5.24081166
H	-3.19566912	-1.84502040	-5.04441599
H	-1.71245039	-0.98868355	-5.24081166
H	3.19566912	-1.84502040	-5.04441599
H	1.71245039	-0.98868355	-5.24081166
H	3.19566912	1.84502040	5.04441599
H	1.71245039	0.98868355	5.24081166
H	-3.19566912	1.84502040	5.04441599
H	-1.71245039	0.98868355	5.24081166
H	0.00000000	-3.69004080	5.04441599
H	0.00000000	-1.97736710	5.24081166

$[Mn(Tb^{5NH2})_2]^+$ $^3A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.58975217	-1.18458391
N	0.00000000	1.43529063	-2.54114249
N	-1.37676574	-0.79487609	-1.18458391
N	-1.24299820	-0.71764531	-2.54114249
N	1.37676574	-0.79487609	-1.18458391
N	1.24299820	-0.71764531	-2.54114249
C	0.00000000	2.90623563	-0.94384848
C	0.00000000	3.62549440	-2.13054857
C	0.00000000	2.64960054	-3.13688864
C	-2.51687389	-1.45311808	-0.94384848
C	-3.13977054	-1.81274747	-2.13054857
C	-2.29462103	-1.32480000	-3.13688864
C	2.51687389	-1.45311808	-0.94384848
C	3.13977054	-1.81274747	-2.13054857
C	2.29462103	-1.32480000	-3.13688864
H	0.00000000	4.70132445	-2.25752888
N	0.00000000	2.81872929	-4.48473485
H	-4.07146647	-2.35066249	-2.25752888
H	-2.83485438	-1.63670395	0.07301323
N	-2.44109094	-1.40936465	-4.48473485
H	0.00000000	3.27340791	0.07301323
H	0.00000000	0.00000000	-4.29279644
H	4.07146647	-2.35066249	-2.25752888
N	2.44109094	-1.40936465	-4.48473485
H	2.83485438	-1.63670395	0.07301323

B	0.00000000	0.00000000	-3.08425138
N	1.37676574	0.79487609	1.18458391
N	1.24299820	0.71764531	2.54114249
N	-1.37676574	0.79487609	1.18458391
N	-1.24299820	0.71764531	2.54114249
N	0.00000000	-1.58975217	1.18458391
N	0.00000000	-1.43529063	2.54114249
C	2.51687389	1.45311808	0.94384848
C	3.13977054	1.81274747	2.13054857
C	2.29462103	1.32480000	3.13688864
C	-2.51687389	1.45311808	0.94384848
C	-3.13977054	1.81274747	2.13054857
C	-2.29462103	1.32480000	3.13688864
C	0.00000000	-2.90623563	0.94384848
C	0.00000000	-3.62549440	2.13054857
C	0.00000000	-2.64960054	3.13688864
H	4.07146647	2.35066249	2.25752888
N	2.44109094	1.40936465	4.48473485
H	-4.07146647	2.35066249	2.25752888
H	-2.83485438	1.63670395	-0.07301323
N	-2.44109094	1.40936465	4.48473485
H	2.83485438	1.63670395	-0.07301323
H	0.00000000	0.00000000	4.29279644
H	0.00000000	-4.70132445	2.25752888
N	0.00000000	-2.81872929	4.48473485
H	0.00000000	-3.27340791	-0.07301323
B	0.00000000	0.00000000	3.08425138
H	0.00000000	3.74493500	-4.86850530
H	0.00000000	2.03826429	-5.11289470
H	-3.24320882	-1.87246723	-4.86850530
H	-1.76518872	-1.01913241	-5.11289470
H	3.24320882	-1.87246723	-4.86850530
H	1.76518872	-1.01913241	-5.11289470
H	3.24320882	1.87246723	4.86850530
H	1.76518872	1.01913241	5.11289470
H	-3.24320882	1.87246723	4.86850530
H	-1.76518872	1.01913241	5.11289470
H	0.00000000	-3.74493500	4.86850530
H	0.00000000	-2.03826429	5.11289470

$[Mn(Tb^{5NH2})_2]^+$ ^1E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.58050000	1.16930000	0.00000000
N	1.43470000	2.52710000	0.00000000
N	-0.79030000	1.16930000	1.36880000
N	-0.71740000	2.52710000	1.24250000
N	-0.79030000	1.16930000	-1.36880000
N	-0.71740000	2.52710000	-1.24250000
C	2.89740000	0.92270000	0.00000000
C	3.62380000	2.10490000	0.00000000
C	2.65230000	3.11620000	0.00000000
C	-1.44870000	0.92270000	2.50920000
C	-1.81190000	2.10490000	3.13830000
C	-1.32620000	3.11620000	2.29700000
C	-1.44870000	0.92270000	-2.50920000
C	-1.81190000	2.10490000	-3.13830000
C	-1.32620000	3.11620000	-2.29700000
H	4.70020000	2.22740000	0.00000000
N	2.83180000	4.46170000	0.00000000
H	-2.35010000	2.22740000	4.07050000
H	-1.62940000	-0.09600000	2.82220000
N	-1.41590000	4.46170000	2.45240000
H	3.25880000	-0.09600000	0.00000000
H	0.00000000	4.28300000	0.00000000
H	-2.35010000	2.22740000	-4.07050000
N	-1.41590000	4.46170000	-2.45240000
H	-1.62940000	-0.09600000	-2.82220000
B	0.00000000	3.07350000	0.00000000
N	0.79030000	-1.16930000	-1.36880000
N	0.71740000	-2.52710000	-1.24250000
N	0.79030000	-1.16930000	1.36880000
N	0.71740000	-2.52710000	1.24250000
N	-1.58050000	-1.16930000	0.00000000
N	-1.43470000	-2.52710000	0.00000000
C	1.44870000	-0.92270000	-2.50920000
C	1.81190000	-2.10490000	-3.13830000
C	1.32620000	-3.11620000	-2.29700000
C	1.44870000	-0.92270000	2.50920000
C	1.81190000	-2.10490000	3.13830000
C	1.32620000	-3.11620000	2.29700000
C	-2.89740000	-0.92270000	0.00000000
C	-3.62380000	-2.10490000	0.00000000
C	-2.65230000	-3.11620000	0.00000000
H	2.35010000	-2.22740000	-4.07050000
N	1.41590000	-4.46170000	-2.45240000
H	2.35010000	-2.22740000	4.07050000
H	1.62940000	0.09600000	2.82220000
N	1.41590000	-4.46170000	2.45240000
H	1.62940000	0.09600000	-2.82220000
H	0.00000000	-4.28300000	0.00000000
H	-4.70020000	-2.22740000	0.00000000
N	-2.83180000	-4.46170000	0.00000000
H	-3.25880000	0.09600000	0.00000000
B	0.00000000	-3.07350000	0.00000000
H	3.76080000	4.83900000	0.00000000
H	2.05540000	5.09530000	0.00000000
H	-1.88040000	4.83900000	3.25690000
H	-1.02770000	5.09530000	1.78000000
H	-1.88040000	4.83900000	-3.25690000
H	-1.02770000	5.09530000	-1.78000000
H	1.88040000	-4.83900000	-3.25690000
H	1.02770000	-5.09530000	-1.78000000
H	1.88040000	-4.83900000	3.25690000
H	1.02770000	-5.09530000	1.78000000
H	-3.76080000	-4.83900000	0.00000000
H	-2.05540000	-5.09530000	0.00000000

$[Mn(Tb^{5NO2})_2]^+$ ^5E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.42568976	-0.82312251	-1.29029341
N	-1.26541732	-0.73058899	-2.62361741
N	1.42568976	-0.82312251	-1.29029341
N	1.26541732	-0.73058899	-2.62361741
N	0.00000000	1.64624502	-1.29029341
N	0.00000000	1.46117798	-2.62361741
C	-2.56553597	-1.48121316	-1.03122834
C	-3.18046004	-1.83623976	-2.21987422
C	-2.33129672	-1.34597503	-3.19997028

C	2.56553597	-1.48121316	-1.03122834
C	3.18046004	-1.83623976	-2.21987422
C	2.33129672	-1.34597503	-3.19997028
C	0.00000000	2.96242578	-1.03122834
C	0.00000000	3.67247899	-2.21987422
C	0.00000000	2.69194953	-3.19997028
H	-4.10730817	-2.37135544	-2.37583863
N	-2.59101374	-1.49592217	-4.63571335
H	4.10730817	-2.37135544	-2.37583863
H	2.87972808	-1.66261194	-0.01181759
N	2.59101374	-1.49592217	-4.63571335
H	-2.87972808	-1.66261194	-0.01181759
H	0.00000000	0.00000000	-4.34898236
H	0.00000000	4.74271087	-2.37583863
N	0.00000000	2.99184486	-4.63571335
H	0.00000000	3.32522336	-0.01181759
B	0.00000000	0.00000000	-3.18202958
N	-1.42568976	0.82312251	1.29029341
N	-1.26541732	0.73058899	2.62361741
N	0.00000000	-1.64624502	1.29029341
N	0.00000000	-1.46117798	2.62361741
N	1.42568976	0.82312251	1.29029341
N	1.26541732	0.73058899	2.62361741
C	-2.56553597	1.48121316	1.03122834
C	-3.18046004	1.83623976	2.21987422
C	-2.33129672	1.34597503	3.19997028
C	0.00000000	-2.96242578	1.03122834
C	0.00000000	-3.67247899	2.21987422
C	0.00000000	-2.69194953	3.19997028
C	2.56553597	1.48121316	1.03122834
C	3.18046004	1.83623976	2.21987422
C	2.33129672	1.34597503	3.19997028
H	-4.10730817	2.37135544	2.37583863
N	-2.59101374	1.49592217	4.63571335
H	0.00000000	-4.74271087	2.37583863
H	0.00000000	-3.32522336	0.01181759
N	0.00000000	-2.99184486	4.63571335
H	-2.87972808	1.66261194	0.01181759
H	0.00000000	0.00000000	4.34898236
H	4.10730817	2.37135544	2.37583863
N	2.59101374	1.49592217	4.63571335
H	2.87972808	1.66261194	0.01181759
B	0.00000000	0.00000000	3.18202958
O	-3.62716449	-2.09414435	-4.88817376
O	-1.79824272	-1.03821613	-5.43618601
O	3.62716449	-2.09414435	-4.88817376
O	1.79824272	-1.03821613	-5.43618601
O	0.00000000	4.18828922	-4.88817376
O	0.00000000	2.07643226	-5.43618601
O	-3.62716449	2.09414435	4.88817376
O	-1.79824272	1.03821613	5.43618601
O	0.00000000	-4.18828922	4.88817376
O	0.00000000	-2.07643226	5.43618601
O	3.62716449	2.09414435	4.88817376
O	1.79824272	1.03821613	5.43618601

$[Mn(Tb^{5NO2})_2]^+$ $^3A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.37703456	-0.79503114	-1.17175983
N	-1.25431942	-0.72418171	-2.51147310
N	1.37703456	-0.79503114	-1.17175983
N	1.25431942	-0.72418171	-2.51147310
N	0.00000000	1.59006280	-1.17175983
N	0.00000000	1.44836342	-2.51147310
C	-2.51372528	-1.45129983	-0.87740869
C	-3.15628828	-1.82228377	-2.04440116
C	-2.33083316	-1.34570727	-3.05279603
C	2.51372528	-1.45129983	-0.87740869
C	3.15628828	-1.82228377	-2.04440116
C	2.33083316	-1.34570727	-3.05279603
C	0.00000000	2.90260018	-0.87740869
C	0.00000000	3.64456807	-2.04440116
C	0.00000000	2.69141454	-3.05279603
H	-4.08664433	-2.35942513	-2.16959920
N	-2.61657511	-1.51068039	-4.48118830
H	4.08664433	-2.35942513	-2.16959920
H	2.80579990	-1.61992956	0.14976245
N	2.61657511	-1.51068039	-4.48118830
H	-2.80579990	-1.61992956	0.14976245
H	0.00000000	0.00000000	-4.25422312
H	0.00000000	4.71885027	-2.16959920
N	0.00000000	3.02136078	-4.48118830
H	0.00000000	3.23985860	0.14976245
B	0.00000000	0.00000000	-3.08709359
N	-1.37703456	0.79503114	1.17175983
N	-1.25431942	0.72418171	2.51147310
N	0.00000000	-1.59006280	1.17175983
N	0.00000000	-1.44836342	2.51147310
N	1.37703456	0.79503114	1.17175983
N	1.25431942	0.72418171	2.51147310
C	-2.51372528	1.45129983	0.87740869
C	-3.15628828	1.82228377	2.04440116
C	-2.33083316	1.34570727	3.05279603
C	0.00000000	-2.90260018	0.87740869
C	0.00000000	-3.64456807	2.04440116
C	0.00000000	-2.69141454	3.05279603
C	2.51372528	1.45129983	0.87740869
C	3.15628828	1.82228377	2.04440116
C	2.33083316	1.34570727	3.05279603
H	-4.08664433	2.35942513	2.16959920
N	-2.61657511	1.51068039	4.48118830
H	0.00000000	-4.71885027	2.16959920
H	0.00000000	-3.23985860	-0.14976245
N	0.00000000	-3.02136078	4.48118830
H	-2.80579990	1.61992956	-0.14976245
H	0.00000000	0.00000000	4.25422312
H	4.08664433	2.35942513	2.16959920
N	2.61657511	1.51068039	4.48118830
H	2.80579990	1.61992956	-0.14976245
B	0.00000000	0.00000000	3.08709359
O	-3.65615282	-2.11088064	-4.71120048
O	-1.83484591	-1.05934882	-5.29659117
O	3.65615282	-2.11088064	-4.71120048
O	1.83484591	-1.05934882	-5.29659117
O	0.00000000	4.22176127	-4.71120048
O	0.00000000	2.11869764	-5.29659117
O	-3.65615282	2.11088064	4.71120048
O	-1.83484591	1.05934882	5.29659117
O	0.00000000	-4.22176127	4.71120048

O	0.00000000	-2.11869764	5.29659117
O	3.65615282	2.11088064	4.71120048
O	1.83484591	1.05934882	5.29659117

$[Mn(Tb^{5NO2})_2]^+$ ^1E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-0.78760000	1.15810000	1.36420000
N	-0.72320000	2.50090000	1.25270000
N	-0.78760000	1.15810000	-1.36420000
N	-0.72320000	2.50090000	-1.25270000
N	1.57530000	1.15810000	0.00000000
N	1.44640000	2.50090000	0.00000000
C	-1.44410000	0.85350000	2.50130000
C	-1.81970000	2.01310000	3.15180000
C	-1.34690000	3.03120000	2.33290000
C	-1.44410000	0.85350000	-2.50130000
C	-1.81970000	2.01310000	-3.15180000
C	-1.34690000	3.03120000	-2.33290000
C	2.88830000	0.85350000	0.00000000
C	3.63940000	2.01310000	0.00000000
C	2.69380000	3.03120000	0.00000000
H	-2.35720000	2.13090000	4.08290000
N	-1.51870000	4.45560000	2.63050000
H	-2.35720000	2.13090000	-4.08290000
H	-1.60820000	-0.17640000	-2.78540000
N	-1.51870000	4.45560000	-2.63050000
H	-1.60820000	-0.17640000	2.78540000
H	0.00000000	4.24870000	0.00000000
H	4.71450000	2.13090000	0.00000000
N	3.03750000	4.45560000	0.00000000
H	3.21640000	-0.17640000	0.00000000
B	0.00000000	3.08080000	0.00000000
N	0.78760000	-1.15810000	1.36420000
N	0.72320000	-2.50090000	1.25270000
N	-1.57530000	-1.15810000	0.00000000
N	-1.44640000	-2.50090000	0.00000000
N	0.78760000	-1.15810000	-1.36420000
N	0.72320000	-2.50090000	-1.25270000
C	1.44410000	-0.85350000	2.50130000
C	1.81970000	-2.01310000	3.15180000
C	1.34690000	-3.03120000	2.33290000
C	-2.88830000	-0.85350000	0.00000000
C	-3.63940000	-2.01310000	0.00000000
C	-2.69380000	-3.03120000	0.00000000
C	1.44410000	-0.85350000	-2.50130000
C	1.81970000	-2.01310000	-3.15180000
C	1.34690000	-3.03120000	-2.33290000
H	2.35720000	-2.13090000	4.08290000
N	1.51870000	-4.45560000	2.63050000
H	-4.71450000	-2.13090000	0.00000000
H	-3.21640000	0.17640000	0.00000000
N	-3.03750000	-4.45560000	0.00000000
H	1.60820000	0.17640000	2.78540000
H	0.00000000	-4.24870000	0.00000000
H	2.35720000	-2.13090000	-4.08290000
N	1.51870000	-4.45560000	-2.63050000
H	1.60820000	0.17640000	-2.78540000
B	0.00000000	-3.08080000	0.00000000
O	-2.12030000	4.67480000	3.67250000
O	-1.07180000	5.28100000	1.85640000
O	-2.12030000	4.67480000	-3.67250000
O	-1.07180000	5.28100000	-1.85640000
O	4.24060000	4.67480000	0.00000000
O	2.14350000	5.28100000	0.00000000
O	2.12030000	-4.67480000	3.67250000
O	1.07180000	-5.28100000	1.85640000
O	-4.24060000	-4.67480000	0.00000000
O	-2.14350000	-5.28100000	0.00000000
O	2.12030000	-4.67480000	-3.67250000
O	1.07180000	-5.28100000	-1.85640000

$[Mn(Tb^{3,5\text{-}CH3})_2]^+$ ^5E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.48930000	0.85990000	1.28840000
N	1.26080000	0.72790000	2.61830000
N	0.00000000	-1.71970000	1.28840000
N	0.00000000	-1.45580000	2.61830000
N	-1.48930000	0.85990000	1.28840000
N	-1.26080000	0.72790000	2.61830000
C	2.65370000	1.53210000	1.13870000
C	3.16040000	1.82470000	2.40800000
C	2.25960000	1.30460000	3.32630000
C	0.00000000	-3.06420000	1.13870000
C	0.00000000	-3.64940000	2.40800000
C	0.00000000	-2.60920000	3.32630000
C	-2.65370000	1.53210000	1.13870000
C	-3.16040000	1.82470000	2.40800000
C	-2.25960000	1.30460000	3.32630000
H	4.07930000	2.35520000	2.63010000
C	2.33130000	1.34600000	4.81240000
H	0.00000000	-4.71040000	2.63010000
C	0.00000000	-3.79900000	-0.15570000
C	0.00000000	-2.69190000	4.81240000
C	3.29000000	1.89950000	-0.15570000
H	0.00000000	0.00000000	4.32080000
H	-4.07930000	2.35520000	2.63010000
C	-2.33130000	1.34600000	4.81240000
C	-3.29000000	1.89950000	-0.15570000
B	0.00000000	0.00000000	3.12670000
N	0.00000000	1.71970000	-1.28840000
N	0.00000000	1.45580000	-2.61830000
N	1.48930000	-0.85990000	-1.28840000
N	1.26080000	-0.72790000	-2.61830000
N	-1.48930000	-0.85990000	-1.28840000
N	-1.26080000	-0.72790000	-2.61830000
C	0.00000000	3.06420000	-1.13870000
C	0.00000000	3.64940000	-2.40800000
C	0.00000000	2.60920000	-3.32630000
C	2.65370000	-1.53210000	-1.13870000
C	3.16040000	-1.82470000	-2.40800000
C	2.25960000	-1.30460000	-3.32630000
C	-2.65370000	-1.53210000	-1.13870000
C	-3.16040000	-1.82470000	-2.40800000
C	-2.25960000	-1.30460000	-3.32630000
H	0.00000000	4.71040000	-2.63010000
C	0.00000000	2.69190000	-4.81240000
H	4.07930000	-2.35520000	-2.63010000
C	3.29000000	-1.89950000	0.15570000

C	2.33130000	-1.34600000	-4.81240000
C	0.00000000	3.79900000	0.15570000
H	0.00000000	0.00000000	-4.32080000
H	-4.07930000	-2.35520000	-2.63010000
C	-2.33130000	-1.34600000	-4.81240000
C	-3.29000000	-1.89950000	0.15570000
B	0.00000000	0.00000000	-3.12670000
H	-0.87870000	-3.57090000	-0.76370000
H	0.00000000	-4.87280000	0.04690000
H	0.87870000	-3.57090000	-0.76370000
H	4.22000000	2.43640000	0.04690000
H	2.65320000	2.54650000	-0.76370000
H	3.53190000	1.02450000	-0.76370000
H	-4.22000000	2.43640000	0.04690000
H	-3.53190000	1.02450000	-0.76370000
H	-2.65320000	2.54650000	-0.76370000
H	3.53190000	-1.02450000	0.76370000
H	4.22000000	-2.43640000	-0.04690000
H	2.65320000	-2.54650000	0.76370000
H	-2.65320000	-2.54650000	0.76370000
H	-4.22000000	-2.43640000	-0.04690000
H	-3.53190000	-1.02450000	0.76370000
H	-0.87870000	3.57090000	0.76370000
H	0.00000000	4.87280000	-0.04690000
H	0.87870000	3.57090000	0.76370000
H	-3.24100000	-1.87120000	-5.11350000
H	-1.47910000	-1.87500000	-5.25110000
H	-2.36340000	-0.34350000	-5.25110000
H	3.24100000	-1.87120000	-5.11350000
H	2.36340000	-0.34350000	-5.25110000
H	1.47910000	-1.87500000	-5.25110000
H	0.88430000	2.21850000	-5.25110000
H	0.00000000	3.74230000	-5.11350000
H	-0.88430000	2.21850000	-5.25110000
H	-2.36340000	0.34350000	5.25110000
H	-3.24100000	1.87120000	5.11350000
H	-1.47910000	1.87500000	5.25110000
H	-0.88430000	-2.21850000	5.25110000
H	0.88430000	-2.21850000	5.25110000
H	0.00000000	-3.74230000	5.11350000
H	2.36340000	0.34350000	5.25110000
H	1.47910000	1.87500000	5.25110000
H	3.24100000	1.87120000	5.11350000

$[Mn(Tb^{3,5\text{-}CH3})_2]^+$ $^3A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.43180000	0.82670000	1.17360000
N	1.24790000	0.72050000	2.51260000
N	0.00000000	-1.65340000	1.17360000
N	0.00000000	-1.44100000	2.51260000
N	-1.43180000	0.82670000	1.17360000
N	-1.24790000	0.72050000	2.51260000
C	2.59590000	1.49870000	0.98070000
C	3.13690000	1.81110000	2.23030000
C	2.26270000	1.30640000	3.18300000
C	0.00000000	-2.99750000	0.98070000
C	0.00000000	-3.62220000	2.23030000
C	0.00000000	-2.61280000	3.18300000
C	-2.59590000	1.49870000	0.98070000
C	-3.13690000	1.81110000	2.23030000
C	-2.26270000	1.30640000	3.18300000
H	4.06170000	2.34500000	2.41630000
C	2.36810000	1.36720000	4.66630000
H	0.00000000	-4.69010000	2.41630000
C	0.00000000	-3.70790000	-0.32610000
C	0.00000000	-2.73450000	4.66630000
C	3.21120000	1.85400000	-0.32610000
H	0.00000000	0.00000000	4.23360000
H	-4.06170000	2.34500000	2.41630000
C	-2.36810000	1.36720000	4.66630000
C	-3.21120000	1.85400000	-0.32610000
B	0.00000000	0.00000000	3.03880000
N	0.00000000	1.65340000	-1.17360000
N	0.00000000	1.44100000	-2.51260000
N	1.43180000	-0.82670000	-1.17360000
N	1.24790000	-0.72050000	-2.51260000
N	-1.43180000	-0.82670000	-1.17360000
N	-1.24790000	-0.72050000	-2.51260000
C	0.00000000	2.99750000	-0.98070000
C	0.00000000	3.62220000	-2.23030000
C	0.00000000	2.61280000	-3.18300000
C	2.59590000	-1.49870000	-0.98070000
C	3.13690000	-1.81110000	-2.23030000
C	2.26270000	-1.30640000	-3.18300000
C	-2.59590000	-1.49870000	-0.98070000
C	-3.13690000	-1.81110000	-2.23030000
C	-2.26270000	-1.30640000	-3.18300000
H	0.00000000	4.69010000	-2.41630000
C	0.00000000	2.73450000	-4.66630000
H	4.06170000	-2.34500000	-2.41630000
C	3.21120000	-1.85400000	0.32610000
C	2.36810000	-1.36720000	-4.66630000
C	0.00000000	3.70790000	0.32610000
H	0.00000000	0.00000000	-4.23360000
H	-4.06170000	-2.34500000	-2.41630000
C	-2.36810000	-1.36720000	-4.66630000
C	-3.21120000	-1.85400000	0.32610000
B	0.00000000	0.00000000	-3.03880000
H	-0.88000000	-3.47120000	-0.92900000
H	0.00000000	-4.78480000	-0.13890000
H	0.88000000	-3.47120000	-0.92900000
H	4.14370000	2.39240000	-0.13890000
H	2.56610000	2.49770000	-0.92900000
H	3.44620000	0.97350000	-0.92900000
H	-4.14370000	2.39240000	-0.13890000
H	-3.44620000	0.97350000	-0.92900000
H	-2.56610000	2.49770000	-0.92900000
H	3.44620000	-0.97350000	0.92900000
H	4.14370000	-2.39240000	0.13890000
H	2.56610000	-2.49770000	0.92900000
H	-2.56610000	-2.49770000	0.92900000
H	-4.14370000	-2.39240000	0.13890000
H	-3.44620000	-0.97350000	0.92900000
H	-0.88000000	3.47120000	0.92900000
H	0.00000000	4.78480000	0.13890000
H	0.88000000	3.47120000	0.92900000
H	-3.28370000	-1.89580000	-4.94230000
H	-1.52390000	-1.90060000	-5.11580000
H	-2.40790000	-0.36940000	-5.11580000

H	3.28370000	-1.89580000	-4.94230000
H	2.40790000	-0.36940000	-5.11580000
H	1.52390000	-1.90060000	-5.11580000
H	0.88410000	2.27000000	-5.11580000
H	0.00000000	3.79170000	-4.94230000
H	-0.88410000	2.27000000	-5.11580000
H	-2.40790000	0.36940000	5.11580000
H	-3.28370000	1.89580000	4.94230000
H	-1.52390000	1.90060000	5.11580000
H	-0.88410000	-2.27000000	5.11580000
H	0.88410000	-2.27000000	5.11580000
H	0.00000000	-3.79170000	4.94230000
H	2.40790000	0.36940000	5.11580000
H	1.52390000	1.90060000	5.11580000
H	3.28370000	1.89580000	4.94230000

$[Mn(Tb^{3,5\text{-}CH3})_2]^+$ ^1E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.37390000	0.79320000	-1.12580000
N	-1.22550000	0.70760000	-2.46760000
N	0.00000000	-1.58640000	-1.12580000
N	0.00000000	-1.41510000	-2.46760000
N	1.37390000	0.79320000	-1.12580000
N	1.22550000	0.70760000	-2.46760000
C	-2.52750000	1.45930000	-0.89290000
C	-3.10080000	1.79030000	-2.11730000
C	-2.25230000	1.30030000	-3.09800000
C	0.00000000	-2.91850000	-0.89290000
C	0.00000000	-3.58050000	-2.11730000
C	0.00000000	-2.60070000	-3.09800000
C	2.52750000	1.45930000	-0.89290000
C	3.10080000	1.79030000	-2.11730000
C	2.25230000	1.30030000	-3.09800000
H	-4.03460000	2.32940000	-2.27160000
C	-2.36310000	1.36430000	-4.56540000
H	0.00000000	-4.65880000	-2.27160000
C	0.00000000	-3.53960000	0.44150000
C	0.00000000	-2.72870000	-4.56540000
C	-3.06540000	1.76980000	0.44150000
H	0.00000000	0.00000000	-4.21510000
H	4.03460000	2.32940000	-2.27160000
C	2.36310000	1.36430000	-4.56540000
C	3.06540000	1.76980000	0.44150000
B	0.00000000	0.00000000	-3.01260000
N	0.00000000	1.58640000	1.12580000
N	0.00000000	1.41510000	2.46760000
N	-1.37390000	-0.79320000	1.12580000
N	-1.22550000	-0.70760000	2.46760000
N	1.37390000	-0.79320000	1.12580000
N	1.22550000	-0.70760000	2.46760000
C	0.00000000	2.91850000	0.89290000
C	0.00000000	3.58050000	2.11730000
C	0.00000000	2.60070000	3.09800000
C	-2.52750000	-1.45930000	0.89290000
C	-3.10080000	-1.79030000	2.11730000
C	-2.25230000	-1.30030000	3.09800000
C	2.52750000	-1.45930000	0.89290000
C	3.10080000	-1.79030000	2.11730000
C	2.25230000	-1.30030000	3.09800000
H	0.00000000	4.65880000	2.27160000
C	0.00000000	2.72870000	4.56540000
H	-4.03460000	-2.32940000	2.27160000
C	-3.06540000	-1.76980000	-0.44150000
C	-2.36310000	-1.36430000	4.56540000
C	0.00000000	3.53960000	-0.44150000
H	0.00000000	0.00000000	4.21510000
H	4.03460000	-2.32940000	2.27160000
C	2.36310000	-1.36430000	4.56540000
C	3.06540000	-1.76980000	-0.44150000
B	0.00000000	0.00000000	3.01260000
H	0.88690000	-3.24900000	1.03090000
H	0.00000000	-4.63250000	0.33380000
H	-0.88690000	-3.24900000	1.03090000
H	-4.01190000	2.31630000	0.33380000
H	-2.37030000	2.39260000	1.03090000
H	-3.25720000	0.85640000	1.03090000
H	4.01190000	2.31630000	0.33380000
H	3.25720000	0.85640000	1.03090000
H	2.37030000	2.39260000	1.03090000
H	-3.25720000	-0.85640000	-1.03090000
H	-4.01190000	-2.31630000	-0.33380000
H	-2.37030000	-2.39260000	-1.03090000
H	2.37030000	-2.39260000	-1.03090000
H	4.01190000	-2.31630000	-0.33380000
H	3.25720000	-0.85640000	-1.03090000
H	0.88690000	3.24900000	-1.03090000
H	0.00000000	4.63250000	-0.33380000
H	-0.88690000	3.24900000	-1.03090000
H	3.28140000	-1.89450000	4.84940000
H	1.50760000	-1.89380000	5.01430000
H	2.39390000	-0.35880000	5.01430000
H	-3.28140000	-1.89450000	4.84940000
H	-2.39390000	-0.35880000	5.01430000
H	-1.50760000	-1.89380000	5.01430000
H	-0.88620000	2.25250000	5.01430000
H	0.00000000	3.78900000	4.84940000
H	0.88620000	2.25250000	5.01430000
H	2.39390000	0.35880000	-5.01430000
H	3.28140000	1.89450000	-4.84940000
H	1.50760000	1.89380000	-5.01430000
H	0.88620000	-2.25250000	-5.01430000
H	-0.88620000	-2.25250000	-5.01430000
H	0.00000000	-3.78900000	-4.84940000
H	-2.39390000	0.35880000	-5.01430000
H	-1.50760000	1.89380000	-5.01430000
H	-3.28140000	1.89450000	-4.84940000

$[Mn(Tb^{3,5\text{-}CF3})_2]^+$ ^5E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.54539601	0.89223465	1.22369064
N	1.28546573	0.74216421	2.54388098
N	0.00000000	-1.78446929	1.22369064
N	0.00000000	-1.48432842	2.54388098
N	-1.54539601	0.89223465	1.22369064
N	-1.28546573	0.74216421	2.54388098
C	2.71833749	1.56943283	1.11448274
C	3.20260875	1.84902733	2.38634332
C	2.28144187	1.31719096	3.26474528

C	0.00000000	-3.13886565	1.11448274
C	0.00000000	-3.69805413	2.38634332
C	0.00000000	-2.63438193	3.26474528
C	-2.71833749	1.56943283	1.11448274
C	-3.20260875	1.84902733	2.38634332
C	-2.28144187	1.31719096	3.26474528
H	4.11194535	2.37403254	2.64002296
C	2.41235926	1.39277653	4.77275226
H	0.00000000	-4.74806562	2.64002296
C	0.00000000	-4.03883951	-0.12690517
C	0.00000000	-2.78555252	4.77275226
C	3.49773778	2.01941976	-0.12690517
H	0.00000000	0.00000000	4.22569835
H	-4.11194535	2.37403254	2.64002296
C	-2.41235926	1.39277653	4.77275226
C	-3.49773778	2.01941976	-0.12690517
B	0.00000000	0.00000000	3.04092976
N	0.00000000	1.78446929	-1.22369064
N	0.00000000	1.48432842	-2.54388098
N	1.54539601	-0.89223465	-1.22369064
N	1.28546573	-0.74216421	-2.54388098
N	-1.54539601	-0.89223465	-1.22369064
N	-1.28546573	-0.74216421	-2.54388098
C	0.00000000	3.13886565	-1.11448274
C	0.00000000	3.69805413	-2.38634332
C	0.00000000	2.63438193	-3.26474528
C	2.71833749	-1.56943283	-1.11448274
C	3.20260875	-1.84902733	-2.38634332
C	2.28144187	-1.31719096	-3.26474528
C	-2.71833749	-1.56943283	-1.11448274
C	-3.20260875	-1.84902733	-2.38634332
C	-2.28144187	-1.31719096	-3.26474528
H	0.00000000	4.74806562	-2.64002296
C	0.00000000	2.78555252	-4.77275226
H	4.11194535	-2.37403254	-2.64002296
C	3.49773778	-2.01941976	0.12690517
C	2.41235926	-1.39277653	-4.77275226
C	0.00000000	4.03883951	0.12690517
H	0.00000000	0.00000000	-4.22569835
H	-4.11194535	-2.37403254	-2.64002296
C	-2.41235926	-1.39277653	-4.77275226
C	-3.49773778	-2.01941976	0.12690517
B	0.00000000	0.00000000	-3.04092976
F	-1.07809228	-3.88222263	-0.91214864
F	0.00000000	-5.32049993	0.29458398
F	1.07809228	-3.88222263	-0.91214864
F	4.60768812	2.66025023	0.29458398
F	2.82305743	2.87476652	-0.91214864
F	3.90114971	1.00745611	-0.91214864
F	-4.60768812	2.66025023	0.29458398
F	-3.90114971	1.00745611	-0.91214864
F	-2.82305743	2.87476652	-0.91214864
F	3.90114971	-1.00745611	0.91214864
F	4.60768812	-2.66025023	-0.29458398
F	2.82305743	-2.87476652	0.91214864
F	-2.82305743	-2.87476652	0.91214864
F	-4.60768812	-2.66025023	-0.29458398
F	-3.90114971	-1.00745611	0.91214864
F	-1.07809228	3.88222263	0.91214864
F	0.00000000	5.32049993	-0.29458398
F	1.07809228	3.88222263	0.91214864
F	-3.55028244	-2.04975643	-5.07111827
F	-1.39276065	-2.06136711	-5.33875231
F	-2.48157671	-0.17548258	-5.33875231
F	3.55028244	-2.04975643	-5.07111827
F	2.48157671	-0.17548258	-5.33875231
F	1.39276065	-2.06136711	-5.33875231
F	1.08881606	2.23684969	-5.33875231
F	0.00000000	4.09951339	-5.07111827
F	-1.08881606	2.23684969	-5.33875231
F	-2.48157671	0.17548258	5.33875231
F	-3.55028244	2.04975643	5.07111827
F	-1.39276065	2.06136711	5.33875231
F	-1.08881606	-2.23684969	5.33875231
F	1.08881606	-2.23684969	5.33875231
F	0.00000000	-4.09951339	5.07111827
F	2.48157671	0.17548258	5.33875231
F	1.39276065	2.06136711	5.33875231
F	3.55028244	2.04975643	5.07111827

$[Mn(Tb^{3,5\text{-}CF3})_2]^+$ $^3A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.48930639	0.85985164	1.13434647
N	1.27080699	0.73370055	2.46432235
N	0.00000000	-1.71970276	1.13434647
N	0.00000000	-1.46740163	2.46432235
N	-1.48930639	0.85985164	1.13434647
N	-1.27080699	0.73370055	2.46432235
C	2.66711207	1.53985817	0.98829831
C	3.17815018	1.83490623	2.24479106
C	2.27948709	1.31606223	3.15268194
C	0.00000000	-3.07971581	0.98829831
C	0.00000000	-3.66981194	2.24479106
C	0.00000000	-2.63212499	3.15268194
C	-2.66711207	1.53985817	0.98829831
C	-3.17815018	1.83490623	2.24479106
C	-2.27948709	1.31606223	3.15268194
H	4.09242612	2.36276319	2.47128156
C	2.44359395	1.41080983	4.65650261
H	0.00000000	-4.72552637	2.47128156
C	0.00000000	-3.98448137	-0.25366270
C	0.00000000	-2.82161913	4.65650261
C	3.45066165	1.99224068	-0.25366270
H	0.00000000	0.00000000	4.15982478
H	-4.09242612	2.36276319	2.47128156
C	-2.44359395	1.41080983	4.65650261
C	-3.45066165	1.99224068	-0.25366270
B	0.00000000	0.00000000	2.97471222
N	0.00000000	1.71970276	-1.13434647
N	0.00000000	1.46740163	-2.46432235
N	1.48930639	-0.85985164	-1.13434647
N	1.27080699	-0.73370055	-2.46432235
N	-1.48930639	-0.85985164	-1.13434647
N	-1.27080699	-0.73370055	-2.46432235
C	0.00000000	3.07971581	-0.98829831
C	0.00000000	3.66981194	-2.24479106
C	0.00000000	2.63212499	-3.15268194
C	2.66711207	-1.53985817	-0.98829831
C	3.17815018	-1.83490623	-2.24479106

C	2.27948709	-1.31606223	-3.15268194
C	-2.66711207	-1.53985817	-0.98829831
C	-3.17815018	-1.83490623	-2.24479106
C	-2.27948709	-1.31606223	-3.15268194
H	0.00000000	4.72552637	-2.47128156
C	0.00000000	2.82161913	-4.65650261
H	4.09242612	-2.36276319	-2.47128156
C	3.45066165	-1.99224068	0.25366270
C	2.44359395	-1.41080983	-4.65650261
C	0.00000000	3.98448137	0.25366270
H	0.00000000	0.00000000	-4.15982478
H	-4.09242612	-2.36276319	-2.47128156
C	-2.44359395	-1.41080983	-4.65650261
C	-3.45066165	-1.99224068	0.25366270
B	0.00000000	0.00000000	-2.97471222
F	-1.07889822	-3.83759658	-1.03891200
F	0.00000000	-5.26459500	0.17413794
F	1.07889822	-3.83759658	-1.03891200
F	4.55927264	2.63229750	0.17413794
F	2.78400680	2.85315174	-1.03891200
F	3.86290501	0.98444484	-1.03891200
F	-4.55927264	2.63229750	0.17413794
F	-3.86290501	0.98444484	-1.03891200
F	-2.78400680	2.85315174	-1.03891200
F	3.86290501	-0.98444484	1.03891200
F	4.55927264	-2.63229750	-0.17413794
F	2.78400680	-2.85315174	1.03891200
F	-2.78400680	-2.85315174	1.03891200
F	-4.55927264	-2.63229750	-0.17413794
F	-3.86290501	-0.98444484	1.03891200
F	-1.07889822	3.83759658	1.03891200
F	0.00000000	5.26459500	-0.17413794
F	1.07889822	3.83759658	1.03891200
F	-3.58737618	-2.07117276	-4.92178022
F	-1.43590553	-2.08654854	-5.23478115
F	-2.52495707	-0.20025655	-5.23478115
F	3.58737618	-2.07117276	-4.92178022
F	2.52495707	-0.20025655	-5.23478115
F	1.43590553	-2.08654854	-5.23478115
F	1.08905154	2.28680508	-5.23478115
F	0.00000000	4.14234500	-4.92178022
F	-1.08905154	2.28680508	-5.23478115
F	-2.52495707	0.20025655	5.23478115
F	-3.58737618	2.07117276	4.92178022
F	-1.43590553	2.08654854	5.23478115
F	-1.08905154	-2.28680508	5.23478115
F	1.08905154	-2.28680508	5.23478115
F	0.00000000	-4.14234500	4.92178022
F	2.52495707	0.20025655	5.23478115
F	1.43590553	2.08654854	5.23478115
F	3.58737618	2.07117276	4.92178022

$[Mn(Tb^{3,5\text{-}CF3})_2]^+$ ^1E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.85330000	1.12590000	-1.47800000
N	0.73210000	2.45880000	-1.26800000
N	0.85330000	1.12590000	1.47800000
N	0.73210000	2.45880000	1.26800000
N	-1.70660000	1.12590000	0.00000000
N	-1.46420000	2.45880000	0.00000000
C	1.53500000	0.97660000	-2.65860000
C	1.83280000	2.22920000	-3.17450000
C	1.31540000	3.14270000	-2.27830000
C	1.53500000	0.97660000	2.65860000
C	1.83280000	2.22920000	3.17450000
C	1.31540000	3.14270000	2.27830000
C	-3.06990000	0.97660000	0.00000000
C	-3.66560000	2.22920000	0.00000000
C	-2.63080000	3.14270000	0.00000000
H	2.36090000	2.45280000	-4.08920000
C	1.41310000	4.64580000	-2.44750000
H	2.36090000	2.45280000	4.08920000
C	1.98680000	-0.26600000	3.44130000
C	1.41310000	4.64580000	2.44750000
C	1.98680000	-0.26600000	-3.44130000
H	0.00000000	4.15730000	0.00000000
H	-4.72190000	2.45280000	0.00000000
C	-2.82620000	4.64580000	0.00000000
C	-3.97370000	-0.26600000	0.00000000
B	0.00000000	2.97200000	0.00000000
N	-0.85330000	-1.12590000	-1.47800000
N	-0.73210000	-2.45880000	-1.26800000
N	1.70660000	-1.12590000	0.00000000
N	1.46420000	-2.45880000	0.00000000
N	-0.85330000	-1.12590000	1.47800000
N	-0.73210000	-2.45880000	1.26800000
C	-1.53500000	-0.97660000	-2.65860000
C	-1.83280000	-2.22920000	-3.17450000
C	-1.31540000	-3.14270000	-2.27830000
C	3.06990000	-0.97660000	0.00000000
C	3.66560000	-2.22920000	0.00000000
C	2.63080000	-3.14270000	0.00000000
C	-1.53500000	-0.97660000	2.65860000
C	-1.83280000	-2.22920000	3.17450000
C	-1.31540000	-3.14270000	2.27830000
H	-2.36090000	-2.45280000	-4.08920000
C	-1.41310000	-4.64580000	-2.44750000
H	4.72190000	-2.45280000	0.00000000
C	3.97370000	0.26600000	0.00000000
C	2.82620000	-4.64580000	0.00000000
C	-1.98680000	0.26600000	-3.44130000
H	0.00000000	-4.15730000	0.00000000
H	-2.36090000	-2.45280000	4.08920000
C	-1.41310000	-4.64580000	2.44750000
C	-1.98680000	0.26600000	3.44130000
B	0.00000000	-2.97200000	0.00000000
F	0.97970000	-1.05170000	3.85450000
F	2.62730000	0.16090000	4.55060000
F	2.84830000	-1.05170000	2.77570000
F	2.62730000	0.16090000	-4.55060000
F	0.97970000	-1.05170000	-3.85450000
F	2.84830000	-1.05170000	-2.77570000
F	-5.25460000	0.16090000	0.00000000
F	-3.82790000	-1.05170000	1.07880000
F	-3.82790000	-1.05170000	-1.07880000
F	3.82790000	1.05170000	-1.07880000
F	5.25460000	-0.16090000	0.00000000
F	3.82790000	1.05170000	1.07880000
F	-0.97970000	1.05170000	3.85450000

F	-2.62730000	-0.16090000	4.55060000
F	-2.84830000	1.05170000	2.77570000
F	-2.84830000	1.05170000	-2.77570000
F	-2.62730000	-0.16090000	-4.55060000
F	-0.97970000	1.05170000	-3.85450000
F	-2.07380000	-4.90670000	3.59200000
F	-0.20330000	-5.22540000	2.53050000
F	-2.08980000	-5.22540000	1.44130000
F	4.14770000	-4.90670000	0.00000000
F	2.29310000	-5.22540000	-1.08920000
F	2.29310000	-5.22540000	1.08920000
F	-0.20330000	-5.22540000	-2.53050000
F	-2.07380000	-4.90670000	-3.59200000
F	-2.08980000	-5.22540000	-1.44130000
F	-2.29310000	5.22540000	1.08920000
F	-4.14770000	4.90670000	0.00000000
F	-2.29310000	5.22540000	-1.08920000
F	0.20330000	5.22540000	2.53050000
F	2.08980000	5.22540000	1.44130000
F	2.07380000	4.90670000	3.59200000
F	2.08980000	5.22540000	-1.44130000
F	0.20330000	5.22540000	-2.53050000
F	2.07380000	4.90670000	-3.59200000

$[Mn(Tb^{3,5\text{-}NH2})_2]^+$ ^5E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.68401134	1.30442827
N	0.00000000	1.44801152	2.66762643
N	1.45839662	-0.84200567	1.30442827
N	1.25401461	-0.72400549	2.66762643
N	-1.45839662	-0.84200567	1.30442827
N	-1.25401461	-0.72400549	2.66762643
C	0.00000000	3.02690127	1.14759654
C	0.00000000	3.66365496	2.39787780
C	0.00000000	2.62768202	3.32721941
C	2.62137316	-1.51345063	1.14759654
C	3.17281819	-1.83182748	2.39787780
C	2.27563944	-1.31384127	3.32721941
C	-2.62137316	-1.51345063	1.14759654
C	-3.17281819	-1.83182748	2.39787780
C	-2.27563944	-1.31384127	3.32721941
H	0.00000000	4.72820295	2.59816980
N	0.00000000	2.71943394	4.68546501
H	4.09474391	-2.36410147	2.59816980
N	3.12998606	-1.80709850	-0.06960903
N	2.35509911	-1.35971724	4.68546501
N	0.00000000	3.61419647	-0.06960903
H	0.00000000	0.00000000	4.38228137
H	-4.09474391	-2.36410147	2.59816980
N	-2.35509911	-1.35971724	4.68546501
N	-3.12998606	-1.80709850	-0.06960903
B	0.00000000	0.00000000	3.17201331
N	-1.45839662	0.84200567	-1.30442827
N	-1.25401461	0.72400549	-2.66762643
N	1.45839662	0.84200567	-1.30442827
N	1.25401461	0.72400549	-2.66762643
N	0.00000000	-1.68401134	-1.30442827
N	0.00000000	-1.44801152	-2.66762643
C	-2.62137316	1.51345063	-1.14759654
C	-3.17281819	1.83182748	-2.39787780
C	-2.27563944	1.31384127	-3.32721941
C	2.62137316	1.51345063	-1.14759654
C	3.17281819	1.83182748	-2.39787780
C	2.27563944	1.31384127	-3.32721941
C	0.00000000	-3.02690127	-1.14759654
C	0.00000000	-3.66365496	-2.39787780
C	0.00000000	-2.62768202	-3.32721941
H	-4.09474391	2.36410147	-2.59816980
N	-2.35509911	1.35971724	-4.68546501
H	4.09474391	2.36410147	-2.59816980
N	3.12998606	1.80709850	0.06960903
N	2.35509911	1.35971724	-4.68546501
N	-3.12998606	1.80709850	0.06960903
H	0.00000000	0.00000000	-4.38228137
H	0.00000000	-4.72820295	-2.59816980
N	0.00000000	-2.71943394	-4.68546501
N	0.00000000	-3.61419647	0.06960903
B	0.00000000	0.00000000	-3.17201331
H	0.00000000	3.62123770	5.12220081
H	0.00000000	1.90182281	5.26317839
H	3.13608377	-1.81061911	5.12220081
H	1.64702661	-0.95091141	5.26317839
H	-3.13608377	-1.81061911	5.12220081
H	-1.64702661	-0.95091141	5.26317839
H	-3.13608377	1.81061911	-5.12220081
H	-1.64702661	0.95091141	-5.26317839
H	3.13608377	1.81061911	-5.12220081
H	1.64702661	0.95091141	-5.26317839
H	0.00000000	-3.62123770	-5.12220081
H	0.00000000	-1.90182281	-5.26317839
H	0.00000000	4.61297354	-0.14426483
H	3.99495273	-2.30648677	-0.14426483
H	-3.99495273	-2.30648677	-0.14426483
H	-3.99495273	2.30648677	0.14426483
H	3.99495273	2.30648677	0.14426483
H	0.00000000	-4.61297354	0.14426483
H	2.64922800	-1.52953233	-0.90621551
H	0.00000000	3.05906519	-0.90621551
H	-2.64922800	-1.52953233	-0.90621551
H	2.64922800	1.52953233	0.90621551
H	-2.64922800	1.52953233	0.90621551
H	0.00000000	-3.05906519	0.90621551

$[Mn(Tb^{3,5\text{-}NH2})_2]^+$ $^3A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.62091701	1.19304439
N	0.00000000	1.43580128	2.56548623
N	1.40375537	-0.81045877	1.19304439
N	1.24344059	-0.71790091	2.56548623
N	-1.40375537	-0.81045877	1.19304439
N	-1.24344059	-0.71790091	2.56548623
C	0.00000000	2.96326188	0.99546072
C	0.00000000	3.63831584	2.22577454
C	0.00000000	2.63366701	3.18746952
C	2.56625988	-1.48163068	0.99546072
C	3.15087374	-1.81915792	2.22577454
C	2.28082273	-1.31683377	3.18746952
C	-2.56625988	-1.48163068	0.99546072

C	-3.15087374	-1.81915792	2.22577454
C	-2.28082273	-1.31683377	3.18746952
H	0.00000000	4.70884564	2.39063389
N	0.00000000	2.76328316	4.54246756
H	4.07798011	-2.35442282	2.39063389
N	3.05181017	-1.76196338	-0.23191405
N	2.39307340	-1.38164158	4.54246756
N	0.00000000	3.52392677	-0.23191405
H	0.00000000	0.00000000	4.29647422
H	-4.07798011	-2.35442282	2.39063389
N	-2.39307340	-1.38164158	4.54246756
N	-3.05181017	-1.76196338	-0.23191405
B	0.00000000	0.00000000	3.08608287
N	-1.40375537	0.81045877	-1.19304439
N	-1.24344059	0.71790091	-2.56548623
N	1.40375537	0.81045877	-1.19304439
N	1.24344059	0.71790091	-2.56548623
N	0.00000000	-1.62091701	-1.19304439
N	0.00000000	-1.43580128	-2.56548623
C	-2.56625988	1.48163068	-0.99546072
C	-3.15087374	1.81915792	-2.22577454
C	-2.28082273	1.31683377	-3.18746952
C	2.56625988	1.48163068	-0.99546072
C	3.15087374	1.81915792	-2.22577454
C	2.28082273	1.31683377	-3.18746952
C	0.00000000	-2.96326188	-0.99546072
C	0.00000000	-3.63831584	-2.22577454
C	0.00000000	-2.63366701	-3.18746952
H	-4.07798011	2.35442282	-2.39063389
N	-2.39307340	1.38164158	-4.54246756
H	4.07798011	2.35442282	-2.39063389
N	3.05181017	1.76196338	0.23191405
N	2.39307340	1.38164158	-4.54246756
N	-3.05181017	1.76196338	0.23191405
H	0.00000000	0.00000000	-4.29647422
H	0.00000000	-4.70884564	-2.39063389
N	0.00000000	-2.76328316	-4.54246756
N	0.00000000	-3.52392677	0.23191405
B	0.00000000	0.00000000	-3.08608287
H	0.00000000	3.67679232	4.95422513
H	0.00000000	1.96205165	5.14302446
H	3.18419550	-1.83839616	4.95422513
H	1.69918656	-0.98102583	5.14302446
H	-3.18419550	-1.83839616	4.95422513
H	-1.69918656	-0.98102583	5.14302446
H	-3.18419550	1.83839616	-4.95422513
H	-1.69918656	0.98102583	-5.14302446
H	3.18419550	1.83839616	-4.95422513
H	1.69918656	0.98102583	-5.14302446
H	0.00000000	-3.67679232	-4.95422513
H	0.00000000	-1.96205165	-5.14302446
H	0.00000000	4.52120521	-0.32552233
H	3.91547877	-2.26060287	-0.32552233
H	-3.91547877	-2.26060287	-0.32552233
H	-3.91547877	2.26060287	0.32552233
H	3.91547877	2.26060287	0.32552233
H	0.00000000	-4.52120521	0.32552233
H	2.55512017	-1.47519906	-1.05529374
H	0.00000000	2.95039864	-1.05529374
H	-2.55512017	-1.47519906	-1.05529374
H	2.55512017	1.47519906	1.05529374
H	-2.55512017	1.47519906	1.05529374
H	0.00000000	-2.95039864	1.05529374

$[Mn(Tb^{3,5\text{-}NO2})_2]^+$ ^1E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.67320000	1.15100000	0.00000000
N	1.45170000	2.47770000	0.00000000
N	-0.83660000	1.15100000	1.44900000
N	-0.72590000	2.47770000	1.25720000
N	-0.83660000	1.15100000	-1.44900000
N	-0.72590000	2.47770000	-1.25720000
C	3.02900000	1.00430000	0.00000000
C	3.66800000	2.22760000	0.00000000
C	2.63610000	3.13870000	0.00000000
C	-1.51450000	1.00430000	2.62320000
C	-1.83400000	2.22760000	3.17660000
C	-1.31800000	3.13870000	2.28290000
C	-1.51450000	1.00430000	-2.62320000
C	-1.83400000	2.22760000	-3.17660000
C	-1.31800000	3.13870000	-2.28290000
H	4.72900000	2.42640000	0.00000000
N	2.87040000	4.59500000	0.00000000
H	-2.36450000	2.42640000	4.09540000
N	-1.90490000	-0.23460000	3.29940000
N	-1.43520000	4.59500000	2.48590000
N	3.80990000	-0.23460000	0.00000000
H	0.00000000	4.16800000	0.00000000
H	-2.36450000	2.42640000	-4.09540000
N	-1.43520000	4.59500000	-2.48590000
N	-1.90490000	-0.23460000	-3.29940000
B	0.00000000	3.00270000	0.00000000
N	0.83660000	-1.15100000	-1.44900000
N	0.72590000	-2.47770000	-1.25720000
N	0.83660000	-1.15100000	1.44900000
N	0.72590000	-2.47770000	1.25720000
N	-1.67320000	-1.15100000	0.00000000
N	-1.45170000	-2.47770000	0.00000000
C	1.51450000	-1.00430000	-2.62320000
C	1.83400000	-2.22760000	-3.17660000
C	1.31800000	-3.13870000	-2.28290000
C	1.51450000	-1.00430000	2.62320000
C	1.83400000	-2.22760000	3.17660000
C	1.31800000	-3.13870000	2.28290000
C	-3.02900000	-1.00430000	0.00000000
C	-3.66800000	-2.22760000	0.00000000
C	-2.63610000	-3.13870000	0.00000000
H	2.36450000	-2.42640000	-4.09540000
N	1.43520000	-4.59500000	-2.48590000
H	2.36450000	-2.42640000	4.09540000
N	1.90490000	0.23460000	3.29940000
N	1.43520000	-4.59500000	2.48590000
N	1.90490000	0.23460000	-3.29940000
H	0.00000000	-4.16800000	0.00000000
H	-4.72900000	-2.42640000	0.00000000
N	-2.87040000	-4.59500000	0.00000000
N	-3.80990000	0.23460000	0.00000000
B	0.00000000	-3.00270000	0.00000000
O	4.05410000	4.89100000	0.00000000

O	1.92360000	5.35460000	0.00000000
O	-2.02710000	4.89100000	3.51100000
O	-0.96180000	5.35460000	1.66580000
O	-2.02710000	4.89100000	-3.51100000
O	-0.96180000	5.35460000	-1.66580000
O	2.02710000	-4.89100000	-3.51100000
O	0.96180000	-5.35460000	-1.66580000
O	2.02710000	-4.89100000	3.51100000
O	0.96180000	-5.35460000	1.66580000
O	-4.05410000	-4.89100000	0.00000000
O	-1.92360000	-5.35460000	0.00000000
O	5.01770000	-0.07320000	0.00000000
O	-2.50880000	-0.07320000	4.34540000
O	-2.50880000	-0.07320000	-4.34540000
O	2.50880000	0.07320000	-4.34540000
O	2.50880000	0.07320000	4.34540000
O	-5.01770000	0.07320000	0.00000000
O	-1.61470000	-1.30820000	2.79670000
O	3.22940000	-1.30820000	0.00000000
O	-1.61470000	-1.30820000	-2.79670000
O	1.61470000	1.30820000	2.79670000
O	1.61470000	1.30820000	-2.79670000
O	-3.22940000	1.30820000	0.00000000

$[Mn(Tb^{3,5\text{-}NO2})_2]^+$ ^5E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.76750493	1.78753217
N	0.00000000	1.47436031	3.09100368
N	1.53070446	-0.88375246	1.78753217
N	1.27683326	-0.73717989	3.09100368
N	-1.53070446	-0.88375246	1.78753217
N	-1.27683326	-0.73717989	3.09100368
C	0.00000000	3.10463370	1.71591808
C	0.00000000	3.71448455	2.95983546
C	0.00000000	2.63720509	3.81446942
C	2.68869139	-1.55231659	1.71591808
C	3.21683780	-1.85724228	2.95983546
C	2.28388667	-1.31860228	3.81446942
C	-2.68869139	-1.55231659	1.71591808
C	-3.21683780	-1.85724228	2.95983546
C	-2.28388667	-1.31860228	3.81446942
H	0.00000000	4.76650956	3.20376818
N	0.00000000	2.77951937	5.25970805
H	4.12791804	-2.38325452	3.20376818
N	3.29772043	-1.90393952	0.45526442
N	2.40713417	-1.38975969	5.25970805
N	0.00000000	3.80787905	0.45526442
H	0.00000000	0.00000000	4.76922583
H	-4.12791804	-2.38325452	3.20376818
N	-2.40713417	-1.38975969	5.25970805
N	-3.29772043	-1.90393952	0.45526442
B	0.00000000	0.00000000	3.57548239
N	-1.53070446	0.88375246	-1.78753217
N	-1.27683326	0.73717989	-3.09100368
N	1.53070446	0.88375246	-1.78753217
N	1.27683326	0.73717989	-3.09100368
N	0.00000000	-1.76750493	-1.78753217
N	0.00000000	-1.47436031	-3.09100368
C	-2.68869139	1.55231659	-1.71591808
C	-3.21683780	1.85724228	-2.95983546
C	-2.28388667	1.31860228	-3.81446942
C	2.68869139	1.55231659	-1.71591808
C	3.21683780	1.85724228	-2.95983546
C	2.28388667	1.31860228	-3.81446942
C	0.00000000	-3.10463370	-1.71591808
C	0.00000000	-3.71448455	-2.95983546
C	0.00000000	-2.63720509	-3.81446942
H	-4.12791804	2.38325452	-3.20376818
N	-2.40713417	1.38975969	-5.25970805
H	4.12791804	2.38325452	-3.20376818
N	3.29772043	1.90393952	-0.45526442
N	2.40713417	1.38975969	-5.25970805
N	-3.29772043	1.90393952	-0.45526442
H	0.00000000	0.00000000	-4.76922583
H	0.00000000	-4.76650956	-3.20376818
N	0.00000000	-2.77951937	-5.25970805
N	0.00000000	-3.80787905	-0.45526442
B	0.00000000	0.00000000	-3.57548239
O	0.00000000	3.92618985	5.67537148
O	0.00000000	1.77661101	5.96354766
O	3.40018025	-1.96309466	5.67537148
O	1.53859026	-0.88830550	5.96354766
O	-3.40018025	-1.96309466	5.67537148
O	-1.53859026	-0.88830550	5.96354766
O	-3.40018025	1.96309466	-5.67537148
O	-1.53859026	0.88830550	-5.96354766
O	3.40018025	1.96309466	-5.67537148
O	1.53859026	0.88830550	-5.96354766
O	0.00000000	-3.92618985	-5.67537148
O	0.00000000	-1.77661101	-5.96354766
O	0.00000000	5.02567835	0.51056767
O	4.35236539	-2.51283944	0.51056767
O	-4.35236539	-2.51283944	0.51056767
O	-4.35236539	2.51283944	-0.51056767
O	4.35236539	2.51283944	-0.51056767
O	0.00000000	-5.02567835	-0.51056767
O	2.70997067	-1.56460250	-0.56627522
O	0.00000000	3.12920446	-0.56627522
O	-2.70997067	-1.56460250	-0.56627522
O	2.70997067	1.56460250	0.56627522
O	-2.70997067	1.56460250	0.56627522
O	0.00000000	-3.12920446	0.56627522

$[Mn(Tb^{3,5\text{-}NO2})_2]^+$ $^3A_{2g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.69117376	1.17278431
N	0.00000000	1.45553060	2.49488499
N	1.46459911	-0.84558661	1.17278431
N	1.26052666	-0.72776530	2.49488499
N	-1.46459911	-0.84558661	1.17278431
N	-1.26052666	-0.72776530	2.49488499
C	0.00000000	3.04329412	1.03343977
C	0.00000000	3.67406388	2.26221051
C	0.00000000	2.63700030	3.16461277
C	2.63556993	-1.52164706	1.03343977
C	3.18183273	-1.83703194	2.26221051
C	2.28370887	-1.31850015	3.16461277
C	-2.63556993	-1.52164706	1.03343977

C	-3.18183273	-1.83703194	2.26221051
C	-2.28370887	-1.31850015	3.16461277
H	0.00000000	4.73394717	2.46737782
N	0.00000000	2.86245097	4.62292737
H	4.09971818	-2.36697332	2.46737782
N	3.31105411	-1.91163799	-0.20489161
N	2.47895516	-1.43122549	4.62292737
N	0.00000000	3.82327599	-0.20489161
H	0.00000000	0.00000000	4.18002083
H	-4.09971818	-2.36697332	2.46737782
N	-2.47895516	-1.43122549	4.62292737
N	-3.31105411	-1.91163799	-0.20489161
B	0.00000000	0.00000000	3.01484714
N	-1.46459911	0.84558661	-1.17278431
N	-1.26052666	0.72776530	-2.49488499
N	1.46459911	0.84558661	-1.17278431
N	1.26052666	0.72776530	-2.49488499
N	0.00000000	-1.69117376	-1.17278431
N	0.00000000	-1.45553060	-2.49488499
C	-2.63556993	1.52164706	-1.03343977
C	-3.18183273	1.83703194	-2.26221051
C	-2.28370887	1.31850015	-3.16461277
C	2.63556993	1.52164706	-1.03343977
C	3.18183273	1.83703194	-2.26221051
C	2.28370887	1.31850015	-3.16461277
C	0.00000000	-3.04329412	-1.03343977
C	0.00000000	-3.67406388	-2.26221051
C	0.00000000	-2.63700030	-3.16461277
H	-4.09971818	2.36697332	-2.46737782
N	-2.47895516	1.43122549	-4.62292737
H	4.09971818	2.36697332	-2.46737782
N	3.31105411	1.91163799	0.20489161
N	2.47895516	1.43122549	-4.62292737
N	-3.31105411	1.91163799	0.20489161
H	0.00000000	0.00000000	-4.18002083
H	0.00000000	-4.73394717	-2.46737782
N	0.00000000	-2.86245097	-4.62292737
N	0.00000000	-3.82327599	0.20489161
B	0.00000000	0.00000000	-3.01484714
O	0.00000000	4.04386670	4.92639094
O	0.00000000	1.91115168	5.37674248
O	3.50209133	-2.02193335	4.92639094
O	1.65510609	-0.95557558	5.37674248
O	-3.50209133	-2.02193335	4.92639094
O	-1.65510609	-0.95557558	5.37674248
O	-3.50209133	2.02193335	-4.92639094
O	-1.65510609	0.95557558	-5.37674248
O	3.50209133	2.02193335	-4.92639094
O	1.65510609	0.95557558	-5.37674248
O	0.00000000	-4.04386670	-4.92639094
O	0.00000000	-1.91115168	-5.37674248
O	0.00000000	5.03114581	-0.04609981
O	4.35710047	-2.51557317	-0.04609981
O	-4.35710047	-2.51557317	-0.04609981
O	-4.35710047	2.51557317	0.04609981
O	4.35710047	2.51557317	0.04609981
O	0.00000000	-5.03114581	0.04609981
O	2.80389486	-1.61882940	-1.27574104
O	0.00000000	3.23765881	-1.27574104
O	-2.80389486	-1.61882940	-1.27574104
O	2.80389486	1.61882940	1.27574104
O	-2.80389486	1.61882940	1.27574104
O	0.00000000	-3.23765881	1.27574104

$[Mn(Tb^{3,5\text{-}NO2})_2]^+$ ^1E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.61300000	1.18600000	0.00000000
N	1.43580000	2.55780000	0.00000000
N	-0.80650000	1.18600000	1.39690000
N	-0.71790000	2.55780000	1.24340000
N	-0.80650000	1.18600000	-1.39690000
N	-0.71790000	2.55780000	-1.24340000
C	2.95630000	0.98550000	0.00000000
C	3.63810000	2.21160000	0.00000000
C	2.63700000	3.17590000	0.00000000
C	-1.47820000	0.98550000	2.56020000
C	-1.81910000	2.21160000	3.15070000
C	-1.31850000	3.17590000	2.28370000
C	-1.47820000	0.98550000	-2.56020000
C	-1.81910000	2.21160000	-3.15070000
C	-1.31850000	3.17590000	-2.28370000
H	4.70920000	2.37280000	0.00000000
N	2.77330000	4.52940000	0.00000000
H	-2.35460000	2.37280000	4.07830000
N	-1.75490000	-0.24480000	3.03950000
N	-1.38670000	4.52940000	2.40180000
N	3.50970000	-0.24480000	0.00000000
H	0.00000000	4.29210000	0.00000000
H	-2.35460000	2.37280000	-4.07830000
N	-1.38670000	4.52940000	-2.40180000
N	-1.75490000	-0.24480000	-3.03950000
B	0.00000000	3.08120000	0.00000000
N	0.80650000	-1.18600000	-1.39690000
N	0.71790000	-2.55780000	-1.24340000
N	0.80650000	-1.18600000	1.39690000
N	0.71790000	-2.55780000	1.24340000
N	-1.61300000	-1.18600000	0.00000000
N	-1.43580000	-2.55780000	0.00000000
C	1.47820000	-0.98550000	-2.56020000
C	1.81910000	-2.21160000	-3.15070000
C	1.31850000	-3.17590000	-2.28370000
C	1.47820000	-0.98550000	2.56020000
C	1.81910000	-2.21160000	3.15070000
C	1.31850000	-3.17590000	2.28370000
C	-2.95630000	-0.98550000	0.00000000
C	-3.63810000	-2.21160000	0.00000000
C	-2.63700000	-3.17590000	0.00000000
H	2.35460000	-2.37280000	-4.07830000
N	1.38670000	-4.52940000	-2.40180000
H	2.35460000	-2.37280000	4.07830000
N	1.75490000	0.24480000	3.03950000
N	1.38670000	-4.52940000	2.40180000
N	1.75490000	0.24480000	-3.03950000
H	0.00000000	-4.29210000	0.00000000
H	-4.70920000	-2.37280000	0.00000000
N	-2.77330000	-4.52940000	0.00000000
N	-3.50970000	0.24480000	0.00000000
B	0.00000000	-3.08120000	0.00000000
H	3.68890000	4.93670000	0.00000000

H	1.97530000	5.13440000	0.00000000
H	-1.84450000	4.93670000	3.19470000
H	-0.98760000	5.13440000	1.71060000
H	-1.84450000	4.93670000	-3.19470000
H	-0.98760000	5.13440000	-1.71060000
H	1.84450000	-4.93670000	-3.19470000
H	0.98760000	-5.13440000	-1.71060000
H	1.84450000	-4.93670000	3.19470000
H	0.98760000	-5.13440000	1.71060000
H	-3.68890000	-4.93670000	0.00000000
H	-1.97530000	-5.13440000	0.00000000
H	4.50630000	-0.34580000	0.00000000
H	-2.25320000	-0.34580000	3.90260000
H	-2.25320000	-0.34580000	-3.90260000
H	2.25320000	0.34580000	-3.90260000
H	2.25320000	0.34580000	3.90260000
H	-4.50630000	0.34580000	0.00000000
H	-1.46430000	-1.06300000	2.53630000
H	2.92860000	-1.06300000	0.00000000
H	-1.46430000	-1.06300000	-2.53630000
H	1.46430000	1.06300000	2.53630000
H	1.46430000	1.06300000	-2.53630000
H	-2.92860000	1.06300000	0.00000000

$[Mn(Tb^{3CH3})_2]$ $^6A_{1g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.57157123	0.90734742	1.47972670
N	1.26956131	0.73298140	2.78453491
N	0.00000000	-1.81469431	1.47972670
N	0.00000000	-1.46596333	2.78453491
N	-1.57157123	0.90734742	1.47972670
N	-1.26956131	0.73298140	2.78453491
C	2.73818693	1.58089322	1.43916579
C	3.18157608	1.83688377	2.74809789
C	2.21796971	1.28054544	3.56783419
C	0.00000000	-3.16178590	1.43916579
C	0.00000000	-3.67376754	2.74809789
C	0.00000000	-2.56109088	3.56783419
C	-2.73818693	1.58089322	1.43916579
C	-3.18157608	1.83688377	2.74809789
C	-2.21796971	1.28054544	3.56783419
H	4.08333803	2.35751639	3.05053115
H	2.13862222	1.23473404	4.64666891
H	0.00000000	-4.71503279	3.05053115
C	0.00000000	-3.95189728	0.17305154
H	0.00000000	-2.46946807	4.64666891
C	3.42244327	1.97594837	0.17305154
H	0.00000000	0.00000000	4.46703757
H	-4.08333803	2.35751639	3.05053115
H	-2.13862222	1.23473404	4.64666891
C	-3.42244327	1.97594837	0.17305154
B	0.00000000	0.00000000	3.26036528
N	0.00000000	1.81469431	-1.47972670
N	0.00000000	1.46596333	-2.78453491
N	1.57157123	-0.90734742	-1.47972670
N	1.26956131	-0.73298140	-2.78453491
N	-1.57157123	-0.90734742	-1.47972670
N	-1.26956131	-0.73298140	-2.78453491
C	0.00000000	3.16178590	-1.43916579
C	0.00000000	3.67376754	-2.74809789
C	0.00000000	2.56109088	-3.56783419
C	2.73818693	-1.58089322	-1.43916579
C	3.18157608	-1.83688377	-2.74809789
C	2.21796971	-1.28054544	-3.56783419
C	-2.73818693	-1.58089322	-1.43916579
C	-3.18157608	-1.83688377	-2.74809789
C	-2.21796971	-1.28054544	-3.56783419
H	0.00000000	4.71503279	-3.05053115
H	0.00000000	2.46946807	-4.64666891
H	4.08333803	-2.35751639	-3.05053115
C	3.42244327	-1.97594837	-0.17305154
H	2.13862222	-1.23473404	-4.64666891
C	0.00000000	3.95189728	-0.17305154
H	0.00000000	0.00000000	-4.46703757
H	-4.08333803	-2.35751639	-3.05053115
H	-2.13862222	-1.23473404	-4.64666891
C	-3.42244327	-1.97594837	-0.17305154
B	0.00000000	0.00000000	-3.26036528
H	-0.87636515	-3.74102173	-0.44527831
H	0.00000000	-5.02011352	0.40746172
H	0.87636515	-3.74102173	-0.44527831
H	4.34754565	2.51005650	0.40746172
H	2.80163739	2.62946587	-0.44527831
H	3.67800254	1.11155639	-0.44527831
H	-4.34754565	2.51005650	0.40746172
H	-3.67800254	1.11155639	-0.44527831
H	-2.80163739	2.62946587	-0.44527831
H	3.67800254	-1.11155639	0.44527831
H	4.34754565	-2.51005650	-0.40746172
H	2.80163739	-2.62946587	0.44527831
H	-2.80163739	-2.62946587	0.44527831
H	-4.34754565	-2.51005650	-0.40746172
H	-3.67800254	-1.11155639	0.44527831
H	-0.87636515	3.74102173	0.44527831
H	0.00000000	5.02011352	-0.40746172
H	0.87636515	3.74102173	0.44527831

$[Mn(Tb^{3CH3})_2]$ ^4E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.52297635	0.87929097	1.32909322
N	1.26144267	0.72829395	2.64380763
N	0.00000000	-1.75858141	1.32909322
N	0.00000000	-1.45658842	2.64380763
N	-1.52297635	0.87929097	1.32909322
N	-1.26144267	0.72829395	2.64380763
C	2.69033978	1.55326805	1.24091694
C	3.16890651	1.82956895	2.53319848
C	2.23013126	1.28756709	3.39084504
C	0.00000000	-3.10653662	1.24091694
C	0.00000000	-3.65913843	2.53319848
C	0.00000000	-2.57513366	3.39084504
C	-2.69033978	1.55326805	1.24091694
C	-3.16890651	1.82956895	2.53319848
C	-2.23013126	1.28756709	3.39084504
H	4.07925172	2.35515732	2.79956514
H	2.18112204	1.25927146	4.47202771
H	0.00000000	-4.71031411	2.79956514
C	0.00000000	-3.86567843	-0.04225216

H	0.00000000	-2.51854291	4.47202771
C	3.34777583	1.93283948	-0.04225216
H	0.00000000	0.00000000	4.33998053
H	-4.07925172	2.35515732	2.79956514
H	-2.18112204	1.25927146	4.47202771
C	-3.34777583	1.93283948	-0.04225216
B	0.00000000	0.00000000	3.13246313
N	0.00000000	1.75858141	-1.32909322
N	0.00000000	1.45658842	-2.64380763
N	1.52297635	-0.87929097	-1.32909322
N	1.26144267	-0.72829395	-2.64380763
N	-1.52297635	-0.87929097	-1.32909322
N	-1.26144267	-0.72829395	-2.64380763
C	0.00000000	3.10653662	-1.24091694
C	0.00000000	3.65913843	-2.53319848
C	0.00000000	2.57513366	-3.39084504
C	2.69033978	-1.55326805	-1.24091694
C	3.16890651	-1.82956895	-2.53319848
C	2.23013126	-1.28756709	-3.39084504
C	-2.69033978	-1.55326805	-1.24091694
C	-3.16890651	-1.82956895	-2.53319848
C	-2.23013126	-1.28756709	-3.39084504
H	0.00000000	4.71031411	-2.79956514
H	0.00000000	2.51854291	-4.47202771
H	4.07925172	-2.35515732	-2.79956514
C	3.34777583	-1.93283948	0.04225216
H	2.18112204	-1.25927146	-4.47202771
C	0.00000000	3.86567843	0.04225216
H	0.00000000	0.00000000	-4.33998053
H	-4.07925172	-2.35515732	-2.79956514
H	-2.18112204	-1.25927146	-4.47202771
C	-3.34777583	-1.93283948	0.04225216
B	0.00000000	0.00000000	-3.13246313
H	-0.87694513	-3.63965042	-0.65423136
H	0.00000000	-4.93868796	0.17003153
H	0.87694513	-3.63965042	-0.65423136
H	4.27702907	2.46934425	0.17003153
H	2.71355690	2.57928188	-0.65423136
H	3.59050203	1.06036855	-0.65423136
H	-4.27702907	2.46934425	0.17003153
H	-3.59050203	1.06036855	-0.65423136
H	-2.71355690	2.57928188	-0.65423136
H	3.59050203	-1.06036855	0.65423136
H	4.27702907	-2.46934425	-0.17003153
H	2.71355690	-2.57928188	0.65423136
H	-2.71355690	-2.57928188	0.65423136
H	-4.27702907	-2.46934425	-0.17003153
H	-3.59050203	-1.06036855	0.65423136
H	-0.87694513	3.63965042	0.65423136
H	0.00000000	4.93868796	-0.17003153
H	0.87694513	3.63965042	0.65423136

$[Mn(Tb^{3CH3})_2]$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.44511004	0.83433472	1.19438586
N	1.24452382	0.71852586	2.52536771
N	0.00000000	-1.66866943	1.19438586
N	0.00000000	-1.43705226	2.52536771
N	-1.44511004	0.83433472	1.19438586
N	-1.24452382	0.71852586	2.52536771
C	2.61273805	1.50846526	1.03937661
C	3.14107814	1.81350207	2.30542683
C	2.24257063	1.29474909	3.21703624
C	0.00000000	-3.01692998	1.03937661
C	0.00000000	-3.62700467	2.30542683
C	0.00000000	-2.58949764	3.21703624
C	-2.61273805	1.50846526	1.03937661
C	-3.14107814	1.81350207	2.30542683
C	-2.24257063	1.29474909	3.21703624
H	4.06211802	2.34526488	2.51604467
H	2.23762600	1.29189365	4.29952969
H	0.00000000	-4.69052976	2.51604467
C	0.00000000	-3.74458363	-0.26080395
H	0.00000000	-2.58378782	4.29952969
C	3.24290454	1.87229208	-0.26080395
H	0.00000000	0.00000000	4.25327007
H	-4.06211802	2.34526488	2.51604467
H	-2.23762600	1.29189365	4.29952969
C	-3.24290454	1.87229208	-0.26080395
B	0.00000000	0.00000000	3.04708779
N	0.00000000	1.66866943	-1.19438586
N	0.00000000	1.43705226	-2.52536771
N	1.44511004	-0.83433472	-1.19438586
N	1.24452382	-0.71852586	-2.52536771
N	-1.44511004	-0.83433472	-1.19438586
N	-1.24452382	-0.71852586	-2.52536771
C	0.00000000	3.01692998	-1.03937661
C	0.00000000	3.62700467	-2.30542683
C	0.00000000	2.58949764	-3.21703624
C	2.61273805	-1.50846526	-1.03937661
C	3.14107814	-1.81350207	-2.30542683
C	2.24257063	-1.29474909	-3.21703624
C	-2.61273805	-1.50846526	-1.03937661
C	-3.14107814	-1.81350207	-2.30542683
C	-2.24257063	-1.29474909	-3.21703624
H	0.00000000	4.69052976	-2.51604467
H	0.00000000	2.58378782	-4.29952969
H	4.06211802	-2.34526488	-2.51604467
C	3.24290454	-1.87229208	0.26080395
H	2.23762600	-1.29189365	-4.29952969
C	0.00000000	3.74458363	0.26080395
H	0.00000000	0.00000000	-4.25327007
H	-4.06211802	-2.34526488	-2.51604467
H	-2.23762600	-1.29189365	-4.29952969
C	-3.24290454	-1.87229208	0.26080395
B	0.00000000	0.00000000	-3.04708779
H	-0.87863797	-3.51171494	-0.86753689
H	0.00000000	-4.82094761	-0.06426117
H	0.87863797	-3.51171494	-0.86753689
H	4.17506297	2.41047381	-0.06426117
H	2.60191532	2.51678022	-0.86753689
H	3.48055328	0.99493472	-0.86753689
H	-4.17506297	2.41047381	-0.06426117
H	-3.48055328	0.99493472	-0.86753689
H	-2.60191532	2.51678022	-0.86753689
H	3.48055328	-0.99493472	0.86753689
H	4.17506297	-2.41047381	0.06426117
H	2.60191532	-2.51678022	0.86753689
H	-2.60191532	-2.51678022	0.86753689

H	-4.17506297	-2.41047381	0.06426117
H	-3.48055328	-0.99493472	0.86753689
H	-0.87863797	3.51171494	0.86753689
H	0.00000000	4.82094761	0.06426117
H	0.87863797	3.51171494	0.86753689

$[Mn(Tb^{3CF3})_2]$ $^6A_{1g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.67403688	0.96650573	1.33855067
N	1.29080460	0.74524667	2.61223639
N	0.00000000	-1.93301146	1.33855067
N	0.00000000	-1.49049281	2.61223639
N	-1.67403688	0.96650573	1.33855067
N	-1.29080460	0.74524667	2.61223639
C	2.84349214	1.64169092	1.41889195
C	3.19845313	1.84662751	2.75909101
C	2.18299479	1.26035257	3.48151162
C	0.00000000	-3.28338237	1.41889195
C	0.00000000	-3.69325555	2.75909101
C	0.00000000	-2.52070566	3.48151162
C	-2.84349214	1.64169092	1.41889195
C	-3.19845313	1.84662751	2.75909101
C	-2.18299479	1.26035257	3.48151162
H	4.07347999	2.35182456	3.14409128
H	2.03317096	1.17385166	4.54931617
H	0.00000000	-4.70364965	3.14409128
C	0.00000000	-4.28442644	0.27010424
H	0.00000000	-2.34770333	4.54931617
C	3.71042206	2.14221322	0.27010424
H	0.00000000	0.00000000	4.24580074
H	-4.07347999	2.35182456	3.14409128
H	-2.03317096	1.17385166	4.54931617
C	-3.71042206	2.14221322	0.27010424
B	0.00000000	0.00000000	3.04292846
N	0.00000000	1.93301146	-1.33855067
N	0.00000000	1.49049281	-2.61223639
N	1.67403688	-0.96650573	-1.33855067
N	1.29080460	-0.74524667	-2.61223639
N	-1.67403688	-0.96650573	-1.33855067
N	-1.29080460	-0.74524667	-2.61223639
C	0.00000000	3.28338237	-1.41889195
C	0.00000000	3.69325555	-2.75909101
C	0.00000000	2.52070566	-3.48151162
C	2.84349214	-1.64169092	-1.41889195
C	3.19845313	-1.84662751	-2.75909101
C	2.18299479	-1.26035257	-3.48151162
C	-2.84349214	-1.64169092	-1.41889195
C	-3.19845313	-1.84662751	-2.75909101
C	-2.18299479	-1.26035257	-3.48151162
H	0.00000000	4.70364965	-3.14409128
H	0.00000000	2.34770333	-4.54931617
H	4.07347999	-2.35182456	-3.14409128
C	3.71042206	-2.14221322	-0.27010424
H	2.03317096	-1.17385166	-4.54931617
C	0.00000000	4.28442644	-0.27010424
H	0.00000000	0.00000000	-4.24580074
H	-4.07347999	-2.35182456	-3.14409128
H	-2.03317096	-1.17385166	-4.54931617
C	-3.71042206	-2.14221322	-0.27010424
B	0.00000000	0.00000000	-3.04292846
F	-1.07201309	-4.21365375	-0.53857279
F	0.00000000	-5.53756209	0.80747051
F	1.07201309	-4.21365375	-0.53857279
F	4.79566934	2.76878131	0.80747051
F	3.11312488	3.03521729	-0.53857279
F	4.18513797	1.17843646	-0.53857279
F	-4.79566934	2.76878131	0.80747051
F	-4.18513797	1.17843646	-0.53857279
F	-3.11312488	3.03521729	-0.53857279
F	4.18513797	-1.17843646	0.53857279
F	4.79566934	-2.76878131	-0.80747051
F	3.11312488	-3.03521729	0.53857279
F	-3.11312488	-3.03521729	0.53857279
F	-4.79566934	-2.76878131	-0.80747051
F	-4.18513797	-1.17843646	0.53857279
F	-1.07201309	4.21365375	0.53857279
F	0.00000000	5.53756209	-0.80747051
F	1.07201309	4.21365375	0.53857279

$[Mn(Tb^{3CF3})_2]$ ^4E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.61374613	0.93169698	1.22701440
N	1.28112859	0.73965962	2.51568536
N	0.00000000	-1.86339396	1.22701440
N	0.00000000	-1.47931976	2.51568536
N	-1.61374613	0.93169698	1.22701440
N	-1.28112859	0.73965962	2.51568536
C	2.78831377	1.60983339	1.24658602
C	3.18943859	1.84142305	2.56844486
C	2.20156415	1.27107370	3.34153472
C	0.00000000	-3.21966731	1.24658602
C	0.00000000	-3.68284663	2.56844486
C	0.00000000	-2.54214739	3.34153472
C	-2.78831377	1.60983339	1.24658602
C	-3.18943859	1.84142305	2.56844486
C	-2.20156415	1.27107370	3.34153472
H	4.07811717	2.35450167	2.90929110
H	2.08892190	1.20603940	4.41531685
H	0.00000000	-4.70900387	2.90929110
C	0.00000000	-4.18166287	0.06563227
H	0.00000000	-2.41207933	4.41531685
C	3.62142609	2.09083117	0.06563227
H	0.00000000	0.00000000	4.16369571
H	-4.07811717	2.35450167	2.90929110
H	-2.08892190	1.20603940	4.41531685
C	-3.62142609	2.09083117	0.06563227
B	0.00000000	0.00000000	2.95789338
N	0.00000000	1.86339396	-1.22701440
N	0.00000000	1.47931976	-2.51568536
N	1.61374613	-0.93169698	-1.22701440
N	1.28112859	-0.73965962	-2.51568536
N	-1.61374613	-0.93169698	-1.22701440
N	-1.28112859	-0.73965962	-2.51568536
C	0.00000000	3.21966731	-1.24658602
C	0.00000000	3.68284663	-2.56844486
C	0.00000000	2.54214739	-3.34153472
C	2.78831377	-1.60983339	-1.24658602
C	3.18943859	-1.84142305	-2.56844486

C	2.20156415	-1.27107370	-3.34153472
C	-2.78831377	-1.60983339	-1.24658602
C	-3.18943859	-1.84142305	-2.56844486
C	-2.20156415	-1.27107370	-3.34153472
H	0.00000000	4.70900387	-2.90929110
H	0.00000000	2.41207933	-4.41531685
H	4.07811717	-2.35450167	-2.90929110
C	3.62142609	-2.09083117	-0.06563227
H	2.08892190	-1.20603940	-4.41531685
C	0.00000000	4.18166287	-0.06563227
H	0.00000000	0.00000000	-4.16369571
H	-4.07811717	-2.35450167	-2.90929110
H	-2.08892190	-1.20603940	-4.41531685
C	-3.62142609	-2.09083117	-0.06563227
B	0.00000000	0.00000000	-2.95789338
F	-1.07460659	-4.08455461	-0.73832926
F	0.00000000	-5.45292918	0.55796396
F	1.07460659	-4.08455461	-0.73832926
F	4.72237512	2.72646459	0.55796396
F	3.00002436	2.97291408	-0.73832926
F	4.07463148	1.11164053	-0.73832926
F	-4.72237512	2.72646459	0.55796396
F	-4.07463148	1.11164053	-0.73832926
F	-3.00002436	2.97291408	-0.73832926
F	4.07463148	-1.11164053	0.73832926
F	4.72237512	-2.72646459	-0.55796396
F	3.00002436	-2.97291408	0.73832926
F	-3.00002436	-2.97291408	0.73832926
F	-4.72237512	-2.72646459	-0.55796396
F	-4.07463148	-1.11164053	0.73832926
F	-1.07460659	4.08455461	0.73832926
F	0.00000000	5.45292918	-0.55796396
F	1.07460659	4.08455461	0.73832926

$[Mn(Tb^{3CF3})_2]$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.51217902	0.87305726	1.14808550
N	1.25768657	0.72612591	2.46093774
N	0.00000000	-1.74611400	1.14808550
N	0.00000000	-1.45225182	2.46093774
N	-1.51217902	0.87305726	1.14808550
N	-1.25768657	0.72612591	2.46093774
C	2.69300577	1.55480795	1.08390476
C	3.15962792	1.82421209	2.37663610
C	2.21804908	1.28059148	3.21981760
C	0.00000000	-3.10961538	1.08390476
C	0.00000000	-3.64842418	2.37663610
C	0.00000000	-2.56118243	3.21981760
C	-2.69300577	1.55480795	1.08390476
C	-3.15962792	1.82421209	2.37663610
C	-2.21804908	1.28059148	3.21981760
H	4.06469353	2.34675187	2.65201464
H	2.16042327	1.24732105	4.29936088
H	0.00000000	-4.69350374	2.65201464
C	0.00000000	-4.03178082	-0.12674271
H	0.00000000	-2.49464156	4.29936088
C	3.49162473	2.01589067	-0.12674271
H	0.00000000	0.00000000	4.15275021
H	-4.06469353	2.34675187	2.65201464
H	-2.16042327	1.24732105	4.29936088
C	-3.49162473	2.01589067	-0.12674271
B	0.00000000	0.00000000	2.94859838
N	0.00000000	1.74611400	-1.14808550
N	0.00000000	1.45225182	-2.46093774
N	1.51217902	-0.87305726	-1.14808550
N	1.25768657	-0.72612591	-2.46093774
N	-1.51217902	-0.87305726	-1.14808550
N	-1.25768657	-0.72612591	-2.46093774
C	0.00000000	3.10961538	-1.08390476
C	0.00000000	3.64842418	-2.37663610
C	0.00000000	2.56118243	-3.21981760
C	2.69300577	-1.55480795	-1.08390476
C	3.15962792	-1.82421209	-2.37663610
C	2.21804908	-1.28059148	-3.21981760
C	-2.69300577	-1.55480795	-1.08390476
C	-3.15962792	-1.82421209	-2.37663610
C	-2.21804908	-1.28059148	-3.21981760
H	0.00000000	4.69350374	-2.65201464
H	0.00000000	2.49464156	-4.29936088
H	4.06469353	-2.34675187	-2.65201464
C	3.49162473	-2.01589067	0.12674271
H	2.16042327	-1.24732105	-4.29936088
C	0.00000000	4.03178082	0.12674271
H	0.00000000	0.00000000	-4.15275021
H	-4.06469353	-2.34675187	-2.65201464
H	-2.16042327	-1.24732105	-4.29936088
C	-3.49162473	-2.01589067	0.12674271
B	0.00000000	0.00000000	-2.94859838
F	-1.07756839	-3.91466754	-0.92510396
F	0.00000000	-5.31951884	0.32271504
F	1.07756839	-3.91466754	-0.92510396
F	4.60683879	2.65975968	0.32271504
F	2.85141763	2.89053547	-0.92510396
F	3.92898602	1.02413208	-0.92510396
F	-4.60683879	2.65975968	0.32271504
F	-3.92898602	1.02413208	-0.92510396
F	-2.85141763	2.89053547	-0.92510396
F	3.92898602	-1.02413208	0.92510396
F	4.60683879	-2.65975968	-0.32271504
F	2.85141763	-2.89053547	0.92510396
F	-2.85141763	-2.89053547	0.92510396
F	-4.60683879	-2.65975968	-0.32271504
F	-3.92898602	-1.02413208	0.92510396
F	-1.07756839	3.91466754	0.92510396
F	0.00000000	5.31951884	-0.32271504
F	1.07756839	3.91466754	0.92510396

$[Mn(Tb^{3NH2})_2]$ $^6A_{1g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.77913466	1.47543930
N	0.00000000	1.45999580	2.80273544
N	1.54077576	-0.88956759	1.47543930
N	1.26439336	-0.72999790	2.80273544
N	-1.54077576	-0.88956759	1.47543930
N	-1.26439336	-0.72999790	2.80273544
C	0.00000000	3.12458527	1.41133107
C	0.00000000	3.67767022	2.71017704
C	0.00000000	2.57682755	3.54725131

C	2.70597061	-1.56229264	1.41133107
C	3.18495593	-1.83883485	2.71017704
C	2.23159814	-1.28841378	3.54725131
C	-2.70597061	-1.56229264	1.41133107
C	-3.18495593	-1.83883485	2.71017704
C	-2.23159814	-1.28841378	3.54725131
H	0.00000000	4.72455427	2.99146333
H	0.00000000	2.51831325	4.62870598
H	4.09158367	-2.36227687	2.99146333
N	3.28158158	-1.89462177	0.22368640
H	2.18092307	-1.25915662	4.62870598
N	0.00000000	3.78924354	0.22368640
H	0.00000000	0.00000000	4.49668155
H	-4.09158367	-2.36227687	2.99146333
H	-2.18092307	-1.25915662	4.62870598
N	-3.28158158	-1.89462177	0.22368640
B	0.00000000	0.00000000	3.28806453
N	-1.54077576	0.88956759	-1.47543930
N	-1.26439336	0.72999790	-2.80273544
N	1.54077576	0.88956759	-1.47543930
N	1.26439336	0.72999790	-2.80273544
N	0.00000000	-1.77913466	-1.47543930
N	0.00000000	-1.45999580	-2.80273544
C	-2.70597061	1.56229264	-1.41133107
C	-3.18495593	1.83883485	-2.71017704
C	-2.23159814	1.28841378	-3.54725131
C	2.70597061	1.56229264	-1.41133107
C	3.18495593	1.83883485	-2.71017704
C	2.23159814	1.28841378	-3.54725131
C	0.00000000	-3.12458527	-1.41133107
C	0.00000000	-3.67767022	-2.71017704
C	0.00000000	-2.57682755	-3.54725131
H	-4.09158367	2.36227687	-2.99146333
H	-2.18092307	1.25915662	-4.62870598
H	4.09158367	2.36227687	-2.99146333
N	3.28158158	1.89462177	-0.22368640
H	2.18092307	1.25915662	-4.62870598
N	-3.28158158	1.89462177	-0.22368640
H	0.00000000	0.00000000	-4.49668155
H	0.00000000	-4.72455427	-2.99146333
H	0.00000000	-2.51831325	-4.62870598
N	0.00000000	-3.78924354	-0.22368640
B	0.00000000	0.00000000	-3.28806453
H	0.00000000	4.78965842	0.20736287
H	4.14796592	-2.39482921	0.20736287
H	-4.14796592	-2.39482921	0.20736287
H	-4.14796592	2.39482921	-0.20736287
H	4.14796592	2.39482921	-0.20736287
H	0.00000000	-4.78965842	-0.20736287
H	2.84673811	-1.64356527	-0.64575976
H	0.00000000	3.28713053	-0.64575976
H	-2.84673811	-1.64356527	-0.64575976
H	2.84673811	1.64356527	0.64575976
H	-2.84673811	1.64356527	0.64575976
H	0.00000000	-3.28713053	0.64575976

$[Mn(Tb^{3NH2})_2]$ ^4E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.71466288	1.34715192
N	0.00000000	1.44933129	2.68626935
N	1.48494174	-0.85733170	1.34715192
N	1.25515816	-0.72466591	2.68626935
N	-1.48494174	-0.85733170	1.34715192
N	-1.25515816	-0.72466591	2.68626935
C	0.00000000	3.06027595	1.23065514
C	0.00000000	3.66004544	2.50873726
C	0.00000000	2.59237266	3.38811554
C	2.65027683	-1.53013771	1.23065514
C	3.16969234	-1.83002246	2.50873726
C	2.24506094	-1.29618633	3.38811554
C	-2.65027683	-1.53013771	1.23065514
C	-3.16969234	-1.83002246	2.50873726
C	-2.24506094	-1.29618633	3.38811554
H	0.00000000	4.71708493	2.74939490
H	0.00000000	2.57466745	4.47101487
H	4.08511501	-2.35854247	2.74939490
N	3.18527979	-1.83902217	0.02211273
H	2.22972750	-1.28733373	4.47101487
N	0.00000000	3.67804435	0.02211273
H	0.00000000	0.00000000	4.39746399
H	-4.08511501	-2.35854247	2.74939490
H	-2.22972750	-1.28733373	4.47101487
N	-3.18527979	-1.83902217	0.02211273
B	0.00000000	0.00000000	3.18830351
N	-1.48494174	0.85733170	-1.34715192
N	-1.25515816	0.72466591	-2.68626935
N	1.48494174	0.85733170	-1.34715192
N	1.25515816	0.72466591	-2.68626935
N	0.00000000	-1.71466288	-1.34715192
N	0.00000000	-1.44933129	-2.68626935
C	-2.65027683	1.53013771	-1.23065514
C	-3.16969234	1.83002246	-2.50873726
C	-2.24506094	1.29618633	-3.38811554
C	2.65027683	1.53013771	-1.23065514
C	3.16969234	1.83002246	-2.50873726
C	2.24506094	1.29618633	-3.38811554
C	0.00000000	-3.06027595	-1.23065514
C	0.00000000	-3.66004544	-2.50873726
C	0.00000000	-2.59237266	-3.38811554
H	-4.08511501	2.35854247	-2.74939490
H	-2.22972750	1.28733373	-4.47101487
H	4.08511501	2.35854247	-2.74939490
N	3.18527979	1.83902217	-0.02211273
H	2.22972750	1.28733373	-4.47101487
N	-3.18527979	1.83902217	-0.02211273
H	0.00000000	0.00000000	-4.39746399
H	0.00000000	-4.71708493	-2.74939490
H	0.00000000	-2.57466745	-4.47101487
N	0.00000000	-3.67804435	-0.02211273
B	0.00000000	0.00000000	-3.18830351
H	0.00000000	4.67693890	-0.03437853
H	4.05034806	-2.33846972	-0.03437853
H	-4.05034806	-2.33846972	-0.03437853
H	-4.05034806	2.33846972	0.03437853
H	4.05034806	2.33846972	0.03437853
H	0.00000000	-4.67693890	0.03437853
H	2.71493911	-1.56747064	-0.82281135
H	0.00000000	3.13494180	-0.82281135
H	-2.71493911	-1.56747064	-0.82281135

H	2.71493911	1.56747064	0.82281135
H	-2.71493911	1.56747064	0.82281135
H	0.00000000	-3.13494180	0.82281135

$[Mn(Tb^{3NH2})_2]$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.63869049	1.22895542
N	0.00000000	1.43366870	2.58137689
N	1.41914754	-0.81934524	1.22895542
N	1.24159323	-0.71683408	2.58137689
N	-1.41914754	-0.81934524	1.22895542
N	-1.24159323	-0.71683408	2.58137689
C	0.00000000	2.98282504	1.05757502
C	0.00000000	3.63187152	2.31101706
C	0.00000000	2.60494274	3.23602841
C	2.58320202	-1.49141252	1.05757502
C	3.14529304	-1.81593576	2.31101706
C	2.25594664	-1.30247137	3.23602841
C	-2.58320202	-1.49141252	1.05757502
C	-3.14529304	-1.81593576	2.31101706
C	-2.25594664	-1.30247137	3.23602841
H	0.00000000	4.69855897	2.50327244
H	0.00000000	2.63058085	4.31850704
H	4.06907141	-2.34927975	2.50327244
N	3.08550236	-1.78141541	-0.16763859
H	2.27814986	-1.31529069	4.31850704
N	0.00000000	3.56283135	-0.16763859
H	0.00000000	0.00000000	4.31844354
H	-4.06907141	-2.34927975	2.50327244
H	-2.27814986	-1.31529069	4.31850704
N	-3.08550236	-1.78141541	-0.16763859
B	0.00000000	0.00000000	3.11011704
N	-1.41914754	0.81934524	-1.22895542
N	-1.24159323	0.71683408	-2.58137689
N	1.41914754	0.81934524	-1.22895542
N	1.24159323	0.71683408	-2.58137689
N	0.00000000	-1.63869049	-1.22895542
N	0.00000000	-1.43366870	-2.58137689
C	-2.58320202	1.49141252	-1.05757502
C	-3.14529304	1.81593576	-2.31101706
C	-2.25594664	1.30247137	-3.23602841
C	2.58320202	1.49141252	-1.05757502
C	3.14529304	1.81593576	-2.31101706
C	2.25594664	1.30247137	-3.23602841
C	0.00000000	-2.98282504	-1.05757502
C	0.00000000	-3.63187152	-2.31101706
C	0.00000000	-2.60494274	-3.23602841
H	-4.06907141	2.34927975	-2.50327244
H	-2.27814986	1.31529069	-4.31850704
H	4.06907141	2.34927975	-2.50327244
N	3.08550236	1.78141541	0.16763859
H	2.27814986	1.31529069	-4.31850704
N	-3.08550236	1.78141541	0.16763859
H	0.00000000	0.00000000	-4.31844354
H	0.00000000	-4.69855897	-2.50327244
H	0.00000000	-2.63058085	-4.31850704
N	0.00000000	-3.56283135	0.16763859
B	0.00000000	0.00000000	-3.11011704
H	0.00000000	4.55982563	-0.25164019
H	3.94892489	-2.27991308	-0.25164019
H	-3.94892489	-2.27991308	-0.25164019
H	-3.94892489	2.27991308	0.25164019
H	3.94892489	2.27991308	0.25164019
H	0.00000000	-4.55982563	0.25164019
H	2.59240759	-1.49672705	-0.99431452
H	0.00000000	2.99345409	-0.99431452
H	-2.59240759	-1.49672705	-0.99431452
H	2.59240759	1.49672705	0.99431452
H	-2.59240759	1.49672705	0.99431452
H	0.00000000	-2.99345409	0.99431452

$[Mn(Tb^{3NO2})_2]$ $^6A_{1g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	-1.82790000	-1.63740000
N	0.00000000	-1.46170000	-2.92370000
N	1.58300000	0.91390000	-1.63740000
N	1.26590000	0.73080000	-2.92370000
N	-1.58300000	0.91390000	-1.63740000
N	-1.26590000	0.73080000	-2.92370000
C	0.00000000	-3.16880000	-1.67550000
C	0.00000000	-3.67210000	-2.97830000
C	0.00000000	-2.53440000	-3.75000000
C	2.74420000	1.58440000	-1.67550000
C	3.18010000	1.83600000	-2.97830000
C	2.19490000	1.26720000	-3.75000000
C	-2.74420000	1.58440000	-1.67550000
C	-3.18010000	1.83600000	-2.97830000
C	-2.19490000	1.26720000	-3.75000000
H	0.00000000	-4.70780000	-3.28580000
H	0.00000000	-2.40390000	-4.82410000
H	4.07700000	2.35390000	-3.28580000
N	3.45020000	1.99200000	-0.48470000
H	2.08190000	1.20200000	-4.82410000
N	0.00000000	-3.98390000	-0.48470000
H	0.00000000	0.00000000	-4.59590000
H	-4.07700000	2.35390000	-3.28580000
H	-2.08190000	1.20200000	-4.82410000
N	-3.45020000	1.99200000	-0.48470000
B	0.00000000	0.00000000	-3.39270000
N	-1.58300000	-0.91390000	1.63740000
N	-1.26590000	-0.73080000	2.92370000
N	1.58300000	-0.91390000	1.63740000
N	1.26590000	-0.73080000	2.92370000
N	0.00000000	1.82790000	1.63740000
N	0.00000000	1.46170000	2.92370000
C	-2.74420000	-1.58440000	1.67550000
C	-3.18010000	-1.83600000	2.97830000
C	-2.19490000	-1.26720000	3.75000000
C	2.74420000	-1.58440000	1.67550000
C	3.18010000	-1.83600000	2.97830000
C	2.19490000	-1.26720000	3.75000000
C	0.00000000	3.16880000	1.67550000
C	0.00000000	3.67210000	2.97830000
C	0.00000000	2.53440000	3.75000000
H	-4.07700000	-2.35390000	3.28580000
H	-2.08190000	-1.20200000	4.82410000
H	4.07700000	-2.35390000	3.28580000
N	3.45020000	-1.99200000	0.48470000

H	2.08190000	-1.20200000	4.82410000
N	-3.45020000	-1.99200000	0.48470000
H	0.00000000	0.00000000	4.59590000
H	0.00000000	4.70780000	3.28580000
H	0.00000000	2.40390000	4.82410000
N	0.00000000	3.98390000	0.48470000
B	0.00000000	0.00000000	3.39270000
O	0.00000000	-5.19920000	-0.66350000
O	4.50260000	2.59960000	-0.66350000
O	-4.50260000	2.59960000	-0.66350000
O	-4.50260000	-2.59960000	0.66350000
O	4.50260000	-2.59960000	0.66350000
O	0.00000000	5.19920000	0.66350000
O	2.96560000	1.71220000	0.60310000
O	0.00000000	-3.42440000	0.60310000
O	-2.96560000	1.71220000	0.60310000
O	2.96560000	-1.71220000	-0.60310000
O	-2.96560000	-1.71220000	-0.60310000
O	0.00000000	3.42440000	-0.60310000

$[Mn(Tb^{3NO2})_2]$ ^4E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.80970628	1.39391532
N	0.00000000	1.45737319	2.68352239
N	1.56725156	-0.90485288	1.39391532
N	1.26212213	-0.72868660	2.68352239
N	-1.56725156	-0.90485288	1.39391532
N	-1.26212213	-0.72868660	2.68352239
C	0.00000000	3.15622478	1.42077371
C	0.00000000	3.66379890	2.72152948
C	0.00000000	2.53317625	3.50189288
C	2.73337088	-1.57811239	1.42077371
C	3.17294255	-1.83189945	2.72152948
C	2.19379477	-1.26658786	3.50189288
C	-2.73337088	-1.57811239	1.42077371
C	-3.17294255	-1.83189945	2.72152948
C	-2.19379477	-1.26658786	3.50189288
H	0.00000000	4.70167318	3.02086442
H	0.00000000	2.40871217	4.57634654
H	4.07176863	-2.35083659	3.02086442
N	3.46159604	-1.99855377	0.24520539
H	2.08600613	-1.20435609	4.57634654
N	0.00000000	3.99710701	0.24520539
H	0.00000000	0.00000000	4.35577964
H	-4.07176863	-2.35083659	3.02086442
H	-2.08600613	-1.20435609	4.57634654
N	-3.46159604	-1.99855377	0.24520539
B	0.00000000	0.00000000	3.15223267
N	-1.56725156	0.90485288	-1.39391532
N	-1.26212213	0.72868660	-2.68352239
N	1.56725156	0.90485288	-1.39391532
N	1.26212213	0.72868660	-2.68352239
N	0.00000000	-1.80970628	-1.39391532
N	0.00000000	-1.45737319	-2.68352239
C	-2.73337088	1.57811239	-1.42077371
C	-3.17294255	1.83189945	-2.72152948
C	-2.19379477	1.26658786	-3.50189288
C	2.73337088	1.57811239	-1.42077371
C	3.17294255	1.83189945	-2.72152948
C	2.19379477	1.26658786	-3.50189288
C	0.00000000	-3.15622478	-1.42077371
C	0.00000000	-3.66379890	-2.72152948
C	0.00000000	-2.53317625	-3.50189288
H	-4.07176863	2.35083659	-3.02086442
H	-2.08600613	1.20435609	-4.57634654
H	4.07176863	2.35083659	-3.02086442
N	3.46159604	1.99855377	-0.24520539
H	2.08600613	1.20435609	-4.57634654
N	-3.46159604	1.99855377	-0.24520539
H	0.00000000	0.00000000	-4.35577964
H	0.00000000	-4.70167318	-3.02086442
H	0.00000000	-2.40871217	-4.57634654
N	0.00000000	-3.99710701	-0.24520539
B	0.00000000	0.00000000	-3.15223267
O	0.00000000	5.20759520	0.45886970
O	4.50990993	-2.60379760	0.45886970
O	-4.50990993	-2.60379760	0.45886970
O	-4.50990993	2.60379760	-0.45886970
O	4.50990993	2.60379760	-0.45886970
O	0.00000000	-5.20759520	-0.45886970
O	3.00722911	-1.73622473	-0.85785241
O	0.00000000	3.47244893	-0.85785241
O	-3.00722911	-1.73622473	-0.85785241
O	3.00722911	1.73622473	0.85785241
O	-3.00722911	1.73622473	0.85785241
O	0.00000000	-3.47244893	0.85785241

$[Mn(Tb^{3NO2})_2]$ ^2E_g D_{3d} OPBE

$[Mn(Tb^{5CH3})_2]$ $^6A_{1g}$ D_{3d} OPBE

$[Mn(Tb^{5CH3})_2]$ ^4E_g D_{3d} OPBE

$[Mn(Tb^{5CH3})_2]$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.71301396	1.20521335
N	0.00000000	1.43714963	2.51492704
N	1.48351349	-0.85650671	1.20521335
N	1.24460795	-0.71857455	2.51492704
N	-1.48351349	-0.85650671	1.20521335
N	-1.24460795	-0.71857455	2.51492704
C	0.00000000	3.07064624	1.15691641
C	0.00000000	3.63550644	2.43435822
C	0.00000000	2.55130375	3.27425089
C	2.65925749	-1.53532312	1.15691641
C	3.14844058	-1.81775295	2.43435822
C	2.20949387	-1.27565161	3.27425089
C	-2.65925749	-1.53532312	1.15691641
C	-3.14844058	-1.81775295	2.43435822
C	-2.20949387	-1.27565161	3.27425089
H	0.00000000	4.68785689	2.67566040
H	0.00000000	2.48155766	4.35343803
H	4.05980340	-2.34392871	2.67566040
N	3.37809081	-1.95034149	-0.02746800
H	2.14909200	-1.24077883	4.35343803
N	0.00000000	3.90068351	-0.02746800
H	0.00000000	0.00000000	4.22157923
H	-4.05980340	-2.34392871	2.67566040

H	-2.14909200	-1.24077883	4.35343803
N	-3.37809081	-1.95034149	-0.02746800
B	0.00000000	0.00000000	3.01936843
N	-1.48351349	0.85650671	-1.20521335
N	-1.24460795	0.71857455	-2.51492704
N	1.48351349	0.85650671	-1.20521335
N	1.24460795	0.71857455	-2.51492704
N	0.00000000	-1.71301396	-1.20521335
N	0.00000000	-1.43714963	-2.51492704
C	-2.65925749	1.53532312	-1.15691641
C	-3.14844058	1.81775295	-2.43435822
C	-2.20949387	1.27565161	-3.27425089
C	2.65925749	1.53532312	-1.15691641
C	3.14844058	1.81775295	-2.43435822
C	2.20949387	1.27565161	-3.27425089
C	0.00000000	-3.07064624	-1.15691641
C	0.00000000	-3.63550644	-2.43435822
C	0.00000000	-2.55130375	-3.27425089
H	-4.05980340	2.34392871	-2.67566040
H	-2.14909200	1.24077883	-4.35343803
H	4.05980340	2.34392871	-2.67566040
N	3.37809081	1.95034149	0.02746800
H	2.14909200	1.24077883	-4.35343803
N	-3.37809081	1.95034149	0.02746800
H	0.00000000	0.00000000	-4.22157923
H	0.00000000	-4.68785689	-2.67566040
H	0.00000000	-2.48155766	-4.35343803
N	0.00000000	-3.90068351	0.02746800
B	0.00000000	0.00000000	-3.01936843
O	0.00000000	5.11305239	0.18568459
O	4.42803298	-2.55652620	0.18568459
O	-4.42803298	-2.55652620	0.18568459
O	-4.42803298	2.55652620	-0.18568459
O	4.42803298	2.55652620	-0.18568459
O	0.00000000	-5.11305239	-0.18568459
O	2.93121121	-1.69233583	-1.13468408
O	0.00000000	3.38467113	-1.13468408
O	-2.93121121	-1.69233583	-1.13468408
O	2.93121121	1.69233583	1.13468408
O	-2.93121121	1.69233583	1.13468408
O	0.00000000	-3.38467113	1.13468408

$[Mn(Tb^{5CF3})_2]$ $^6A_{1g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.47474979	0.85144725	1.50663642
N	1.27611093	0.73676290	2.83432944
N	0.00000000	-1.70289397	1.50663642
N	0.00000000	-1.47352580	2.83432944
N	-1.47474979	0.85144725	1.50663642
N	-1.27611093	0.73676290	2.83432944
C	2.61903579	1.51210070	1.32275050
C	3.19292375	1.84343551	2.54752965
C	2.31143352	1.33450670	3.48903176
C	0.00000000	-3.02420194	1.32275050
C	0.00000000	-3.68687103	2.54752965
C	0.00000000	-2.66901393	3.48903176
C	-2.61903579	1.51210070	1.32275050
C	-3.19292375	1.84343551	2.54752965
C	-2.31143352	1.33450670	3.48903176
H	4.11570357	2.37620270	2.73512564
C	2.49151783	1.43847839	4.97859639
H	0.00000000	-4.75240487	2.73512564
H	0.00000000	-3.43541711	0.32046127
C	0.00000000	-2.87695678	4.97859639
H	2.97515832	1.71770882	0.32046127
H	0.00000000	0.00000000	4.54826310
H	-4.11570357	2.37620270	2.73512564
C	-2.49151783	1.43847839	4.97859639
H	-2.97515832	1.71770882	0.32046127
B	0.00000000	0.00000000	3.36010831
N	0.00000000	1.70289397	-1.50663642
N	0.00000000	1.47352580	-2.83432944
N	1.47474979	-0.85144725	-1.50663642
N	1.27611093	-0.73676290	-2.83432944
N	-1.47474979	-0.85144725	-1.50663642
N	-1.27611093	-0.73676290	-2.83432944
C	0.00000000	3.02420194	-1.32275050
C	0.00000000	3.68687103	-2.54752965
C	0.00000000	2.66901393	-3.48903176
C	2.61903579	-1.51210070	-1.32275050
C	3.19292375	-1.84343551	-2.54752965
C	2.31143352	-1.33450670	-3.48903176
C	-2.61903579	-1.51210070	-1.32275050
C	-3.19292375	-1.84343551	-2.54752965
C	-2.31143352	-1.33450670	-3.48903176
H	0.00000000	4.75240487	-2.73512564
C	0.00000000	2.87695678	-4.97859639
H	4.11570357	-2.37620270	-2.73512564
H	2.97515832	-1.71770882	-0.32046127
C	2.49151783	-1.43847839	-4.97859639
H	0.00000000	3.43541711	-0.32046127
H	0.00000000	0.00000000	-4.54826310
H	-4.11570357	-2.37620270	-2.73512564
C	-2.49151783	-1.43847839	-4.97859639
H	-2.97515832	-1.71770882	-0.32046127
B	0.00000000	0.00000000	-3.36010831
F	-3.64361449	-2.10364202	-5.24548747
F	-1.49377159	-2.11902838	-5.58457102
F	-2.58201825	-0.23413024	-5.58457102
F	3.64361449	-2.10364202	-5.24548747
F	2.58201825	-0.23413024	-5.58457102
F	1.49377159	-2.11902838	-5.58457102
F	1.08824666	2.35315809	-5.58457102
F	0.00000000	4.20728404	-5.24548747
F	-1.08824666	2.35315809	-5.58457102
F	-2.58201825	0.23413024	5.58457102
F	-3.64361449	2.10364202	5.24548747
F	-1.49377159	2.11902838	5.58457102
F	-1.08824666	-2.35315809	5.58457102
F	1.08824666	-2.35315809	5.58457102
F	0.00000000	-4.20728404	5.24548747
F	2.58201825	0.23413024	5.58457102
F	1.49377159	2.11902838	5.58457102
F	3.64361449	2.10364202	5.24548747

$[Mn(Tb^{5CF3})_2]$ ^4E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.43969656	0.83120887	1.33729070

N	1.26714244	0.73158490	2.66958015
N	0.00000000	-1.66241826	1.33729070
N	0.00000000	-1.46317033	2.66958015
N	-1.43969656	0.83120887	1.33729070
N	-1.26714244	0.73158490	2.66958015
C	2.58202831	1.49073464	1.12554519
C	3.17620916	1.83378491	2.33712137
C	2.31103558	1.33427704	3.30010543
C	0.00000000	-2.98146929	1.12554519
C	0.00000000	-3.66757034	2.33712137
C	0.00000000	-2.66855408	3.30010543
C	-2.58202831	1.49073464	1.12554519
C	-3.17620916	1.83378491	2.33712137
C	-2.31103558	1.33427704	3.30010543
H	4.10233814	2.36848624	2.50286868
C	2.50404875	1.44571330	4.78687389
H	0.00000000	-4.73697194	2.50286868
H	0.00000000	-3.37026057	0.11548235
C	0.00000000	-2.89142660	4.78687389
H	2.91873162	1.68513055	0.11548235
H	0.00000000	0.00000000	4.39296387
H	-4.10233814	2.36848624	2.50286868
C	-2.50404875	1.44571330	4.78687389
H	-2.91873162	1.68513055	0.11548235
B	0.00000000	0.00000000	3.20487205
N	0.00000000	1.66241826	-1.33729070
N	0.00000000	1.46317033	-2.66958015
N	1.43969656	-0.83120887	-1.33729070
N	1.26714244	-0.73158490	-2.66958015
N	-1.43969656	-0.83120887	-1.33729070
N	-1.26714244	-0.73158490	-2.66958015
C	0.00000000	2.98146929	-1.12554519
C	0.00000000	3.66757034	-2.33712137
C	0.00000000	2.66855408	-3.30010543
C	2.58202831	-1.49073464	-1.12554519
C	3.17620916	-1.83378491	-2.33712137
C	2.31103558	-1.33427704	-3.30010543
C	-2.58202831	-1.49073464	-1.12554519
C	-3.17620916	-1.83378491	-2.33712137
C	-2.31103558	-1.33427704	-3.30010543
H	0.00000000	4.73697194	-2.50286868
C	0.00000000	2.89142660	-4.78687389
H	4.10233814	-2.36848624	-2.50286868
H	2.91873162	-1.68513055	-0.11548235
C	2.50404875	-1.44571330	-4.78687389
H	0.00000000	3.37026057	-0.11548235
H	0.00000000	0.00000000	-4.39296387
H	-4.10233814	-2.36848624	-2.50286868
C	-2.50404875	-1.44571330	-4.78687389
H	-2.91873162	-1.68513055	-0.11548235
B	0.00000000	0.00000000	-3.20487205
F	-3.65775463	-2.11180564	-5.04222308
F	-1.50943894	-2.12842392	-5.39665859
F	-2.59798882	-0.24300084	-5.39665859
F	3.65775463	-2.11180564	-5.04222308
F	2.59798882	-0.24300084	-5.39665859
F	1.50943894	-2.12842392	-5.39665859
F	1.08854935	2.37142476	-5.39665859
F	0.00000000	4.22361075	-5.04222308
F	-1.08854935	2.37142476	-5.39665859
F	-2.59798882	0.24300084	5.39665859
F	-3.65775463	2.11180564	5.04222308
F	-1.50943894	2.12842392	5.39665859
F	-1.08854935	-2.37142476	5.39665859
F	1.08854935	-2.37142476	5.39665859
F	0.00000000	-4.22361075	5.04222308
F	2.59798882	0.24300084	5.39665859
F	1.50943894	2.12842392	5.39665859
F	3.65775463	2.11180564	5.04222308

$[Mn(Tb^{5CF3})_2]$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.37591800	0.79438660	1.19951200
N	1.25065539	0.72206659	2.54145205
N	0.00000000	-1.58877372	1.19951200
N	0.00000000	-1.44413265	2.54145205
N	-1.37591800	0.79438660	1.19951200
N	-1.25065539	0.72206659	2.54145205
C	2.51450952	1.45175280	0.93666437
C	3.14498559	1.81575848	2.12255534
C	2.31386615	1.33591114	3.12466624
C	0.00000000	-2.90350560	0.93666437
C	0.00000000	-3.63151697	2.12255534
C	0.00000000	-2.67182228	3.12466624
C	-2.51450952	1.45175280	0.93666437
C	-3.14498559	1.81575848	2.12255534
C	-2.31386615	1.33591114	3.12466624
H	4.07610418	2.35334013	2.24503924
C	2.54060537	1.46681901	4.60277736
H	0.00000000	-4.70667972	2.24503924
H	0.00000000	-3.25612233	-0.08506524
C	0.00000000	-2.93363854	4.60277736
H	2.81988448	1.62806090	-0.08506524
H	0.00000000	0.00000000	4.29224239
H	-4.07610418	2.35334013	2.24503924
C	-2.54060537	1.46681901	4.60277736
H	-2.81988448	1.62806090	-0.08506524
B	0.00000000	0.00000000	3.10459825
N	0.00000000	1.58877372	-1.19951200
N	0.00000000	1.44413265	-2.54145205
N	1.37591800	-0.79438660	-1.19951200
N	1.25065539	-0.72206659	-2.54145205
N	-1.37591800	-0.79438660	-1.19951200
N	-1.25065539	-0.72206659	-2.54145205
C	0.00000000	2.90350560	-0.93666437
C	0.00000000	3.63151697	-2.12255534
C	0.00000000	2.67182228	-3.12466624
C	2.51450952	-1.45175280	-0.93666437
C	3.14498559	-1.81575848	-2.12255534
C	2.31386615	-1.33591114	-3.12466624
C	-2.51450952	-1.45175280	-0.93666437
C	-3.14498559	-1.81575848	-2.12255534
C	-2.31386615	-1.33591114	-3.12466624
H	0.00000000	4.70667972	-2.24503924
C	0.00000000	2.93363854	-4.60277736
H	4.07610418	-2.35334013	-2.24503924
H	2.81988448	-1.62806090	0.08506524
C	2.54060537	-1.46681901	-4.60277736
H	0.00000000	3.25612233	0.08506524

H	0.00000000	0.00000000	-4.29224239
H	-4.07610418	-2.35334013	-2.24503924
C	-2.54060537	-1.46681901	-4.60277736
H	-2.81988448	-1.62806090	0.08506524
B	0.00000000	0.00000000	-3.10459825
F	-3.69873042	-2.13546304	-4.82591923
F	-1.55736705	-2.15596389	-5.22594072
F	-2.64580263	-0.27073766	-5.22594072
F	3.69873042	-2.13546304	-4.82591923
F	2.64580263	-0.27073766	-5.22594072
F	1.55736705	-2.15596389	-5.22594072
F	1.08843558	2.42670103	-5.22594072
F	0.00000000	4.27092607	-4.82591923
F	-1.08843558	2.42670103	-5.22594072
F	-2.64580263	0.27073766	5.22594072
F	-3.69873042	2.13546304	4.82591923
F	-1.55736705	2.15596389	5.22594072
F	-1.08843558	-2.42670103	5.22594072
F	1.08843558	-2.42670103	5.22594072
F	0.00000000	-4.27092607	4.82591923
F	2.64580263	0.27073766	5.22594072
F	1.55736705	2.15596389	5.22594072
F	3.69873042	2.13546304	4.82591923

$[Mn(Tb^{5NH2})_2]$ $^6A_{1g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.73268718	-1.48089512
N	0.00000000	1.46458112	-2.81918015
N	-1.50055088	-0.86634359	-1.48089512
N	-1.26836431	-0.73229029	-2.81918015
N	1.50055088	-0.86634359	-1.48089512
N	1.26836431	-0.73229029	-2.81918015
C	0.00000000	3.05725911	-1.36240387
C	0.00000000	3.68268100	-2.61171250
C	0.00000000	2.62502713	-3.52202596
C	-2.64766428	-1.52862956	-1.36240387
C	-3.18929518	-1.84134050	-2.61171250
C	-2.27334017	-1.31251357	-3.52202596
C	2.64766428	-1.52862956	-1.36240387
C	3.18929518	-1.84134050	-2.61171250
C	2.27334017	-1.31251357	-3.52202596
H	0.00000000	4.74328503	-2.83571641
N	0.00000000	2.67521219	-4.89002271
H	-4.10780507	-2.37164225	-2.83571641
H	-3.03809813	-1.75404689	-0.37678690
N	-2.31680202	-1.33760609	-4.89002271
H	0.00000000	3.50809378	-0.37678690
H	0.00000000	0.00000000	-4.52172963
H	4.10780507	-2.37164225	-2.83571641
N	2.31680202	-1.33760609	-4.89002271
H	3.03809813	-1.75404689	-0.37678690
B	0.00000000	0.00000000	-3.30671274
N	1.50055088	0.86634359	1.48089512
N	1.26836431	0.73229029	2.81918015
N	-1.50055088	0.86634359	1.48089512
N	-1.26836431	0.73229029	2.81918015
N	0.00000000	-1.73268718	1.48089512
N	0.00000000	-1.46458112	2.81918015
C	2.64766428	1.52862956	1.36240387
C	3.18929518	1.84134050	2.61171250
C	2.27334017	1.31251357	3.52202596
C	-2.64766428	1.52862956	1.36240387
C	-3.18929518	1.84134050	2.61171250
C	-2.27334017	1.31251357	3.52202596
C	0.00000000	-3.05725911	1.36240387
C	0.00000000	-3.68268100	2.61171250
C	0.00000000	-2.62502713	3.52202596
H	4.10780507	2.37164225	2.83571641
N	2.31680202	1.33760609	4.89002271
H	-4.10780507	2.37164225	2.83571641
H	-3.03809813	1.75404689	0.37678690
N	-2.31680202	1.33760609	4.89002271
H	3.03809813	1.75404689	0.37678690
H	0.00000000	0.00000000	4.52172963
H	0.00000000	-4.74328503	2.83571641
N	0.00000000	-2.67521219	4.89002271
H	0.00000000	-3.50809378	0.37678690
B	0.00000000	0.00000000	3.30671274
H	0.00000000	3.56195450	-5.35439532
H	0.00000000	1.83686154	-5.43669455
H	-3.08474299	-1.78097725	-5.35439532
H	-1.59076872	-0.91843051	-5.43669455
H	3.08474299	-1.78097725	-5.35439532
H	1.59076872	-0.91843051	-5.43669455
H	3.08474299	1.78097725	5.35439532
H	1.59076872	0.91843051	5.43669455
H	-3.08474299	1.78097725	5.35439532
H	-1.59076872	0.91843051	5.43669455
H	0.00000000	-3.56195450	5.35439532
H	0.00000000	-1.83686154	5.43669455

$[Mn(Tb^{5NH2})_2]$ ^4E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.68077913	-1.32507041
N	0.00000000	1.45497549	-2.67078139
N	-1.45559727	-0.84038956	-1.32507041
N	-1.26004564	-0.72748801	-2.67078139
N	1.45559727	-0.84038956	-1.32507041
N	1.26004564	-0.72748801	-2.67078139
C	0.00000000	3.00257764	-1.16614102
C	0.00000000	3.66337344	-2.39682738
C	0.00000000	2.63317593	-3.33922592
C	-2.60030821	-1.50128855	-1.16614102
C	-3.17257424	-1.83168672	-2.39682738
C	-2.28039728	-1.31658823	-3.33922592
C	2.60030821	-1.50128855	-1.16614102
C	3.17257424	-1.83168672	-2.39682738
C	2.28039728	-1.31658823	-3.33922592
H	0.00000000	4.73050593	-2.58864937
N	0.00000000	2.71914025	-4.70531762
H	-4.09673838	-2.36525296	-2.58864937
H	-2.96497166	-1.71182701	-0.16875092
N	-2.35484405	-1.35957012	-4.70531762
H	0.00000000	3.42365456	-0.16875092
H	0.00000000	0.00000000	-4.38692649
H	4.09673838	-2.36525296	-2.58864937
N	2.35484405	-1.35957012	-4.70531762
H	2.96497166	-1.71182701	-0.16875092

B	0.00000000	0.00000000	-3.17117880
N	1.45559727	0.84038956	1.32507041
N	1.26004564	0.72748801	2.67078139
N	-1.45559727	0.84038956	1.32507041
N	-1.26004564	0.72748801	2.67078139
N	0.00000000	-1.68077913	1.32507041
N	0.00000000	-1.45497549	2.67078139
C	2.60030821	1.50128855	1.16614102
C	3.17257424	1.83168672	2.39682738
C	2.28039728	1.31658823	3.33922592
C	-2.60030821	1.50128855	1.16614102
C	-3.17257424	1.83168672	2.39682738
C	-2.28039728	1.31658823	3.33922592
C	0.00000000	-3.00257764	1.16614102
C	0.00000000	-3.66337344	2.39682738
C	0.00000000	-2.63317593	3.33922592
H	4.09673838	2.36525296	2.58864937
N	2.35484405	1.35957012	4.70531762
H	-4.09673838	2.36525296	2.58864937
H	-2.96497166	1.71182701	0.16875092
N	-2.35484405	1.35957012	4.70531762
H	2.96497166	1.71182701	0.16875092
H	0.00000000	0.00000000	4.38692649
H	0.00000000	-4.73050593	2.58864937
N	0.00000000	-2.71914025	4.70531762
H	0.00000000	-3.42365456	0.16875092
B	0.00000000	0.00000000	3.17117880
H	0.00000000	3.61749906	-5.14714728
H	0.00000000	1.89483132	-5.27327986
H	-3.13284626	-1.80874953	-5.14714728
H	-1.64097177	-0.94741566	-5.27327986
H	3.13284626	-1.80874953	-5.14714728
H	1.64097177	-0.94741566	-5.27327986
H	3.13284626	1.80874953	5.14714728
H	1.64097177	0.94741566	5.27327986
H	-3.13284626	1.80874953	5.14714728
H	-1.64097177	0.94741566	5.27327986
H	0.00000000	-3.61749906	5.14714728
H	0.00000000	-1.89483132	5.27327986

$[Mn(Tb^{5NH2})_2]$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.59960810	-1.19147697
N	0.00000000	1.43875409	-2.54844725
N	-1.38530084	-0.79980379	-1.19147697
N	-1.24599757	-0.71937678	-2.54844725
N	1.38530084	-0.79980379	-1.19147697
N	1.24599757	-0.71937678	-2.54844725
C	0.00000000	2.91496811	-0.96837955
C	0.00000000	3.62993367	-2.16988866
C	0.00000000	2.64670700	-3.15939244
C	-2.52443689	-1.45748432	-0.96837955
C	-3.14361502	-1.81496684	-2.16988866
C	-2.29211538	-1.32335323	-3.15939244
C	2.52443689	-1.45748432	-0.96837955
C	3.14361502	-1.81496684	-2.16988866
C	2.29211538	-1.32335323	-3.15939244
H	0.00000000	4.70490486	-2.30899348
N	0.00000000	2.78792800	-4.52169523
H	-4.07456692	-2.35245217	-2.30899348
H	-2.84833464	-1.64448656	0.04594899
N	-2.41441671	-1.39396400	-4.52169523
H	0.00000000	3.28897313	0.04594899
H	0.00000000	0.00000000	-4.29424850
H	4.07456692	-2.35245217	-2.30899348
N	2.41441671	-1.39396400	-4.52169523
H	2.84833464	-1.64448656	0.04594899
B	0.00000000	0.00000000	-3.07998621
N	1.38530084	0.79980379	1.19147697
N	1.24599757	0.71937678	2.54844725
N	-1.38530084	0.79980379	1.19147697
N	-1.24599757	0.71937678	2.54844725
N	0.00000000	-1.59960810	1.19147697
N	0.00000000	-1.43875409	2.54844725
C	2.52443689	1.45748432	0.96837955
C	3.14361502	1.81496684	2.16988866
C	2.29211538	1.32335323	3.15939244
C	-2.52443689	1.45748432	0.96837955
C	-3.14361502	1.81496684	2.16988866
C	-2.29211538	1.32335323	3.15939244
C	0.00000000	-2.91496811	0.96837955
C	0.00000000	-3.62993367	2.16988866
C	0.00000000	-2.64670700	3.15939244
H	4.07456692	2.35245217	2.30899348
N	2.41441671	1.39396400	4.52169523
H	-4.07456692	2.35245217	2.30899348
H	-2.84833464	1.64448656	-0.04594899
N	-2.41441671	1.39396400	4.52169523
H	2.84833464	1.64448656	-0.04594899
H	0.00000000	0.00000000	4.29424850
H	0.00000000	-4.70490486	2.30899348
N	0.00000000	-2.78792800	4.52169523
H	0.00000000	-3.28897313	-0.04594899
B	0.00000000	0.00000000	3.07998621
H	0.00000000	3.70340834	-4.92653541
H	0.00000000	1.98811416	-5.12373860
H	-3.20724541	-1.85170391	-4.92653541
H	-1.72175755	-0.99405734	-5.12373860
H	3.20724541	-1.85170391	-4.92653541
H	1.72175755	-0.99405734	-5.12373860
H	3.20724541	1.85170391	4.92653541
H	1.72175755	0.99405734	5.12373860
H	-3.20724541	1.85170391	4.92653541
H	-1.72175755	0.99405734	5.12373860
H	0.00000000	-3.70340834	4.92653541
H	0.00000000	-1.98811416	5.12373860

$[Mn(Tb^{5NO2})_2]$ $^6A_{1g}$ D_{3d} OPBE

[Mn	0.00000000	0.00000000	0.00000000
N	-1.47432327	-0.85120065	-1.45445743
N	-1.27927436	-0.73858962	-2.77919499
N	1.47432327	-0.85120065	-1.45445743
N	1.27927436	-0.73858962	-2.77919499
N	0.00000000	1.70240184	-1.45445743
N	0.00000000	1.47717871	-2.77919499
C	-2.61899980	-1.51208007	-1.24861224
C	-3.20584520	-1.85089532	-2.45817226
C	-2.32943031	-1.34489710	-3.40495555

C	2.61899980	-1.51208007	-1.24861224
C	3.20584520	-1.85089532	-2.45817226
C	2.32943031	-1.34489710	-3.40495555
C	0.00000000	3.02416013	-1.24861224
C	0.00000000	3.70179118	-2.45817226
C	0.00000000	2.68979420	-3.40495555
H	-4.12648820	-2.38242900	-2.65241682
N	-2.55824020	-1.47700091	-4.83819032
H	4.12648820	-2.38242900	-2.65241682
H	2.96053133	-1.70926368	-0.24010095
N	2.55824020	-1.47700091	-4.83819032
H	-2.96053133	-1.70926368	-0.24010095
H	0.00000000	0.00000000	-4.47638972
H	0.00000000	4.76485853	-2.65241682
N	0.00000000	2.95400128	-4.83819032
H	0.00000000	3.41852736	-0.24010095
B	0.00000000	0.00000000	-3.30868974
N	-1.47432327	0.85120065	1.45445743
N	-1.27927436	0.73858962	2.77919499
N	0.00000000	-1.70240184	1.45445743
N	0.00000000	-1.47717871	2.77919499
N	1.47432327	0.85120065	1.45445743
N	1.27927436	0.73858962	2.77919499
C	-2.61899980	1.51208007	1.24861224
C	-3.20584520	1.85089532	2.45817226
C	-2.32943031	1.34489710	3.40495555
C	0.00000000	-3.02416013	1.24861224
C	0.00000000	-3.70179118	2.45817226
C	0.00000000	-2.68979420	3.40495555
C	2.61899980	1.51208007	1.24861224
C	3.20584520	1.85089532	2.45817226
C	2.32943031	1.34489710	3.40495555
H	-4.12648820	2.38242900	2.65241682
N	-2.55824020	1.47700091	4.83819032
H	0.00000000	-4.76485853	2.65241682
H	0.00000000	-3.41852736	0.24010095
N	0.00000000	-2.95400128	4.83819032
H	-2.96053133	1.70926368	0.24010095
H	0.00000000	0.00000000	4.47638972
H	4.12648820	2.38242900	2.65241682
N	2.55824020	1.47700091	4.83819032
H	2.96053133	1.70926368	0.24010095
B	0.00000000	0.00000000	3.30868974
O	-3.59106825	-2.07330429	-5.13247743
O	-1.75455014	-1.01298972	-5.62813818
O	3.59106825	-2.07330429	-5.13247743
O	1.75455014	-1.01298972	-5.62813818
O	0.00000000	4.14660858	-5.13247743
O	0.00000000	2.02597997	-5.62813818
O	-3.59106825	2.07330429	5.13247743
O	-1.75455014	1.01298972	5.62813818
O	0.00000000	-4.14660858	5.13247743
O	0.00000000	-2.02597997	5.62813818
O	3.59106825	2.07330429	5.13247743
O	1.75455014	1.01298972	5.62813818

$Mn(Tb^{5NO2})_2]$ ^4E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.43050581	-0.82590281	-1.28746496
N	-1.27054240	-0.73354815	-2.61872887
N	1.43050581	-0.82590281	-1.28746496
N	1.27054240	-0.73354815	-2.61872887
N	0.00000000	1.65180614	-1.28746496
N	0.00000000	1.46709630	-2.61872887
C	-2.57104629	-1.48439404	-1.04124937
C	-3.18686150	-1.83993501	-2.23055407
C	-2.33434584	-1.34773508	-3.20757614
C	2.57104629	-1.48439404	-1.04124937
C	3.18686150	-1.83993501	-2.23055407
C	2.33434584	-1.34773508	-3.20757614
C	0.00000000	2.96878861	-1.04124937
C	0.00000000	3.67987054	-2.23055407
C	0.00000000	2.69547068	-3.20757614
H	-4.11227450	-2.37422305	-2.39340202
N	-2.59141591	-1.49615448	-4.63257162
H	4.11227450	-2.37422305	-2.39340202
H	2.88437320	-1.66529381	-0.02146872
N	2.59141591	-1.49615448	-4.63257162
H	-2.88437320	-1.66529381	-0.02146872
H	0.00000000	0.00000000	-4.33178675
H	0.00000000	4.74844557	-2.39340202
N	0.00000000	2.99230895	-4.63257162
H	0.00000000	3.33058710	-0.02146872
B	0.00000000	0.00000000	-3.16329618
N	-1.43050581	0.82590281	1.28746496
N	-1.27054240	0.73354815	2.61872887
N	0.00000000	-1.65180614	1.28746496
N	0.00000000	-1.46709630	2.61872887
N	1.43050581	0.82590281	1.28746496
N	1.27054240	0.73354815	2.61872887
C	-2.57104629	1.48439404	1.04124937
C	-3.18686150	1.83993501	2.23055407
C	-2.33434584	1.34773508	3.20757614
C	0.00000000	-2.96878861	1.04124937
C	0.00000000	-3.67987054	2.23055407
C	0.00000000	-2.69547068	3.20757614
C	2.57104629	1.48439404	1.04124937
C	3.18686150	1.83993501	2.23055407
C	2.33434584	1.34773508	3.20757614
H	-4.11227450	2.37422305	2.39340202
N	-2.59141591	1.49615448	4.63257162
H	0.00000000	-4.74844557	2.39340202
H	0.00000000	-3.33058710	0.02146872
N	0.00000000	-2.99230895	4.63257162
H	-2.88437320	1.66529381	0.02146872
H	0.00000000	0.00000000	4.33178675
H	4.11227450	2.37422305	2.39340202
N	2.59141591	1.49615448	4.63257162
H	2.88437320	1.66529381	0.02146872
B	0.00000000	0.00000000	3.16329618
O	-3.62981619	-2.09567526	-4.90039299
O	-1.80096904	-1.03978990	-5.44078351
O	3.62981619	-2.09567526	-4.90039299
O	1.80096904	-1.03978990	-5.44078351
O	0.00000000	4.19135104	-4.90039299
O	0.00000000	2.07957980	-5.44078351
O	-3.62981619	2.09567526	4.90039299
O	-1.80096904	1.03978990	5.44078351
O	0.00000000	-4.19135104	4.90039299

O	0.00000000	-2.07957980	5.44078351
O	3.62981619	2.09567526	4.90039299
O	1.80096904	1.03978990	5.44078351

$[Mn(Tb^{5NO2})_2]$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	-1.36845289	-0.79007698	-1.16777671
N	-1.25490098	-0.72451721	-2.50792603
N	1.36845289	-0.79007698	-1.16777671
N	1.25490098	-0.72451721	-2.50792603
N	0.00000000	1.58015343	-1.16777671
N	0.00000000	1.44903442	-2.50792603
C	-2.50446891	-1.44595566	-0.86998856
C	-3.15481664	-1.82143444	-2.03204857
C	-2.33691711	-1.34921995	-3.04860918
C	2.50446891	-1.44595566	-0.86998856
C	3.15481664	-1.82143444	-2.03204857
C	2.33691711	-1.34921995	-3.04860918
C	0.00000000	2.89191133	-0.86998856
C	0.00000000	3.64286888	-2.03204857
C	0.00000000	2.69843936	-3.04860918
H	-4.08514993	-2.35856258	-2.15132036
N	-2.62741372	-1.51693791	-4.45824688
H	4.08514993	-2.35856258	-2.15132036
H	2.78754805	-1.60939153	0.16010999
N	2.62741372	-1.51693791	-4.45824688
H	-2.78754805	-1.60939153	0.16010999
H	0.00000000	0.00000000	-4.25008231
H	0.00000000	4.71712515	-2.15132036
N	0.00000000	3.03387583	-4.45824688
H	0.00000000	3.21878306	0.16010999
B	0.00000000	0.00000000	-3.08188014
N	-1.36845289	0.79007698	1.16777671
N	-1.25490098	0.72451721	2.50792603
N	0.00000000	-1.58015343	1.16777671
N	0.00000000	-1.44903442	2.50792603
N	1.36845289	0.79007698	1.16777671
N	1.25490098	0.72451721	2.50792603
C	-2.50446891	1.44595566	0.86998856
C	-3.15481664	1.82143444	2.03204857
C	-2.33691711	1.34921995	3.04860918
C	0.00000000	-2.89191133	0.86998856
C	0.00000000	-3.64286888	2.03204857
C	0.00000000	-2.69843936	3.04860918
C	2.50446891	1.44595566	0.86998856
C	3.15481664	1.82143444	2.03204857
C	2.33691711	1.34921995	3.04860918
H	-4.08514993	2.35856258	2.15132036
N	-2.62741372	1.51693791	4.45824688
H	0.00000000	-4.71712515	2.15132036
H	0.00000000	-3.21878306	-0.16010999
N	0.00000000	-3.03387583	4.45824688
H	-2.78754805	1.60939153	-0.16010999
H	0.00000000	0.00000000	4.25008231
H	4.08514993	2.35856258	2.15132036
N	2.62741372	1.51693791	4.45824688
H	2.78754805	1.60939153	-0.16010999
B	0.00000000	0.00000000	3.08188014
O	-3.67225515	-2.12017775	-4.69623429
O	-1.85259610	-1.06959687	-5.28895038
O	3.67225515	-2.12017775	-4.69623429
O	1.85259610	-1.06959687	-5.28895038
O	0.00000000	4.24035497	-4.69623429
O	0.00000000	2.13919374	-5.28895038
O	-3.67225515	2.12017775	4.69623429
O	-1.85259610	1.06959687	5.28895038
O	0.00000000	-4.24035497	4.69623429
O	0.00000000	-2.13919374	5.28895038
O	3.67225515	2.12017775	4.69623429
O	1.85259610	1.06959687	5.28895038

$[Mn(Tb^{3,5\text{-}CH3})_2]$ $^6A_{1g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.55380000	0.89710000	1.47220000
N	1.27720000	0.73740000	2.78880000
N	0.00000000	-1.79410000	1.47220000
N	0.00000000	-1.47480000	2.78880000
N	-1.55380000	0.89710000	1.47220000
N	-1.27720000	0.73740000	2.78880000
C	2.71570000	1.56790000	1.39240000
C	3.18570000	1.83930000	2.68480000
C	2.24860000	1.29820000	3.55220000
C	0.00000000	-3.13580000	1.39240000
C	0.00000000	-3.67850000	2.68480000
C	0.00000000	-2.59640000	3.55220000
C	-2.71570000	1.56790000	1.39240000
C	-3.18570000	1.83930000	2.68480000
C	-2.24860000	1.29820000	3.55220000
H	4.09490000	2.36420000	2.95750000
C	2.26500000	1.30770000	5.04190000
H	0.00000000	-4.72840000	2.95750000
C	0.00000000	-3.89520000	0.10800000
C	0.00000000	-2.61540000	5.04190000
C	3.37330000	1.94760000	0.10800000
H	0.00000000	0.00000000	4.45900000
H	-4.09490000	2.36420000	2.95750000
C	-2.26500000	1.30770000	5.04190000
C	-3.37330000	1.94760000	0.10800000
B	0.00000000	0.00000000	3.26150000
N	0.00000000	1.79410000	-1.47220000
N	0.00000000	1.47480000	-2.78880000
N	1.55380000	-0.89710000	-1.47220000
N	1.27720000	-0.73740000	-2.78880000
N	-1.55380000	-0.89710000	-1.47220000
N	-1.27720000	-0.73740000	-2.78880000
C	0.00000000	3.13580000	-1.39240000
C	0.00000000	3.67850000	-2.68480000
C	0.00000000	2.59640000	-3.55220000
C	2.71570000	-1.56790000	-1.39240000
C	3.18570000	-1.83930000	-2.68480000
C	2.24860000	-1.29820000	-3.55220000
C	-2.71570000	-1.56790000	-1.39240000
C	-3.18570000	-1.83930000	-2.68480000
C	-2.24860000	-1.29820000	-3.55220000
H	0.00000000	4.72840000	-2.95750000
C	0.00000000	2.61540000	-5.04190000
H	4.09490000	-2.36420000	-2.95750000
C	3.37330000	-1.94760000	-0.10800000

C	2.26500000	-1.30770000	-5.04190000
C	0.00000000	3.89520000	-0.10800000
H	0.00000000	0.00000000	-4.45900000
H	-4.09490000	-2.36420000	-2.95750000
C	-2.26500000	-1.30770000	-5.04190000
C	-3.37330000	-1.94760000	-0.10800000
B	0.00000000	0.00000000	-3.26150000
H	-0.87570000	-3.67000000	-0.50600000
H	0.00000000	-4.96860000	0.31840000
H	0.87570000	-3.67000000	-0.50600000
H	4.30290000	2.48430000	0.31840000
H	2.74050000	2.59340000	-0.50600000
H	3.61620000	1.07660000	-0.50600000
H	-4.30290000	2.48430000	0.31840000
H	-3.61620000	1.07660000	-0.50600000
H	-2.74050000	2.59340000	-0.50600000
H	3.61620000	-1.07660000	0.50600000
H	4.30290000	-2.48430000	-0.31840000
H	2.74050000	-2.59340000	0.50600000
H	-2.74050000	-2.59340000	0.50600000
H	-4.30290000	-2.48430000	-0.31840000
H	-3.61620000	-1.07660000	0.50600000
H	-0.87570000	3.67000000	0.50600000
H	0.00000000	4.96860000	-0.31840000
H	0.87570000	3.67000000	0.50600000
H	-3.16340000	-1.82640000	-5.38840000
H	-1.39680000	-1.82660000	-5.46300000
H	-2.28030000	-0.29640000	-5.46300000
H	3.16340000	-1.82640000	-5.38840000
H	2.28030000	-0.29640000	-5.46300000
H	1.39680000	-1.82660000	-5.46300000
H	0.88350000	2.12300000	-5.46300000
H	0.00000000	3.65280000	-5.38840000
H	-0.88350000	2.12300000	-5.46300000
H	-2.28030000	0.29640000	5.46300000
H	-3.16340000	1.82640000	5.38840000
H	-1.39680000	1.82660000	5.46300000
H	-0.88350000	-2.12300000	5.46300000
H	0.88350000	-2.12300000	5.46300000
H	0.00000000	-3.65280000	5.38840000
H	2.28030000	0.29640000	5.46300000
H	1.39680000	1.82660000	5.46300000
H	3.16340000	1.82640000	5.38840000

$[Mn(Tb^{3,5\text{-}CH3})_2]$ ^4E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.51160000	0.87270000	1.32470000
N	1.26970000	0.73310000	2.64970000
N	0.00000000	-1.74550000	1.32470000
N	0.00000000	-1.46610000	2.64970000
N	-1.51160000	0.87270000	1.32470000
N	-1.26970000	0.73310000	2.64970000
C	2.67410000	1.54390000	1.20630000
C	3.17240000	1.83160000	2.48430000
C	2.25730000	1.30320000	3.38210000
C	0.00000000	-3.08780000	1.20630000
C	0.00000000	-3.66320000	2.48430000
C	0.00000000	-2.60650000	3.38210000
C	-2.67410000	1.54390000	1.20630000
C	-3.17240000	1.83160000	2.48430000
C	-2.25730000	1.30320000	3.38210000
H	4.08820000	2.36030000	2.72670000
C	2.30970000	1.33350000	4.87060000
H	0.00000000	-4.72070000	2.72670000
C	0.00000000	-3.82850000	-0.08720000
C	0.00000000	-2.66700000	4.87060000
C	3.31560000	1.91430000	-0.08720000
H	0.00000000	0.00000000	4.33300000
H	-4.08820000	2.36030000	2.72670000
C	-2.30970000	1.33350000	4.87060000
C	-3.31560000	1.91430000	-0.08720000
B	0.00000000	0.00000000	3.13330000
N	0.00000000	1.74550000	-1.32470000
N	0.00000000	1.46610000	-2.64970000
N	1.51160000	-0.87270000	-1.32470000
N	1.26970000	-0.73310000	-2.64970000
N	-1.51160000	-0.87270000	-1.32470000
N	-1.26970000	-0.73310000	-2.64970000
C	0.00000000	3.08780000	-1.20630000
C	0.00000000	3.66320000	-2.48430000
C	0.00000000	2.60650000	-3.38210000
C	2.67410000	-1.54390000	-1.20630000
C	3.17240000	-1.83160000	-2.48430000
C	2.25730000	-1.30320000	-3.38210000
C	-2.67410000	-1.54390000	-1.20630000
C	-3.17240000	-1.83160000	-2.48430000
C	-2.25730000	-1.30320000	-3.38210000
H	0.00000000	4.72070000	-2.72670000
C	0.00000000	2.66700000	-4.87060000
H	4.08820000	-2.36030000	-2.72670000
C	3.31560000	-1.91430000	0.08720000
C	2.30970000	-1.33350000	-4.87060000
C	0.00000000	3.82850000	0.08720000
H	0.00000000	0.00000000	-4.33300000
H	-4.08820000	-2.36030000	-2.72670000
C	-2.30970000	-1.33350000	-4.87060000
C	-3.31560000	-1.91430000	0.08720000
B	0.00000000	0.00000000	-3.13330000
H	-0.87680000	-3.59560000	-0.69640000
H	0.00000000	-4.90410000	0.11290000
H	0.87680000	-3.59560000	-0.69640000
H	4.24710000	2.45210000	0.11290000
H	2.67550000	2.55720000	-0.69640000
H	3.55230000	1.03850000	-0.69640000
H	-4.24710000	2.45210000	0.11290000
H	-3.55230000	1.03850000	-0.69640000
H	-2.67550000	2.55720000	-0.69640000
H	3.55230000	-1.03850000	0.69640000
H	4.24710000	-2.45210000	-0.11290000
H	2.67550000	-2.55720000	0.69640000
H	-2.67550000	-2.55720000	0.69640000
H	-4.24710000	-2.45210000	-0.11290000
H	-3.55230000	-1.03850000	0.69640000
H	-0.87680000	3.59560000	0.69640000
H	0.00000000	4.90410000	-0.11290000
H	0.87680000	3.59560000	0.69640000
H	-3.21630000	-1.85690000	-5.18730000
H	-1.45230000	-1.85840000	-5.30550000
H	-2.33560000	-0.32850000	-5.30550000

H	3.21630000	-1.85690000	-5.18730000
H	2.33560000	-0.32850000	-5.30550000
H	1.45230000	-1.85840000	-5.30550000
H	0.88330000	2.18690000	-5.30550000
H	0.00000000	3.71390000	-5.18730000
H	-0.88330000	2.18690000	-5.30550000
H	-2.33560000	0.32850000	5.30550000
H	-3.21630000	1.85690000	5.18730000
H	-1.45230000	1.85840000	5.30550000
H	-0.88330000	-2.18690000	5.30550000
H	0.88330000	-2.18690000	5.30550000
H	0.00000000	-3.71390000	5.18730000
H	2.33560000	0.32850000	5.30550000
H	1.45230000	1.85840000	5.30550000
H	3.21630000	1.85690000	5.18730000

$[Mn(Tb^{3,5\text{-}CH3})_2]$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.43830000	0.83040000	1.18910000
N	1.25190000	0.72280000	2.52790000
N	0.00000000	-1.66080000	1.18910000
N	0.00000000	-1.44560000	2.52790000
N	-1.43830000	0.83040000	1.18910000
N	-1.25190000	0.72280000	2.52790000
C	2.60060000	1.50150000	1.01220000
C	3.14220000	1.81410000	2.26700000
C	2.26380000	1.30700000	3.21110000
C	0.00000000	-3.00290000	1.01220000
C	0.00000000	-3.62830000	2.26700000
C	0.00000000	-2.61410000	3.21110000
C	-2.60060000	1.50150000	1.01220000
C	-3.14220000	1.81410000	2.26700000
C	-2.26380000	1.30700000	3.21110000
H	4.06670000	2.34790000	2.45950000
C	2.35890000	1.36190000	4.69630000
H	0.00000000	-4.69580000	2.45950000
C	0.00000000	-3.71630000	-0.29540000
C	0.00000000	-2.72380000	4.69630000
C	3.21840000	1.85810000	-0.29540000
H	0.00000000	0.00000000	4.24260000
H	-4.06670000	2.34790000	2.45950000
C	-2.35890000	1.36190000	4.69630000
C	-3.21840000	1.85810000	-0.29540000
B	0.00000000	0.00000000	3.04320000
N	0.00000000	1.66080000	-1.18910000
N	0.00000000	1.44560000	-2.52790000
N	1.43830000	-0.83040000	-1.18910000
N	1.25190000	-0.72280000	-2.52790000
N	-1.43830000	-0.83040000	-1.18910000
N	-1.25190000	-0.72280000	-2.52790000
C	0.00000000	3.00290000	-1.01220000
C	0.00000000	3.62830000	-2.26700000
C	0.00000000	2.61410000	-3.21110000
C	2.60060000	-1.50150000	-1.01220000
C	3.14220000	-1.81410000	-2.26700000
C	2.26380000	-1.30700000	-3.21110000
C	-2.60060000	-1.50150000	-1.01220000
C	-3.14220000	-1.81410000	-2.26700000
C	-2.26380000	-1.30700000	-3.21110000
H	0.00000000	4.69580000	-2.45950000
C	0.00000000	2.72380000	-4.69630000
H	4.06670000	-2.34790000	-2.45950000
C	3.21840000	-1.85810000	0.29540000
C	2.35890000	-1.36190000	-4.69630000
C	0.00000000	3.71630000	0.29540000
H	0.00000000	0.00000000	-4.24260000
H	-4.06670000	-2.34790000	-2.45950000
C	-2.35890000	-1.36190000	-4.69630000
C	-3.21840000	-1.85810000	0.29540000
B	0.00000000	0.00000000	-3.04320000
H	-0.87880000	-3.47760000	-0.89960000
H	0.00000000	-4.79460000	-0.10870000
H	0.87880000	-3.47760000	-0.89960000
H	4.15230000	2.39730000	-0.10870000
H	2.57230000	2.49990000	-0.89960000
H	3.45110000	0.97770000	-0.89960000
H	-4.15230000	2.39730000	-0.10870000
H	-3.45110000	0.97770000	-0.89960000
H	-2.57230000	2.49990000	-0.89960000
H	3.45110000	-0.97770000	0.89960000
H	4.15230000	-2.39730000	0.10870000
H	2.57230000	-2.49990000	0.89960000
H	-2.57230000	-2.49990000	0.89960000
H	-4.15230000	-2.39730000	0.10870000
H	-3.45110000	-0.97770000	0.89960000
H	-0.87880000	3.47760000	0.89960000
H	0.00000000	4.79460000	0.10870000
H	0.87880000	3.47760000	0.89960000
H	-3.27370000	-1.89000000	-4.97990000
H	-1.51240000	-1.89320000	-5.14640000
H	-2.39580000	-0.36320000	-5.14640000
H	3.27370000	-1.89000000	-4.97990000
H	2.39580000	-0.36320000	-5.14640000
H	1.51240000	-1.89320000	-5.14640000
H	0.88340000	2.25640000	-5.14640000
H	0.00000000	3.78010000	-4.97990000
H	-0.88340000	2.25640000	-5.14640000
H	-2.39580000	0.36320000	5.14640000
H	-3.27370000	1.89000000	4.97990000
H	-1.51240000	1.89320000	5.14640000
H	-0.88340000	-2.25640000	5.14640000
H	0.88340000	-2.25640000	5.14640000
H	0.00000000	-3.78010000	4.97990000
H	2.39580000	0.36320000	5.14640000
H	1.51240000	1.89320000	5.14640000
H	3.27370000	1.89000000	4.97990000

$[Mn(Tb^{3,5\text{-}CF3})_2]$ $^6A_{1g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.62166950	0.93627119	1.35240771
N	1.31166530	0.75729021	2.65727043
N	0.00000000	-1.87254291	1.35240771
N	0.00000000	-1.51458043	2.65727043
N	-1.62166950	0.93627119	1.35240771
N	-1.31166530	0.75729021	2.65727043
C	2.79096124	1.61136218	1.30815632
C	3.23736194	1.86909214	2.60195448
C	2.28555305	1.31956485	3.43329299

C	0.00000000	-3.22272490	1.30815632
C	0.00000000	-3.73818376	2.60195448
C	0.00000000	-2.63912971	3.43329299
C	-2.79096124	1.61136218	1.30815632
C	-3.23736194	1.86909214	2.60195448
C	-2.28555305	1.31956485	3.43329299
H	4.13562180	2.38770225	2.90087824
C	2.38525957	1.37713034	4.93774761
H	0.00000000	-4.77540503	2.90087824
C	0.00000000	-4.15541144	0.09190592
C	0.00000000	-2.75426068	4.93774761
C	3.59869210	2.07770598	0.09190592
H	0.00000000	0.00000000	4.30478071
H	-4.13562180	2.38770225	2.90087824
C	-2.38525957	1.37713034	4.93774761
C	-3.59869210	2.07770598	0.09190592
B	0.00000000	0.00000000	3.11704820
N	0.00000000	1.87254291	-1.35240771
N	0.00000000	1.51458043	-2.65727043
N	1.62166950	-0.93627119	-1.35240771
N	1.31166530	-0.75729021	-2.65727043
N	-1.62166950	-0.93627119	-1.35240771
N	-1.31166530	-0.75729021	-2.65727043
C	0.00000000	3.22272490	-1.30815632
C	0.00000000	3.73818376	-2.60195448
C	0.00000000	2.63912971	-3.43329299
C	2.79096124	-1.61136218	-1.30815632
C	3.23736194	-1.86909214	-2.60195448
C	2.28555305	-1.31956485	-3.43329299
C	-2.79096124	-1.61136218	-1.30815632
C	-3.23736194	-1.86909214	-2.60195448
C	-2.28555305	-1.31956485	-3.43329299
H	0.00000000	4.77540503	-2.90087824
C	0.00000000	2.75426068	-4.93774761
H	4.13562180	-2.38770225	-2.90087824
C	3.59869210	-2.07770598	-0.09190592
C	2.38525957	-1.37713034	-4.93774761
C	0.00000000	4.15541144	-0.09190592
H	0.00000000	0.00000000	-4.30478071
H	-4.13562180	-2.38770225	-2.90087824
C	-2.38525957	-1.37713034	-4.93774761
C	-3.59869210	-2.07770598	-0.09190592
B	0.00000000	0.00000000	-3.11704820
F	-1.07156858	-4.03638836	-0.70899750
F	0.00000000	-5.43308027	0.55533342
F	1.07156858	-4.03638836	-0.70899750
F	4.70518585	2.71654040	0.55533342
F	2.95983070	2.94620015	-0.70899750
F	4.03139928	1.09018821	-0.70899750
F	-4.70518585	2.71654040	0.55533342
F	-4.03139928	1.09018821	-0.70899750
F	-2.95983070	2.94620015	-0.70899750
F	4.03139928	-1.09018821	0.70899750
F	4.70518585	-2.71654040	-0.55533342
F	2.95983070	-2.94620015	0.70899750
F	-2.95983070	-2.94620015	0.70899750
F	-4.70518585	-2.71654040	-0.55533342
F	-4.03139928	-1.09018821	0.70899750
F	-1.07156858	4.03638836	0.70899750
F	0.00000000	5.43308027	-0.55533342
F	1.07156858	4.03638836	0.70899750
F	-3.52155764	-2.03317254	-5.27806203
F	-1.36246102	-2.04281945	-5.50802235
F	-2.45036425	-0.15851610	-5.50802235
F	3.52155764	-2.03317254	-5.27806203
F	2.45036425	-0.15851610	-5.50802235
F	1.36246102	-2.04281945	-5.50802235
F	1.08790323	2.20133608	-5.50802235
F	0.00000000	4.06634456	-5.27806203
F	-1.08790323	2.20133608	-5.50802235
F	-2.45036425	0.15851610	5.50802235
F	-3.52155764	2.03317254	5.27806203
F	-1.36246102	2.04281945	5.50802235
F	-1.08790323	-2.20133608	5.50802235
F	1.08790323	-2.20133608	5.50802235
F	0.00000000	-4.06634456	5.27806203
F	2.45036425	0.15851610	5.50802235
F	1.36246102	2.04281945	5.50802235
F	3.52155764	2.03317254	5.27806203

$[Mn(Tb^{3,5\text{-}CF3})_2]$ ^4E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.57087060	0.90694260	1.24170965
N	1.29712245	0.74889376	2.55409145
N	0.00000000	-1.81388520	1.24170965
N	0.00000000	-1.49778805	2.55409145
N	-1.57087060	0.90694260	1.24170965
N	-1.29712245	0.74889376	2.55409145
C	2.74193350	1.58305596	1.16166048
C	3.21675737	1.85719571	2.44136876
C	2.28398774	1.31866102	3.30108494
C	0.00000000	-3.16611193	1.16166048
C	0.00000000	-3.71439142	2.44136876
C	0.00000000	-2.63732204	3.30108494
C	-2.74193350	1.58305596	1.16166048
C	-3.21675737	1.85719571	2.44136876
C	-2.28398774	1.31866102	3.30108494
H	4.12189759	2.37977888	2.71163122
C	2.40202655	1.38681058	4.80293548
H	0.00000000	-4.75955723	2.71163122
C	0.00000000	-4.07117171	-0.06978790
C	0.00000000	-2.77362169	4.80293548
C	3.52573814	2.03558559	-0.06978790
H	0.00000000	0.00000000	4.20926369
H	-4.12189759	2.37977888	2.71163122
C	-2.40202655	1.38681058	4.80293548
C	-3.52573814	2.03558559	-0.06978790
B	0.00000000	0.00000000	3.02036223
N	0.00000000	1.81388520	-1.24170965
N	0.00000000	1.49778805	-2.55409145
N	1.57087060	-0.90694260	-1.24170965
N	1.29712245	-0.74889376	-2.55409145
N	-1.57087060	-0.90694260	-1.24170965
N	-1.29712245	-0.74889376	-2.55409145
C	0.00000000	3.16611193	-1.16166048
C	0.00000000	3.71439142	-2.44136876
C	0.00000000	2.63732204	-3.30108494
C	2.74193350	-1.58305596	-1.16166048
C	3.21675737	-1.85719571	-2.44136876

C	2.28398774	-1.31866102	-3.30108494
C	-2.74193350	-1.58305596	-1.16166048
C	-3.21675737	-1.85719571	-2.44136876
C	-2.28398774	-1.31866102	-3.30108494
H	0.00000000	4.75955723	-2.71163122
C	0.00000000	2.77362169	-4.80293548
H	4.12189759	-2.37977888	-2.71163122
C	3.52573814	-2.03558559	0.06978790
C	2.40202655	-1.38681058	-4.80293548
C	0.00000000	4.07117171	0.06978790
H	0.00000000	0.00000000	-4.20926369
H	-4.12189759	-2.37977888	-2.71163122
C	-2.40202655	-1.38681058	-4.80293548
C	-3.52573814	-2.03558559	0.06978790
B	0.00000000	0.00000000	-3.02036223
F	-1.07648146	-3.93223570	-0.86258432
F	0.00000000	-5.35992258	0.36027763
F	1.07648146	-3.93223570	-0.86258432
F	4.64182905	2.67996102	0.36027763
F	2.86717547	2.89837840	-0.86258432
F	3.94365693	1.03385782	-0.86258432
F	-4.64182905	2.67996102	0.36027763
F	-3.94365693	1.03385782	-0.86258432
F	-2.86717547	2.89837840	-0.86258432
F	3.94365693	-1.03385782	0.86258432
F	4.64182905	-2.67996102	-0.36027763
F	2.86717547	-2.89837840	0.86258432
F	-2.86717547	-2.89837840	0.86258432
F	-4.64182905	-2.67996102	-0.36027763
F	-3.94365693	-1.03385782	0.86258432
F	-1.07648146	3.93223570	0.86258432
F	0.00000000	5.35992258	-0.36027763
F	1.07648146	3.93223570	0.86258432
F	-3.54245855	-2.04523937	-5.12360683
F	-1.38465048	-2.05603723	-5.37978895
F	-2.47290561	-0.17112375	-5.37978895
F	3.54245855	-2.04523937	-5.12360683
F	2.47290561	-0.17112375	-5.37978895
F	1.38465048	-2.05603723	-5.37978895
F	1.08825513	2.22716099	-5.37978895
F	0.00000000	4.09047875	-5.12360683
F	-1.08825513	2.22716099	-5.37978895
F	-2.47290561	0.17112375	5.37978895
F	-3.54245855	2.04523937	5.12360683
F	-1.38465048	2.05603723	5.37978895
F	-1.08825513	-2.22716099	5.37978895
F	1.08825513	-2.22716099	5.37978895
F	0.00000000	-4.09047875	5.12360683
F	2.47290561	0.17112375	5.37978895
F	1.38465048	2.05603723	5.37978895
F	3.54245855	2.04523937	5.12360683

$[Mn(Tb^{3,5\text{-}CF3})_2]$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.49415313	0.86264940	1.14542215
N	1.27445196	0.73580509	2.47308235
N	0.00000000	-1.72529934	1.14542215
N	0.00000000	-1.47161018	2.47308235
N	-1.49415313	0.86264940	1.14542215
N	-1.27445196	0.73580509	2.47308235
C	2.67060782	1.54187592	1.01313630
C	3.18255558	1.83744946	2.27359788
C	2.28248382	1.31779264	3.17448087
C	0.00000000	-3.08375237	1.01313630
C	0.00000000	-3.67489892	2.27359788
C	0.00000000	-2.63558528	3.17448087
C	-2.67060782	1.54187592	1.01313630
C	-3.18255558	1.83744946	2.27359788
C	-2.28248382	1.31779264	3.17448087
H	4.09542126	2.36449254	2.50364763
C	2.44298116	1.41045581	4.66973468
H	0.00000000	-4.72898507	2.50364763
C	0.00000000	-3.98630491	-0.22176443
C	0.00000000	-2.82091162	4.66973468
C	3.45224177	1.99315246	-0.22176443
H	0.00000000	0.00000000	4.15945012
H	-4.09542126	2.36449254	2.50364763
C	-2.44298116	1.41045581	4.66973468
C	-3.45224177	1.99315246	-0.22176443
B	0.00000000	0.00000000	2.97150594
N	0.00000000	1.72529934	-1.14542215
N	0.00000000	1.47161018	-2.47308235
N	1.49415313	-0.86264940	-1.14542215
N	1.27445196	-0.73580509	-2.47308235
N	-1.49415313	-0.86264940	-1.14542215
N	-1.27445196	-0.73580509	-2.47308235
C	0.00000000	3.08375237	-1.01313630
C	0.00000000	3.67489892	-2.27359788
C	0.00000000	2.63558528	-3.17448087
C	2.67060782	-1.54187592	-1.01313630
C	3.18255558	-1.83744946	-2.27359788
C	2.28248382	-1.31779264	-3.17448087
C	-2.67060782	-1.54187592	-1.01313630
C	-3.18255558	-1.83744946	-2.27359788
C	-2.28248382	-1.31779264	-3.17448087
H	0.00000000	4.72898507	-2.50364763
C	0.00000000	2.82091162	-4.66973468
H	4.09542126	-2.36449254	-2.50364763
C	3.45224177	-1.99315246	0.22176443
C	2.44298116	-1.41045581	-4.66973468
C	0.00000000	3.98630491	0.22176443
H	0.00000000	0.00000000	-4.15945012
H	-4.09542126	-2.36449254	-2.50364763
C	-2.44298116	-1.41045581	-4.66973468
C	-3.45224177	-1.99315246	0.22176443
B	0.00000000	0.00000000	-2.97150594
F	-1.07795893	-3.85477315	-1.01380994
F	0.00000000	-5.27599083	0.20791586
F	1.07795893	-3.85477315	-1.01380994
F	4.56914232	2.63799568	0.20791586
F	2.79935188	2.86092694	-1.01380994
F	3.87731133	0.99384673	-1.01380994
F	-4.56914232	2.63799568	0.20791586
F	-3.87731133	0.99384673	-1.01380994
F	-2.79935188	2.86092694	-1.01380994
F	3.87731133	-0.99384673	1.01380994
F	4.56914232	-2.63799568	-0.20791586
F	2.79935188	-2.86092694	1.01380994
F	-2.79935188	-2.86092694	1.01380994

F	-4.56914232	-2.63799568	-0.20791586
F	-3.87731133	-0.99384673	1.01380994
F	-1.07795893	3.85477315	1.01380994
F	0.00000000	5.27599083	-0.20791586
F	1.07795893	3.85477315	1.01380994
F	-3.59137676	-2.07348209	-4.94667801
F	-1.44068294	-2.08827683	-5.26424416
F	-2.52884229	-0.20353004	-5.26424416
F	3.59137676	-2.07348209	-4.94667801
F	2.52884229	-0.20353004	-5.26424416
F	1.44068294	-2.08827683	-5.26424416
F	1.08815935	2.29180634	-5.26424416
F	0.00000000	4.14696471	-4.94667801
F	-1.08815935	2.29180634	-5.26424416
F	-2.52884229	0.20353004	5.26424416
F	-3.59137676	2.07348209	4.94667801
F	-1.44068294	2.08827683	5.26424416
F	-1.08815935	-2.29180634	5.26424416
F	1.08815935	-2.29180634	5.26424416
F	0.00000000	-4.14696471	4.94667801
F	2.52884229	0.20353004	5.26424416
F	1.44068294	2.08827683	5.26424416
F	3.59137676	2.07348209	4.94667801

$[Mn(Tb^{3,5\text{-}NH2})_2]$ $^6A_{1g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.76192422	1.48106393
N	0.00000000	1.46564423	2.83218891
N	1.52587148	-0.88096211	1.48106393
N	1.26928508	-0.73282212	2.83218891
N	-1.52587148	-0.88096211	1.48106393
N	-1.26928508	-0.73282212	2.83218891
C	0.00000000	3.09926890	1.39424288
C	0.00000000	3.69082821	2.67191806
C	0.00000000	2.61051815	3.54863882
C	2.68404574	-1.54963472	1.39424288
C	3.19635070	-1.84541411	2.67191806
C	2.26077485	-1.30525908	3.54863882
C	-2.68404574	-1.54963472	1.39424288
C	-3.19635070	-1.84541411	2.67191806
C	-2.26077485	-1.30525908	3.54863882
H	0.00000000	4.74496146	2.92477853
N	0.00000000	2.64024998	4.91849244
H	4.10925713	-2.37248047	2.92477853
N	3.23822715	-1.86959116	0.19269619
N	2.28652356	-1.32012472	4.91849244
N	0.00000000	3.73918231	0.19269619
H	0.00000000	0.00000000	4.51870856
H	-4.10925713	-2.37248047	2.92477853
N	-2.28652356	-1.32012472	4.91849244
N	-3.23822715	-1.86959116	0.19269619
B	0.00000000	0.00000000	3.30169825
N	-1.52587148	0.88096211	-1.48106393
N	-1.26928508	0.73282212	-2.83218891
N	1.52587148	0.88096211	-1.48106393
N	1.26928508	0.73282212	-2.83218891
N	0.00000000	-1.76192422	-1.48106393
N	0.00000000	-1.46564423	-2.83218891
C	-2.68404574	1.54963472	-1.39424288
C	-3.19635070	1.84541411	-2.67191806
C	-2.26077485	1.30525908	-3.54863882
C	2.68404574	1.54963472	-1.39424288
C	3.19635070	1.84541411	-2.67191806
C	2.26077485	1.30525908	-3.54863882
C	0.00000000	-3.09926890	-1.39424288
C	0.00000000	-3.69082821	-2.67191806
C	0.00000000	-2.61051815	-3.54863882
H	-4.10925713	2.37248047	-2.92477853
N	-2.28652356	1.32012472	-4.91849244
H	4.10925713	2.37248047	-2.92477853
N	3.23822715	1.86959116	-0.19269619
N	2.28652356	1.32012472	-4.91849244
N	-3.23822715	1.86959116	-0.19269619
H	0.00000000	0.00000000	-4.51870856
H	0.00000000	-4.74496146	-2.92477853
N	0.00000000	-2.64024998	-4.91849244
N	0.00000000	-3.73918231	-0.19269619
B	0.00000000	0.00000000	-3.30169825
H	0.00000000	3.51912131	5.39681364
H	0.00000000	1.79179628	5.44880689
H	3.04764819	-1.75956039	5.39681364
H	1.55174137	-0.89589814	5.44880689
H	-3.04764819	-1.75956039	5.39681364
H	-1.55174137	-0.89589814	5.44880689
H	-3.04764819	1.75956039	-5.39681364
H	-1.55174137	0.89589814	-5.44880689
H	3.04764819	1.75956039	-5.39681364
H	1.55174137	0.89589814	-5.44880689
H	0.00000000	-3.51912131	-5.39681364
H	0.00000000	-1.79179628	-5.44880689
H	0.00000000	4.73848539	0.15340055
H	4.10364838	-2.36924243	0.15340055
H	-4.10364838	-2.36924243	0.15340055
H	-4.10364838	2.36924243	-0.15340055
H	4.10364838	2.36924243	-0.15340055
H	0.00000000	-4.73848539	-0.15340055
H	2.78372263	-1.60718327	-0.66366553
H	0.00000000	3.21436654	-0.66366553
H	-2.78372263	-1.60718327	-0.66366553
H	2.78372263	1.60718327	0.66366553
H	-2.78372263	1.60718327	0.66366553
H	0.00000000	-3.21436654	0.66366553

$[Mn(Tb^{3,5\text{-}NH2})_2]$ ^4E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.57087060	0.90694260	1.24170965
N	1.29712245	0.74889376	2.55409145
N	0.00000000	-1.81388520	1.24170965
N	0.00000000	-1.49778805	2.55409145
N	-1.57087060	0.90694260	1.24170965
N	-1.29712245	0.74889376	2.55409145
C	2.74193350	1.58305596	1.16166048
C	3.21675737	1.85719571	2.44136876
C	2.28398774	1.31866102	3.30108494
C	0.00000000	-3.16611193	1.16166048
C	0.00000000	-3.71439142	2.44136876
C	0.00000000	-2.63732204	3.30108494
C	-2.74193350	1.58305596	1.16166048

C	-3.21675737	1.85719571	2.44136876
C	-2.28398774	1.31866102	3.30108494
H	4.12189759	2.37977888	2.71163122
C	2.40202655	1.38681058	4.80293548
H	0.00000000	-4.75955723	2.71163122
C	0.00000000	-4.07117171	-0.06978790
C	0.00000000	-2.77362169	4.80293548
C	3.52573814	2.03558559	-0.06978790
H	0.00000000	0.00000000	4.20926369
H	-4.12189759	2.37977888	2.71163122
C	-2.40202655	1.38681058	4.80293548
C	-3.52573814	2.03558559	-0.06978790
B	0.00000000	0.00000000	3.02036223
N	0.00000000	1.81388520	-1.24170965
N	0.00000000	1.49778805	-2.55409145
N	1.57087060	-0.90694260	-1.24170965
N	1.29712245	-0.74889376	-2.55409145
N	-1.57087060	-0.90694260	-1.24170965
N	-1.29712245	-0.74889376	-2.55409145
C	0.00000000	3.16611193	-1.16166048
C	0.00000000	3.71439142	-2.44136876
C	0.00000000	2.63732204	-3.30108494
C	2.74193350	-1.58305596	-1.16166048
C	3.21675737	-1.85719571	-2.44136876
C	2.28398774	-1.31866102	-3.30108494
C	-2.74193350	-1.58305596	-1.16166048
C	-3.21675737	-1.85719571	-2.44136876
C	-2.28398774	-1.31866102	-3.30108494
H	0.00000000	4.75955723	-2.71163122
C	0.00000000	2.77362169	-4.80293548
H	4.12189759	-2.37977888	-2.71163122
C	3.52573814	-2.03558559	0.06978790
C	2.40202655	-1.38681058	-4.80293548
C	0.00000000	4.07117171	0.06978790
H	0.00000000	0.00000000	-4.20926369
H	-4.12189759	-2.37977888	-2.71163122
C	-2.40202655	-1.38681058	-4.80293548
C	-3.52573814	-2.03558559	0.06978790
B	0.00000000	0.00000000	-3.02036223
F	-1.07648146	-3.93223570	-0.86258432
F	0.00000000	-5.35992258	0.36027763
F	1.07648146	-3.93223570	-0.86258432
F	4.64182905	2.67996102	0.36027763
F	2.86717547	2.89837840	-0.86258432
F	3.94365693	1.03385782	-0.86258432
F	-4.64182905	2.67996102	0.36027763
F	-3.94365693	1.03385782	-0.86258432
F	-2.86717547	2.89837840	-0.86258432
F	3.94365693	-1.03385782	0.86258432
F	4.64182905	-2.67996102	-0.36027763
F	2.86717547	-2.89837840	0.86258432
F	-2.86717547	-2.89837840	0.86258432
F	-4.64182905	-2.67996102	-0.36027763
F	-3.94365693	-1.03385782	0.86258432
F	-1.07648146	3.93223570	0.86258432
F	0.00000000	5.35992258	-0.36027763
F	1.07648146	3.93223570	0.86258432
F	-3.54245855	-2.04523937	-5.12360683
F	-1.38465048	-2.05603723	-5.37978895
F	-2.47290561	-0.17112375	-5.37978895
F	3.54245855	-2.04523937	-5.12360683
F	2.47290561	-0.17112375	-5.37978895
F	1.38465048	-2.05603723	-5.37978895
F	1.08825513	2.22716099	-5.37978895
F	0.00000000	4.09047875	-5.12360683
F	-1.08825513	2.22716099	-5.37978895
F	-2.47290561	0.17112375	5.37978895
F	-3.54245855	2.04523937	5.12360683
F	-1.38465048	2.05603723	5.37978895
F	-1.08825513	-2.22716099	5.37978895
F	1.08825513	-2.22716099	5.37978895
F	0.00000000	-4.09047875	5.12360683
F	2.47290561	0.17112375	5.37978895
F	1.38465048	2.05603723	5.37978895
F	3.54245855	2.04523937	5.12360683

$[Mn(Tb^{3,5\text{-}NH2})_2]$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	1.49415313	0.86264940	1.14542215
N	1.27445196	0.73580509	2.47308235
N	0.00000000	-1.72529934	1.14542215
N	0.00000000	-1.47161018	2.47308235
N	-1.49415313	0.86264940	1.14542215
N	-1.27445196	0.73580509	2.47308235
C	2.67060782	1.54187592	1.01313630
C	3.18255558	1.83744946	2.27359788
C	2.28248382	1.31779264	3.17448087
C	0.00000000	-3.08375237	1.01313630
C	0.00000000	-3.67489892	2.27359788
C	0.00000000	-2.63558528	3.17448087
C	-2.67060782	1.54187592	1.01313630
C	-3.18255558	1.83744946	2.27359788
C	-2.28248382	1.31779264	3.17448087
H	4.09542126	2.36449254	2.50364763
C	2.44298116	1.41045581	4.66973468
H	0.00000000	-4.72898507	2.50364763
C	0.00000000	-3.98630491	-0.22176443
C	0.00000000	-2.82091162	4.66973468
C	3.45224177	1.99315246	-0.22176443
H	0.00000000	0.00000000	4.15945012
H	-4.09542126	2.36449254	2.50364763
C	-2.44298116	1.41045581	4.66973468
C	-3.45224177	1.99315246	-0.22176443
B	0.00000000	0.00000000	2.97150594
N	0.00000000	1.72529934	-1.14542215
N	0.00000000	1.47161018	-2.47308235
N	1.49415313	-0.86264940	-1.14542215
N	1.27445196	-0.73580509	-2.47308235
N	-1.49415313	-0.86264940	-1.14542215
N	-1.27445196	-0.73580509	-2.47308235
C	0.00000000	3.08375237	-1.01313630
C	0.00000000	3.67489892	-2.27359788
C	0.00000000	2.63558528	-3.17448087
C	2.67060782	-1.54187592	-1.01313630
C	3.18255558	-1.83744946	-2.27359788
C	2.28248382	-1.31779264	-3.17448087
C	-2.67060782	-1.54187592	-1.01313630
C	-3.18255558	-1.83744946	-2.27359788
C	-2.28248382	-1.31779264	-3.17448087

H	0.00000000	4.72898507	-2.50364763
C	0.00000000	2.82091162	-4.66973468
H	4.09542126	-2.36449254	-2.50364763
C	3.45224177	-1.99315246	0.22176443
C	2.44298116	-1.41045581	-4.66973468
C	0.00000000	3.98630491	0.22176443
H	0.00000000	0.00000000	-4.15945012
H	-4.09542126	-2.36449254	-2.50364763
C	-2.44298116	-1.41045581	-4.66973468
C	-3.45224177	-1.99315246	0.22176443
B	0.00000000	0.00000000	-2.97150594
F	-1.07795893	-3.85477315	-1.01380994
F	0.00000000	-5.27599083	0.20791586
F	1.07795893	-3.85477315	-1.01380994
F	4.56914232	2.63799568	0.20791586
F	2.79935188	2.86092694	-1.01380994
F	3.87731133	0.99384673	-1.01380994
F	-4.56914232	2.63799568	0.20791586
F	-3.87731133	0.99384673	-1.01380994
F	-2.79935188	2.86092694	-1.01380994
F	3.87731133	-0.99384673	1.01380994
F	4.56914232	-2.63799568	-0.20791586
F	2.79935188	-2.86092694	1.01380994
F	-2.79935188	-2.86092694	1.01380994
F	-4.56914232	-2.63799568	-0.20791586
F	-3.87731133	-0.99384673	1.01380994
F	-1.07795893	3.85477315	1.01380994
F	0.00000000	5.27599083	-0.20791586
F	1.07795893	3.85477315	1.01380994
F	-3.59137676	-2.07348209	-4.94667801
F	-1.44068294	-2.08827683	-5.26424416
F	-2.52884229	-0.20353004	-5.26424416
F	3.59137676	-2.07348209	-4.94667801
F	2.52884229	-0.20353004	-5.26424416
F	1.44068294	-2.08827683	-5.26424416
F	1.08815935	2.29180634	-5.26424416
F	0.00000000	4.14696471	-4.94667801
F	-1.08815935	2.29180634	-5.26424416
F	-2.52884229	0.20353004	5.26424416
F	-3.59137676	2.07348209	4.94667801
F	-1.44068294	2.08827683	5.26424416
F	-1.08815935	-2.29180634	5.26424416
F	1.08815935	-2.29180634	5.26424416
F	0.00000000	-4.14696471	4.94667801
F	2.52884229	0.20353004	5.26424416
F	1.44068294	2.08827683	5.26424416
F	3.59137676	2.07348209	4.94667801

$[Mn(Tb^{3,5\text{-}NO2})_2]$ $^6A_{1g}$ D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.76742449	1.75523331
N	0.00000000	1.47732159	3.06047598
N	1.53063461	-0.88371225	1.75523331
N	1.27939765	-0.73866053	3.06047598
N	-1.53063461	-0.88371225	1.75523331
N	-1.27939765	-0.73866053	3.06047598
C	0.00000000	3.10379072	1.67753580
C	0.00000000	3.71526826	2.91876178
C	0.00000000	2.64558038	3.78248753
C	2.68796165	-1.55189536	1.67753580
C	3.21751674	-1.85763440	2.91876178
C	2.29113957	-1.32279019	3.78248753
C	-2.68796165	-1.55189536	1.67753580
C	-3.21751674	-1.85763440	2.91876178
C	-2.29113957	-1.32279019	3.78248753
H	0.00000000	4.76682230	3.15874261
N	0.00000000	2.83203069	5.23624750
H	4.12818950	-2.38341115	3.15874261
N	3.29920054	-1.90479414	0.42064987
N	2.45261060	-1.41601534	5.23624750
N	0.00000000	3.80958829	0.42064987
H	0.00000000	0.00000000	4.71856822
H	-4.12818950	-2.38341115	3.15874261
N	-2.45261060	-1.41601534	5.23624750
N	-3.29920054	-1.90479414	0.42064987
B	0.00000000	0.00000000	3.55333897
N	-1.53063461	0.88371225	-1.75523331
N	-1.27939765	0.73866053	-3.06047598
N	1.53063461	0.88371225	-1.75523331
N	1.27939765	0.73866053	-3.06047598
N	0.00000000	-1.76742449	-1.75523331
N	0.00000000	-1.47732159	-3.06047598
C	-2.68796165	1.55189536	-1.67753580
C	-3.21751674	1.85763440	-2.91876178
C	-2.29113957	1.32279019	-3.78248753
C	2.68796165	1.55189536	-1.67753580
C	3.21751674	1.85763440	-2.91876178
C	2.29113957	1.32279019	-3.78248753
C	0.00000000	-3.10379072	-1.67753580
C	0.00000000	-3.71526826	-2.91876178
C	0.00000000	-2.64558038	-3.78248753
H	-4.12818950	2.38341115	-3.15874261
N	-2.45261060	1.41601534	-5.23624750
H	4.12818950	2.38341115	-3.15874261
N	3.29920054	1.90479414	-0.42064987
N	2.45261060	1.41601534	-5.23624750
N	-3.29920054	1.90479414	-0.42064987
H	0.00000000	0.00000000	-4.71856822
H	0.00000000	-4.76682230	-3.15874261
N	0.00000000	-2.83203069	-5.23624750
N	0.00000000	-3.80958829	-0.42064987
B	0.00000000	0.00000000	-3.55333897
O	0.00000000	4.00577070	5.58739577
O	0.00000000	1.86563344	5.97448892
O	3.46909924	-2.00288508	5.58739577
O	1.61568609	-0.93281672	5.97448892
O	-3.46909924	-2.00288508	5.58739577
O	-1.61568609	-0.93281672	5.97448892
O	-3.46909924	2.00288508	-5.58739577
O	-1.61568609	0.93281672	-5.97448892
O	3.46909924	2.00288508	-5.58739577
O	1.61568609	0.93281672	-5.97448892
O	0.00000000	-4.00577070	-5.58739577
O	0.00000000	-1.86563344	-5.97448892
O	0.00000000	5.03051556	0.48073689
O	4.35655436	-2.51525778	0.48073689
O	-4.35655436	-2.51525778	0.48073689
O	-4.35655436	2.51525778	-0.48073689
O	4.35655436	2.51525778	-0.48073689

O	0.00000000	-5.03051556	-0.48073689
O	2.71880845	-1.56970482	-0.60526870
O	0.00000000	3.13940964	-0.60526870
O	-2.71880845	-1.56970482	-0.60526870
O	2.71880845	1.56970482	0.60526870
O	-2.71880845	1.56970482	0.60526870
O	0.00000000	-3.13940964	0.60526870

$[Mn(Tb^{3,5\text{-}NO2})_2]$ ^4E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.75949477	1.33821676
N	0.00000000	1.47187424	2.64897875
N	1.52376747	-0.87974765	1.33821676
N	1.27468057	-0.73593685	2.64897875
N	-1.52376747	-0.87974765	1.33821676
N	-1.27468057	-0.73593685	2.64897875
C	0.00000000	3.10669855	1.25217096
C	0.00000000	3.70361155	2.50024978
C	0.00000000	2.63869049	3.36611606
C	2.69047948	-1.55334901	1.25217096
C	3.20742162	-1.85180551	2.50024978
C	2.28517257	-1.31934525	3.36611606
C	-2.69047948	-1.55334901	1.25217096
C	-3.20742162	-1.85180551	2.50024978
C	-2.28517257	-1.31934525	3.36611606
H	0.00000000	4.75501160	2.73978980
N	0.00000000	2.82616423	4.81781065
H	4.11796051	-2.37750553	2.73978980
N	3.36387975	-1.94213712	0.02984824
N	2.44752997	-1.41308212	4.81781065
N	0.00000000	3.88427372	0.02984824
H	0.00000000	0.00000000	4.30947028
H	-4.11796051	-2.37750553	2.73978980
N	-2.44752997	-1.41308212	4.81781065
N	-3.36387975	-1.94213712	0.02984824
B	0.00000000	0.00000000	3.14445376
N	-1.52376747	0.87974765	-1.33821676
N	-1.27468057	0.73593685	-2.64897875
N	1.52376747	0.87974765	-1.33821676
N	1.27468057	0.73593685	-2.64897875
N	0.00000000	-1.75949477	-1.33821676
N	0.00000000	-1.47187424	-2.64897875
C	-2.69047948	1.55334901	-1.25217096
C	-3.20742162	1.85180551	-2.50024978
C	-2.28517257	1.31934525	-3.36611606
C	2.69047948	1.55334901	-1.25217096
C	3.20742162	1.85180551	-2.50024978
C	2.28517257	1.31934525	-3.36611606
C	0.00000000	-3.10669855	-1.25217096
C	0.00000000	-3.70361155	-2.50024978
C	0.00000000	-2.63869049	-3.36611606
H	-4.11796051	2.37750553	-2.73978980
N	-2.44752997	1.41308212	-4.81781065
H	4.11796051	2.37750553	-2.73978980
N	3.36387975	1.94213712	-0.02984824
N	2.44752997	1.41308212	-4.81781065
N	-3.36387975	1.94213712	-0.02984824
H	0.00000000	0.00000000	-4.30947028
H	0.00000000	-4.75501160	-2.73978980
N	0.00000000	-2.82616423	-4.81781065
N	0.00000000	-3.88427372	-0.02984824
B	0.00000000	0.00000000	-3.14445376
O	0.00000000	4.00107743	5.16600557
O	0.00000000	1.86034802	5.55736337
O	3.46503463	-2.00053871	5.16600557
O	1.61110871	-0.93017401	5.55736337
O	-3.46503463	-2.00053871	5.16600557
O	-1.61110871	-0.93017401	5.55736337
O	-3.46503463	2.00053871	-5.16600557
O	-1.61110871	0.93017401	-5.55736337
O	3.46503463	2.00053871	-5.16600557
O	1.61110871	0.93017401	-5.55736337
O	0.00000000	-4.00107743	-5.16600557
O	0.00000000	-1.86034802	-5.55736337
O	0.00000000	5.09961605	0.18097386
O	4.41639690	-2.54980776	0.18097386
O	-4.41639690	-2.54980776	0.18097386
O	-4.41639690	2.54980776	-0.18097386
O	4.41639690	2.54980776	-0.18097386
O	0.00000000	-5.09961605	-0.18097386
O	2.85558649	-1.64867394	-1.04258978
O	0.00000000	3.29734736	-1.04258978
O	-2.85558649	-1.64867394	-1.04258978
O	2.85558649	1.64867394	1.04258978
O	-2.85558649	1.64867394	1.04258978
O	0.00000000	-3.29734736	1.04258978

$[Mn(Tb^{3,5\text{-}NO2})_2]$ ^2E_g D_{3d} OPBE

Mn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.68652176	1.16702263
N	0.00000000	1.45609100	2.48894920
N	1.46057101	-0.84326088	1.16702263
N	1.26101192	-0.72804523	2.48894920
N	-1.46057101	-0.84326088	1.16702263
N	-1.26101192	-0.72804523	2.48894920
C	0.00000000	3.03978726	1.03180779
C	0.00000000	3.67381146	2.26193058
C	0.00000000	2.64061987	3.16402062
C	2.63253298	-1.51989390	1.03180779
C	3.18161418	-1.83690547	2.26193058
C	2.28684424	-1.32030994	3.16402062
C	-2.63253298	-1.51989390	1.03180779
C	-3.18161418	-1.83690547	2.26193058
C	-2.28684424	-1.32030994	3.16402062
H	0.00000000	4.73268984	2.46448534
N	0.00000000	2.86516724	4.60934286
H	4.09862966	-2.36634519	2.46448534
N	3.31236964	-1.91239736	-0.19531562
N	2.48130736	-1.43258336	4.60934286
N	0.00000000	3.82479473	-0.19531562
H	0.00000000	0.00000000	4.16944734
H	-4.09862966	-2.36634519	2.46448534
N	-2.48130736	-1.43258336	4.60934286
N	-3.31236964	-1.91239736	-0.19531562
B	0.00000000	0.00000000	3.00373759
N	-1.46057101	0.84326088	-1.16702263
N	-1.26101192	0.72804523	-2.48894920
N	1.46057101	0.84326088	-1.16702263

N	1.26101192	0.72804523	-2.48894920
N	0.00000000	-1.68652176	-1.16702263
N	0.00000000	-1.45609100	-2.48894920
C	-2.63253298	1.51989390	-1.03180779
C	-3.18161418	1.83690547	-2.26193058
C	-2.28684424	1.32030994	-3.16402062
C	2.63253298	1.51989390	-1.03180779
C	3.18161418	1.83690547	-2.26193058
C	2.28684424	1.32030994	-3.16402062
C	0.00000000	-3.03978726	-1.03180779
C	0.00000000	-3.67381146	-2.26193058
C	0.00000000	-2.64061987	-3.16402062
H	-4.09862966	2.36634519	-2.46448534
N	-2.48130736	1.43258336	-4.60934286
H	4.09862966	2.36634519	-2.46448534
N	3.31236964	1.91239736	0.19531562
N	2.48130736	1.43258336	-4.60934286
N	-3.31236964	1.91239736	0.19531562
H	0.00000000	0.00000000	-4.16944734
H	0.00000000	-4.73268984	-2.46448534
N	0.00000000	-2.86516724	-4.60934286
N	0.00000000	-3.82479473	0.19531562
B	0.00000000	0.00000000	-3.00373759
O	0.00000000	4.04839751	4.92657139
O	0.00000000	1.91683504	5.37181531
O	3.50601518	-2.02419876	4.92657139
O	1.66002797	-0.95841726	5.37181531
O	-3.50601518	-2.02419876	4.92657139
O	-1.66002797	-0.95841726	5.37181531
O	-3.50601518	2.02419876	-4.92657139
O	-1.66002797	0.95841726	-5.37181531
O	3.50601518	2.02419876	-4.92657139
O	1.66002797	0.95841726	-5.37181531
O	0.00000000	-4.04839751	-4.92657139
O	0.00000000	-1.91683504	-5.37181531
O	0.00000000	5.03769491	-0.02695629
O	4.36277166	-2.51884719	-0.02695629
O	-4.36277166	-2.51884719	-0.02695629
O	-4.36277166	2.51884719	0.02695629
O	4.36277166	2.51884719	0.02695629
O	0.00000000	-5.03769491	0.02695629
O	2.82407292	-1.63047924	-1.27771487
O	0.00000000	3.26095901	-1.27771487
O	-2.82407292	-1.63047924	-1.27771487
O	2.82407292	1.63047924	1.27771487
O	-2.82407292	1.63047924	1.27771487
O	0.00000000	-3.26095901	1.27771487

$[Fe(Tb^{3CH3})_2]^+$ $^6A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.50546376	0.86917998	1.31058895
N	1.25538888	0.72479926	2.63163179
N	0.00000000	-1.73835996	1.31058895
N	0.00000000	-1.44959799	2.63163179
N	-1.50546376	0.86917998	1.31058895
N	-1.25538888	0.72479926	2.63163179
C	2.67786442	1.54606595	1.19814778
C	3.16312049	1.82622826	2.48129201
C	2.23452078	1.29010132	3.35527692
C	0.00000000	-3.09213189	1.19814778
C	0.00000000	-3.65245704	2.48129201
C	0.00000000	-2.58020265	3.35527692
C	-2.67786442	1.54606595	1.19814778
C	-3.16312049	1.82622826	2.48129201
C	-2.23452078	1.29010132	3.35527692
H	4.07558082	2.35303744	2.73470071
H	2.20259023	1.27166585	4.43735232
H	0.00000000	-4.70607487	2.73470071
C	0.00000000	-3.84395729	-0.08654006
H	0.00000000	-2.54333169	4.43735232
C	3.32896464	1.92197865	-0.08654006
H	0.00000000	0.00000000	4.34320427
H	-4.07558082	2.35303744	2.73470071
H	-2.20259023	1.27166585	4.43735232
C	-3.32896464	1.92197865	-0.08654006
B	0.00000000	0.00000000	3.14246511
N	0.00000000	1.73835996	-1.31058895
N	0.00000000	1.44959799	-2.63163179
N	1.50546376	-0.86917998	-1.31058895
N	1.25538888	-0.72479926	-2.63163179
N	-1.50546376	-0.86917998	-1.31058895
N	-1.25538888	-0.72479926	-2.63163179
C	0.00000000	3.09213189	-1.19814778
C	0.00000000	3.65245704	-2.48129201
C	0.00000000	2.58020265	-3.35527692
C	2.67786442	-1.54606595	-1.19814778
C	3.16312049	-1.82622826	-2.48129201
C	2.23452078	-1.29010132	-3.35527692
C	-2.67786442	-1.54606595	-1.19814778
C	-3.16312049	-1.82622826	-2.48129201
C	-2.23452078	-1.29010132	-3.35527692
H	0.00000000	4.70607487	-2.73470071
H	0.00000000	2.54333169	-4.43735232
H	4.07558082	-2.35303744	-2.73470071
C	3.32896464	-1.92197865	0.08654006
H	2.20259023	-1.27166585	-4.43735232
C	0.00000000	3.84395729	0.08654006
H	0.00000000	0.00000000	-4.34320427
H	-4.07558082	-2.35303744	-2.73470071
H	-2.20259023	-1.27166585	-4.43735232
C	-3.32896464	-1.92197865	0.08654006
B	0.00000000	0.00000000	-3.14246511
H	-0.87842788	-3.62062015	-0.69710953
H	0.00000000	-4.91580052	0.12538643
H	0.87842788	-3.62062015	-0.69710953
H	4.25720821	2.45790026	0.12538643
H	2.69633483	2.57105053	-0.69710953
H	3.57476271	1.04956910	-0.69710953
H	-4.25720821	2.45790026	0.12538643
H	-3.57476271	1.04956910	-0.69710953
H	-2.69633483	2.57105053	-0.69710953
H	3.57476271	-1.04956910	0.69710953
H	4.25720821	-2.45790026	-0.12538643
H	2.69633483	-2.57105053	0.69710953
H	-2.69633483	-2.57105053	0.69710953
H	-4.25720821	-2.45790026	-0.12538643
H	-3.57476271	-1.04956910	0.69710953
H	-0.87842788	3.62062015	0.69710953
H	0.00000000	4.91580052	-0.12538643

H	0.87842788	3.62062015	0.69710953

$[Fe(Tb^{3CH3})_2]^+$ ^4E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.47472862	0.85143508	1.22409017
N	1.24840321	0.72076587	2.54834723
N	0.00000000	-1.70286963	1.22409017
N	0.00000000	-1.44153174	2.54834723
N	-1.47472862	0.85143508	1.22409017
N	-1.24840321	0.72076587	2.54834723
C	2.64524329	1.52723200	1.07999414
C	3.15067953	1.81904573	2.35383173
C	2.23867218	1.29249797	3.24963250
C	0.00000000	-3.05446347	1.07999414
C	0.00000000	-3.63809147	2.35383173
C	0.00000000	-2.58499593	3.24963250
C	-2.64524329	1.52723200	1.07999414
C	-3.15067953	1.81904573	2.35383173
C	-2.23867218	1.29249797	3.24963250
H	4.06781991	2.34855689	2.58370209
H	2.22423252	1.28416131	4.33212066
H	0.00000000	-4.69711379	2.58370209
C	0.00000000	-3.79500099	-0.21052206
H	0.00000000	-2.56832209	4.33212066
C	3.28656749	1.89750049	-0.21052206
H	0.00000000	0.00000000	4.26910306
H	-4.06781991	2.34855689	2.58370209
H	-2.22423252	1.28416131	4.33212066
C	-3.28656749	1.89750049	-0.21052206
B	0.00000000	0.00000000	3.06855916
N	0.00000000	1.70286963	-1.22409017
N	0.00000000	1.44153174	-2.54834723
N	1.47472862	-0.85143508	-1.22409017
N	1.24840321	-0.72076587	-2.54834723
N	-1.47472862	-0.85143508	-1.22409017
N	-1.24840321	-0.72076587	-2.54834723
C	0.00000000	3.05446347	-1.07999414
C	0.00000000	3.63809147	-2.35383173
C	0.00000000	2.58499593	-3.24963250
C	2.64524329	-1.52723200	-1.07999414
C	3.15067953	-1.81904573	-2.35383173
C	2.23867218	-1.29249797	-3.24963250
C	-2.64524329	-1.52723200	-1.07999414
C	-3.15067953	-1.81904573	-2.35383173
C	-2.23867218	-1.29249797	-3.24963250
H	0.00000000	4.69711379	-2.58370209
H	0.00000000	2.56832209	-4.33212066
H	4.06781991	-2.34855689	-2.58370209
C	3.28656749	-1.89750049	0.21052206
H	2.22423252	-1.28416131	-4.33212066
C	0.00000000	3.79500099	0.21052206
H	0.00000000	0.00000000	-4.26910306
H	-4.06781991	-2.34855689	-2.58370209
H	-2.22423252	-1.28416131	-4.33212066
C	-3.28656749	-1.89750049	0.21052206
B	0.00000000	0.00000000	-3.06855916
H	-0.87934759	-3.56944871	-0.81870388
H	0.00000000	-4.86793591	-0.00343330
H	0.87934759	-3.56944871	-0.81870388
H	4.21575617	2.43396769	-0.00343330
H	2.65155902	2.54626175	-0.81870388
H	3.53090661	1.02318696	-0.81870388
H	-4.21575617	2.43396769	-0.00343330
H	-3.53090661	1.02318696	-0.81870388
H	-2.65155902	2.54626175	-0.81870388
H	3.53090661	-1.02318696	0.81870388
H	4.21575617	-2.43396769	0.00343330
H	2.65155902	-2.54626175	0.81870388
H	-2.65155902	-2.54626175	0.81870388
H	-4.21575617	-2.43396769	0.00343330
H	-3.53090661	-1.02318696	0.81870388
H	-0.87934759	3.56944871	0.81870388
H	0.00000000	4.86793591	0.00343330
H	0.87934759	3.56944871	0.81870388

$[Fe(Tb^{3CH3})_2]^+$ ^2E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.41899355	0.81925634	1.13652403
N	1.23626600	0.71375851	2.46935430
N	0.00000000	-1.63851268	1.13652403
N	0.00000000	-1.42751701	2.46935430
N	-1.41899355	0.81925634	1.13652403
N	-1.23626600	0.71375851	2.46935430
C	2.58589553	1.49296777	0.94324045
C	3.12811489	1.80601792	2.19762707
C	2.24606743	1.29676790	3.13076818
C	0.00000000	-2.98593501	0.94324045
C	0.00000000	-3.61203637	2.19762707
C	0.00000000	-2.59353580	3.13076818
C	-2.58589553	1.49296777	0.94324045
C	-3.12811489	1.80601792	2.19762707
C	-2.24606743	1.29676790	3.13076818
H	4.05199380	2.33941959	2.38727626
H	2.26275398	1.30640157	4.21307906
H	0.00000000	-4.67883918	2.38727626
C	0.00000000	-3.70164936	-0.36087560
H	0.00000000	-2.61280314	4.21307906
C	3.20572243	1.85082494	-0.36087560
H	0.00000000	0.00000000	4.21248585
H	-4.05199380	2.33941959	2.38727626
H	-2.26275398	1.30640157	4.21307906
C	-3.20572243	1.85082494	-0.36087560
B	0.00000000	0.00000000	3.01279235
N	0.00000000	1.63851268	-1.13652403
N	0.00000000	1.42751701	-2.46935430
N	1.41899355	-0.81925634	-1.13652403
N	1.23626600	-0.71375851	-2.46935430
N	-1.41899355	-0.81925634	-1.13652403
N	-1.23626600	-0.71375851	-2.46935430
C	0.00000000	2.98593501	-0.94324045
C	0.00000000	3.61203637	-2.19762707
C	0.00000000	2.59353580	-3.13076818
C	2.58589553	-1.49296777	-0.94324045
C	3.12811489	-1.80601792	-2.19762707
C	2.24606743	-1.29676790	-3.13076818
C	-2.58589553	-1.49296777	-0.94324045
C	-3.12811489	-1.80601792	-2.19762707
C	-2.24606743	-1.29676790	-3.13076818

H	0.00000000	4.67883918	-2.38727626
H	0.00000000	2.61280314	-4.21307906
H	4.05199380	-2.33941959	-2.38727626
C	3.20572243	-1.85082494	0.36087560
H	2.26275398	-1.30640157	-4.21307906
C	0.00000000	3.70164936	0.36087560
H	0.00000000	0.00000000	-4.21248585
H	-4.05199380	-2.33941959	-2.38727626
H	-2.26275398	-1.30640157	-4.21307906
C	-3.20572243	-1.85082494	0.36087560
B	0.00000000	0.00000000	-3.01279235
H	-0.88092189	-3.46969933	-0.96458006
H	0.00000000	-4.77745400	-0.16815983
H	0.88092189	-3.46969933	-0.96458006
H	4.13739666	2.38872727	-0.16815983
H	2.56438660	2.49774995	-0.96458006
H	3.44530849	0.97194885	-0.96458006
H	-4.13739666	2.38872727	-0.16815983
H	-3.44530849	0.97194885	-0.96458006
H	-2.56438660	2.49774995	-0.96458006
H	3.44530849	-0.97194885	0.96458006
H	4.13739666	-2.38872727	0.16815983
H	2.56438660	-2.49774995	0.96458006
H	-2.56438660	-2.49774995	0.96458006
H	-4.13739666	-2.38872727	0.16815983
H	-3.44530849	-0.97194885	0.96458006
H	-0.88092189	3.46969933	0.96458006
H	0.00000000	4.77745400	0.16815983
H	0.88092189	3.46969933	0.96458006

$[Fe(Tb^{3CF3})_2]^+$ $^6A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.58166211	0.91317313	1.21808453
N	1.27286867	0.73489120	2.52084854
N	0.00000000	-1.82634626	1.21808453
N	0.00000000	-1.46978240	2.52084854
N	-1.58166211	0.91317313	1.21808453
N	-1.27286867	0.73489120	2.52084854
C	2.76104527	1.59409037	1.19875686
C	3.18394097	1.83824905	2.50525316
C	2.21178415	1.27697402	3.31148486
C	0.00000000	-3.18818074	1.19875686
C	0.00000000	-3.67649809	2.50525316
C	0.00000000	-2.55394805	3.31148486
C	-2.76104527	1.59409037	1.19875686
C	-3.18394097	1.83824905	2.50525316
C	-2.21178415	1.27697402	3.31148486
H	4.07935862	2.35521870	2.82241395
H	2.12842445	1.22884641	4.38933318
H	0.00000000	-4.71043741	2.82241395
C	0.00000000	-4.13188687	-0.00556589
H	0.00000000	-2.45769282	4.38933318
C	3.57831878	2.06594343	-0.00556589
H	0.00000000	0.00000000	4.19714183
H	-4.07935862	2.35521870	2.82241395
H	-2.12842445	1.22884641	4.38933318
C	-3.57831878	2.06594343	-0.00556589
B	0.00000000	0.00000000	2.99853419
N	0.00000000	1.82634626	-1.21808453
N	0.00000000	1.46978240	-2.52084854
N	1.58166211	-0.91317313	-1.21808453
N	1.27286867	-0.73489120	-2.52084854
N	-1.58166211	-0.91317313	-1.21808453
N	-1.27286867	-0.73489120	-2.52084854
C	0.00000000	3.18818074	-1.19875686
C	0.00000000	3.67649809	-2.50525316
C	0.00000000	2.55394805	-3.31148486
C	2.76104527	-1.59409037	-1.19875686
C	3.18394097	-1.83824905	-2.50525316
C	2.21178415	-1.27697402	-3.31148486
C	-2.76104527	-1.59409037	-1.19875686
C	-3.18394097	-1.83824905	-2.50525316
C	-2.21178415	-1.27697402	-3.31148486
H	0.00000000	4.71043741	-2.82241395
H	0.00000000	2.45769282	-4.38933318
H	4.07935862	-2.35521870	-2.82241395
C	3.57831878	-2.06594343	0.00556589
H	2.12842445	-1.22884641	-4.38933318
C	0.00000000	4.13188687	0.00556589
H	0.00000000	0.00000000	-4.19714183
H	-4.07935862	-2.35521870	-2.82241395
H	-2.12842445	-1.22884641	-4.38933318
C	-3.57831878	-2.06594343	0.00556589
B	0.00000000	0.00000000	-2.99853419
F	-1.07548979	-4.00705078	-0.80192737
F	0.00000000	-5.40143389	0.46324176
F	1.07548979	-4.00705078	-0.80192737
F	4.67777924	2.70071694	0.46324176
F	2.93246271	2.93492709	-0.80192737
F	4.00795303	1.07212369	-0.80192737
F	-4.67777924	2.70071694	0.46324176
F	-4.00795303	1.07212369	-0.80192737
F	-2.93246271	2.93492709	-0.80192737
F	4.00795303	-1.07212369	0.80192737
F	4.67777924	-2.70071694	-0.46324176
F	2.93246271	-2.93492709	0.80192737
F	-2.93246271	-2.93492709	0.80192737
F	-4.67777924	-2.70071694	-0.46324176
F	-4.00795303	-1.07212369	0.80192737
F	-1.07548979	4.00705078	0.80192737
F	0.00000000	5.40143389	-0.46324176
F	1.07548979	4.00705078	0.80192737

$[Fe(Tb^{3CF3})_2]^+$ ^4E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.53959199	0.88888390	1.16682842
N	1.26248832	0.72889774	2.47489002
N	0.00000000	-1.77776726	1.16682842
N	0.00000000	-1.45779548	2.47489002
N	-1.53959199	0.88888390	1.16682842
N	-1.26248832	0.72889774	2.47489002
C	2.71988639	1.57032713	1.10823580
C	3.16982305	1.83009813	2.40289440
C	2.21752626	1.28028932	3.23756197
C	0.00000000	-3.14065427	1.10823580
C	0.00000000	-3.66019626	2.40289440
C	0.00000000	-2.56057864	3.23756197
C	-2.71988639	1.57032713	1.10823580

C	-3.16982305	1.83009813	2.40289440
C	-2.21752626	1.28028932	3.23756197
H	4.07255604	2.35129115	2.69075730
H	2.15600887	1.24477253	4.31725184
H	0.00000000	-4.70258230	2.69075730
C	0.00000000	-4.06397755	-0.10912482
H	0.00000000	-2.48954506	4.31725184
C	3.51950761	2.03198877	-0.10912482
H	0.00000000	0.00000000	4.16351103
H	-4.07255604	2.35129115	2.69075730
H	-2.15600887	1.24477253	4.31725184
C	-3.51950761	2.03198877	-0.10912482
B	0.00000000	0.00000000	2.96487111
N	0.00000000	1.77776726	-1.16682842
N	0.00000000	1.45779548	-2.47489002
N	1.53959199	-0.88888390	-1.16682842
N	1.26248832	-0.72889774	-2.47489002
N	-1.53959199	-0.88888390	-1.16682842
N	-1.26248832	-0.72889774	-2.47489002
C	0.00000000	3.14065427	-1.10823580
C	0.00000000	3.66019626	-2.40289440
C	0.00000000	2.56057864	-3.23756197
C	2.71988639	-1.57032713	-1.10823580
C	3.16982305	-1.83009813	-2.40289440
C	2.21752626	-1.28028932	-3.23756197
C	-2.71988639	-1.57032713	-1.10823580
C	-3.16982305	-1.83009813	-2.40289440
C	-2.21752626	-1.28028932	-3.23756197
H	0.00000000	4.70258230	-2.69075730
H	0.00000000	2.48954506	-4.31725184
H	4.07255604	-2.35129115	-2.69075730
C	3.51950761	-2.03198877	0.10912482
H	2.15600887	-1.24477253	-4.31725184
C	0.00000000	4.06397755	0.10912482
H	0.00000000	0.00000000	-4.16351103
H	-4.07255604	-2.35129115	-2.69075730
H	-2.15600887	-1.24477253	-4.31725184
C	-3.51950761	-2.03198877	0.10912482
B	0.00000000	0.00000000	-2.96487111
F	-1.07826902	-3.92577074	-0.90009399
F	0.00000000	-5.34146117	0.33618154
F	1.07826902	-3.92577074	-0.90009399
F	4.62584102	2.67073059	0.33618154
F	2.86068299	2.89669403	-0.90009399
F	3.93895202	1.02907724	-0.90009399
F	-4.62584102	2.67073059	0.33618154
F	-3.93895202	1.02907724	-0.90009399
F	-2.86068299	2.89669403	-0.90009399
F	3.93895202	-1.02907724	0.90009399
F	4.62584102	-2.67073059	-0.33618154
F	2.86068299	-2.89669403	0.90009399
F	-2.86068299	-2.89669403	0.90009399
F	-4.62584102	-2.67073059	-0.33618154
F	-3.93895202	-1.02907724	0.90009399
F	-1.07826902	3.92577074	0.90009399
F	0.00000000	5.34146117	-0.33618154
F	1.07826902	3.92577074	0.90009399

$[Fe(Tb^{3CF3})_2]^+$ ^2E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.48186563	0.85555578	1.10080245
N	1.24839369	0.72076058	2.41928937
N	0.00000000	-1.71111104	1.10080245
N	0.00000000	-1.44152063	2.41928937
N	-1.48186563	0.85555578	1.10080245
N	-1.24839369	0.72076058	2.41928937
C	2.66508321	1.53868657	0.99623808
C	3.14784103	1.81740687	2.27575322
C	2.22240686	1.28310719	3.14602277
C	0.00000000	-3.07737314	0.99623808
C	0.00000000	-3.63481374	2.27575322
C	0.00000000	-2.56621437	3.14602277
C	-2.66508321	1.53868657	0.99623808
C	-3.14784103	1.81740687	2.27575322
C	-2.22240686	1.28310719	3.14602277
H	4.05768246	2.34270419	2.52972284
H	2.18942271	1.26406369	4.22723984
H	0.00000000	-4.68540838	2.52972284
C	0.00000000	-3.99955657	-0.22606770
H	0.00000000	-2.52812790	4.22723984
C	3.46371751	1.99977828	-0.22606770
H	0.00000000	0.00000000	4.13033108
H	-4.05768246	2.34270419	2.52972284
H	-2.18942271	1.26406369	4.22723984
C	-3.46371751	1.99977828	-0.22606770
B	0.00000000	0.00000000	2.93245795
N	0.00000000	1.71111104	-1.10080245
N	0.00000000	1.44152063	-2.41928937
N	1.48186563	-0.85555578	-1.10080245
N	1.24839369	-0.72076058	-2.41928937
N	-1.48186563	-0.85555578	-1.10080245
N	-1.24839369	-0.72076058	-2.41928937
C	0.00000000	3.07737314	-0.99623808
C	0.00000000	3.63481374	-2.27575322
C	0.00000000	2.56621437	-3.14602277
C	2.66508321	-1.53868657	-0.99623808
C	3.14784103	-1.81740687	-2.27575322
C	2.22240686	-1.28310719	-3.14602277
C	-2.66508321	-1.53868657	-0.99623808
C	-3.14784103	-1.81740687	-2.27575322
C	-2.22240686	-1.28310719	-3.14602277
H	0.00000000	4.68540838	-2.52972284
H	0.00000000	2.52812790	-4.22723984
H	4.05768246	-2.34270419	-2.52972284
C	3.46371751	-1.99977828	0.22606770
H	2.18942271	-1.26406369	-4.22723984
C	0.00000000	3.99955657	0.22606770
H	0.00000000	0.00000000	-4.13033108
H	-4.05768246	-2.34270419	-2.52972284
H	-2.18942271	-1.26406369	-4.22723984
C	-3.46371751	-1.99977828	0.22606770
B	0.00000000	0.00000000	-2.93245795
F	-1.07844736	-3.86886725	-1.01753535
F	0.00000000	-5.27701056	0.22112412
F	1.07844736	-3.86886725	-1.01753535
F	4.57002499	2.63850528	0.22112412
F	2.81131340	2.86839628	-1.01753535
F	3.88976076	1.00047097	-1.01753535
F	-4.57002499	2.63850528	0.22112412

F	-3.88976076	1.00047097	-1.01753535
F	-2.81131340	2.86839628	-1.01753535
F	3.88976076	-1.00047097	1.01753535
F	4.57002499	-2.63850528	-0.22112412
F	2.81131340	-2.86839628	1.01753535
F	-2.81131340	-2.86839628	1.01753535
F	-4.57002499	-2.63850528	-0.22112412
F	-3.88976076	-1.00047097	1.01753535
F	-1.07844736	3.86886725	1.01753535
F	0.00000000	5.27701056	-0.22112412
F	1.07844736	3.86886725	1.01753535

$[Fe(Tb^{3NH2})_2]^+$ $^6A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.70986747	1.32851165
N	0.00000000	1.44716272	2.66831912
N	1.48078876	-0.85493347	1.32851165
N	1.25327958	-0.72358162	2.66831912
N	-1.48078876	-0.85493347	1.32851165
N	-1.25327958	-0.72358162	2.66831912
C	0.00000000	3.06313774	1.20359090
C	0.00000000	3.66068416	2.48011882
C	0.00000000	2.59857780	3.36052953
C	2.65275496	-1.53156861	1.20359090
C	3.17024586	-1.83034208	2.48011882
C	2.25043473	-1.29928890	3.36052953
C	-2.65275496	-1.53156861	1.20359090
C	-3.17024586	-1.83034208	2.48011882
C	-2.25043473	-1.29928890	3.36052953
H	0.00000000	4.71767497	2.71729395
H	0.00000000	2.58824402	4.44341986
H	4.08562619	-2.35883722	2.71729395
N	3.18597830	-1.83942541	0.00119700
H	2.24148476	-1.29412201	4.44341986
N	0.00000000	3.67885081	0.00119700
H	0.00000000	0.00000000	4.38662486
H	-4.08562619	-2.35883722	2.71729395
H	-2.24148476	-1.29412201	4.44341986
N	-3.18597830	-1.83942541	0.00119700
B	0.00000000	0.00000000	3.18376264
N	-1.48078876	0.85493347	-1.32851165
N	-1.25327958	0.72358162	-2.66831912
N	1.48078876	0.85493347	-1.32851165
N	1.25327958	0.72358162	-2.66831912
N	0.00000000	-1.70986747	-1.32851165
N	0.00000000	-1.44716272	-2.66831912
C	-2.65275496	1.53156861	-1.20359090
C	-3.17024586	1.83034208	-2.48011882
C	-2.25043473	1.29928890	-3.36052953
C	2.65275496	1.53156861	-1.20359090
C	3.17024586	1.83034208	-2.48011882
C	2.25043473	1.29928890	-3.36052953
C	0.00000000	-3.06313774	-1.20359090
C	0.00000000	-3.66068416	-2.48011882
C	0.00000000	-2.59857780	-3.36052953
H	-4.08562619	2.35883722	-2.71729395
H	-2.24148476	1.29412201	-4.44341986
H	4.08562619	2.35883722	-2.71729395
N	3.18597830	1.83942541	-0.00119700
H	2.24148476	1.29412201	-4.44341986
N	-3.18597830	1.83942541	-0.00119700
H	0.00000000	0.00000000	-4.38662486
H	0.00000000	-4.71767497	-2.71729395
H	0.00000000	-2.58824402	-4.44341986
N	0.00000000	-3.67885081	-0.00119700
B	0.00000000	0.00000000	-3.18376264
H	0.00000000	4.68013407	-0.04896424
H	4.05311513	-2.34006730	-0.04896424
H	-4.05311513	-2.34006730	-0.04896424
H	-4.05311513	2.34006730	0.04896424
H	4.05311513	2.34006730	0.04896424
H	0.00000000	-4.68013407	0.04896424
H	2.72745944	-1.57469973	-0.85235744
H	0.00000000	3.14939892	-0.85235744
H	-2.72745944	-1.57469973	-0.85235744
H	2.72745944	1.57469973	0.85235744
H	-2.72745944	1.57469973	0.85235744
H	0.00000000	-3.14939892	0.85235744

$[Fe(Tb^{3NH2})_2]^+$ ^4E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.66339671	1.24183612
N	0.00000000	1.43714486	2.58799161
N	1.44054377	-0.83169836	1.24183612
N	1.24460425	-0.71857243	2.58799161
N	-1.44054377	-0.83169836	1.24183612
N	-1.24460425	-0.71857243	2.58799161
C	0.00000000	3.01385176	1.07679579
C	0.00000000	3.64278527	2.33862635
C	0.00000000	2.60545551	3.24821484
C	2.61007258	-1.50692588	1.07679579
C	3.15474467	-1.82139263	2.33862635
C	2.25639062	-1.30272749	3.24821484
C	-2.61007258	-1.50692588	1.07679579
C	-3.15474467	-1.82139263	2.33862635
C	-2.25639062	-1.30272749	3.24821484
H	0.00000000	4.70609075	2.54591355
H	0.00000000	2.62367826	4.33095329
H	4.07559405	-2.35304537	2.54591355
N	3.12077573	-1.80178080	-0.13643407
H	2.27217174	-1.31183887	4.33095329
N	0.00000000	3.60356159	-0.13643407
H	0.00000000	0.00000000	4.31916216
H	-4.07559405	-2.35304537	2.54591355
H	-2.27217174	-1.31183887	4.33095329
N	-3.12077573	-1.80178080	-0.13643407
B	0.00000000	0.00000000	3.11651850
N	-1.44054377	0.83169836	-1.24183612
N	-1.24460425	0.71857243	-2.58799161
N	1.44054377	0.83169836	-1.24183612
N	1.24460425	0.71857243	-2.58799161
N	0.00000000	-1.66339671	-1.24183612
N	0.00000000	-1.43714486	-2.58799161
C	-2.61007258	1.50692588	-1.07679579
C	-3.15474467	1.82139263	-2.33862635
C	-2.25639062	1.30272749	-3.24821484
C	2.61007258	1.50692588	-1.07679579
C	3.15474467	1.82139263	-2.33862635

C	2.25639062	1.30272749	-3.24821484
C	0.00000000	-3.01385176	-1.07679579
C	0.00000000	-3.64278527	-2.33862635
C	0.00000000	-2.60545551	-3.24821484
H	-4.07559405	2.35304537	-2.54591355
H	-2.27217174	1.31183887	-4.33095329
H	4.07559405	2.35304537	-2.54591355
N	3.12077573	1.80178080	0.13643407
H	2.27217174	1.31183887	-4.33095329
N	-3.12077573	1.80178080	0.13643407
H	0.00000000	0.00000000	-4.31916216
H	0.00000000	-4.70609075	-2.54591355
H	0.00000000	-2.62367826	-4.33095329
N	0.00000000	-3.60356159	0.13643407
B	0.00000000	0.00000000	-3.11651850
H	0.00000000	4.60363515	-0.20610078
H	3.98686531	-2.30181784	-0.20610078
H	-3.98686531	-2.30181784	-0.20610078
H	-3.98686531	2.30181784	0.20610078
H	3.98686531	2.30181784	0.20610078
H	0.00000000	-4.60363515	0.20610078
H	2.64575289	-1.52752622	-0.97730677
H	0.00000000	3.05505244	-0.97730677
H	-2.64575289	-1.52752622	-0.97730677
H	2.64575289	1.52752622	0.97730677
H	-2.64575289	1.52752622	0.97730677
H	0.00000000	-3.05505244	0.97730677

$[Fe(Tb^{3NH2})_2]^+$ ^2E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.61228560	1.16152607
N	0.00000000	1.42649464	2.51449153
N	1.39628074	-0.80614280	1.16152607
N	1.23538069	-0.71324732	2.51449153
N	-1.39628074	-0.80614280	1.16152607
N	-1.23538069	-0.71324732	2.51449153
C	0.00000000	2.95771822	0.95760127
C	0.00000000	3.62078367	2.20298394
C	0.00000000	2.61273117	3.14241061
C	2.56145919	-1.47885938	0.95760127
C	3.13569059	-1.81039210	2.20298394
C	2.26269153	-1.30636559	3.14241061
C	-2.56145919	-1.47885938	0.95760127
C	-3.13569059	-1.81039210	2.20298394
C	-2.26269153	-1.30636559	3.14241061
H	0.00000000	4.68995666	2.37661281
H	0.00000000	2.65971364	4.22406531
H	4.06162165	-2.34497807	2.37661281
N	3.05659182	-1.76472410	-0.26398272
H	2.30337944	-1.32985682	4.22406531
N	0.00000000	3.52944820	-0.26398272
H	0.00000000	0.00000000	4.26297889
H	-4.06162165	-2.34497807	2.37661281
H	-2.30337944	-1.32985682	4.22406531
N	-3.05659182	-1.76472410	-0.26398272
B	0.00000000	0.00000000	3.06104114
N	-1.39628074	0.80614280	-1.16152607
N	-1.23538069	0.71324732	-2.51449153
N	1.39628074	0.80614280	-1.16152607
N	1.23538069	0.71324732	-2.51449153
N	0.00000000	-1.61228560	-1.16152607
N	0.00000000	-1.42649464	-2.51449153
C	-2.56145919	1.47885938	-0.95760127
C	-3.13569059	1.81039210	-2.20298394
C	-2.26269153	1.30636559	-3.14241061
C	2.56145919	1.47885938	-0.95760127
C	3.13569059	1.81039210	-2.20298394
C	2.26269153	1.30636559	-3.14241061
C	0.00000000	-2.95771822	-0.95760127
C	0.00000000	-3.62078367	-2.20298394
C	0.00000000	-2.61273117	-3.14241061
H	-4.06162165	2.34497807	-2.37661281
H	-2.30337944	1.32985682	-4.22406531
H	4.06162165	2.34497807	-2.37661281
N	3.05659182	1.76472410	0.26398272
H	2.30337944	1.32985682	-4.22406531
N	-3.05659182	1.76472410	0.26398272
H	0.00000000	0.00000000	-4.26297889
H	0.00000000	-4.68995666	-2.37661281
H	0.00000000	-2.65971364	-4.22406531
N	0.00000000	-3.52944820	0.26398272
B	0.00000000	0.00000000	-3.06104114
H	0.00000000	4.52876821	-0.34395939
H	3.92202840	-2.26438437	-0.34395939
H	-3.92202840	-2.26438437	-0.34395939
H	-3.92202840	2.26438437	0.34395939
H	3.92202840	2.26438437	0.34395939
H	0.00000000	-4.52876821	0.34395939
H	2.57404408	-1.48612498	-1.09834072
H	0.00000000	2.97224996	-1.09834072
H	-2.57404408	-1.48612498	-1.09834072
H	2.57404408	1.48612498	1.09834072
H	-2.57404408	1.48612498	1.09834072
H	0.00000000	-2.97224996	1.09834072

$[Fe(Tb^{3NO2})_2]^+$ $^6A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.77510868	1.39556264
N	0.00000000	1.44855287	2.69699048
N	1.53728901	-0.88755460	1.39556264
N	1.25448346	-0.72427643	2.69699048
N	-1.53728901	-0.88755460	1.39556264
N	-1.25448346	-0.72427643	2.69699048
C	0.00000000	3.12727561	1.38960040
C	0.00000000	3.65770754	2.67431735
C	0.00000000	2.54204156	3.48403580
C	2.70830005	-1.56363781	1.38960040
C	3.16766771	-1.82885350	2.67431735
C	2.20147261	-1.27102078	3.48403580
C	-2.70830005	-1.56363781	1.38960040
C	-3.16766771	-1.82885350	2.67431735
C	-2.20147261	-1.27102078	3.48403580
H	0.00000000	4.70212456	2.95265241
H	0.00000000	2.44774376	4.56207622
H	4.07215916	-2.35106255	2.95265241
N	3.41723352	-1.97294053	0.19397680
H	2.11980839	-1.22387214	4.56207622
N	0.00000000	3.94588159	0.19397680

H	0.00000000	0.00000000	4.39035397
H	-4.07215916	-2.35106255	2.95265241
H	-2.11980839	-1.22387214	4.56207622
N	-3.41723352	-1.97294053	0.19397680
B	0.00000000	0.00000000	3.19197070
N	-1.53728901	0.88755460	-1.39556264
N	-1.25448346	0.72427643	-2.69699048
N	1.53728901	0.88755460	-1.39556264
N	1.25448346	0.72427643	-2.69699048
N	0.00000000	-1.77510868	-1.39556264
N	0.00000000	-1.44855287	-2.69699048
C	-2.70830005	1.56363781	-1.38960040
C	-3.16766771	1.82885350	-2.67431735
C	-2.20147261	1.27102078	-3.48403580
C	2.70830005	1.56363781	-1.38960040
C	3.16766771	1.82885350	-2.67431735
C	2.20147261	1.27102078	-3.48403580
C	0.00000000	-3.12727561	-1.38960040
C	0.00000000	-3.65770754	-2.67431735
C	0.00000000	-2.54204156	-3.48403580
H	-4.07215916	2.35106255	-2.95265241
H	-2.11980839	1.22387214	-4.56207622
H	4.07215916	2.35106255	-2.95265241
N	3.41723352	1.97294053	-0.19397680
H	2.11980839	1.22387214	-4.56207622
N	-3.41723352	1.97294053	-0.19397680
H	0.00000000	0.00000000	-4.39035397
H	0.00000000	-4.70212456	-2.95265241
H	0.00000000	-2.44774376	-4.56207622
N	0.00000000	-3.94588159	-0.19397680
B	0.00000000	0.00000000	-3.19197070
O	0.00000000	5.15427001	0.37992175
O	4.46372863	-2.57713501	0.37992175
O	-4.46372863	-2.57713501	0.37992175
O	-4.46372863	2.57713501	-0.37992175
O	4.46372863	2.57713501	-0.37992175
O	0.00000000	-5.15427001	-0.37992175
O	2.93203725	-1.69281262	-0.89301465
O	0.00000000	3.38562471	-0.89301465
O	-2.93203725	-1.69281262	-0.89301465
O	2.93203725	1.69281262	0.89301465
O	-2.93203725	1.69281262	0.89301465
O	0.00000000	-3.38562471	0.89301465

$[Fe(Tb^{3NO2})_2]^+$ ^4E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.80113150	1.39702423
N	0.00000000	1.45680644	2.69039269
N	1.55982561	-0.90056548	1.39702423
N	1.26163159	-0.72840296	2.69039269
N	-1.55982561	-0.90056548	1.39702423
N	-1.26163159	-0.72840296	2.69039269
C	0.00000000	3.14985455	1.41389917
C	0.00000000	3.66601403	2.70931025
C	0.00000000	2.53829392	3.49887340
C	2.72785421	-1.57492727	1.41389917
C	3.17486082	-1.83300702	2.70931025
C	2.19822716	-1.26914696	3.49887340
C	-2.72785421	-1.57492727	1.41389917
C	-3.17486082	-1.83300702	2.70931025
C	-2.19822716	-1.26914696	3.49887340
H	0.00000000	4.70500011	3.00720053
H	0.00000000	2.42710426	4.57509980
H	4.07465000	-2.35250032	3.00720053
N	3.44326798	-1.98797181	0.23436625
H	2.10193384	-1.21355213	4.57509980
N	0.00000000	3.97594309	0.23436625
H	0.00000000	0.00000000	4.36971553
H	-4.07465000	-2.35250032	3.00720053
H	-2.10193384	-1.21355213	4.57509980
N	-3.44326798	-1.98797181	0.23436625
B	0.00000000	0.00000000	3.17015008
N	-1.55982561	0.90056548	-1.39702423
N	-1.26163159	0.72840296	-2.69039269
N	1.55982561	0.90056548	-1.39702423
N	1.26163159	0.72840296	-2.69039269
N	0.00000000	-1.80113150	-1.39702423
N	0.00000000	-1.45680644	-2.69039269
C	-2.72785421	1.57492727	-1.41389917
C	-3.17486082	1.83300702	-2.70931025
C	-2.19822716	1.26914696	-3.49887340
C	2.72785421	1.57492727	-1.41389917
C	3.17486082	1.83300702	-2.70931025
C	2.19822716	1.26914696	-3.49887340
C	0.00000000	-3.14985455	-1.41389917
C	0.00000000	-3.66601403	-2.70931025
C	0.00000000	-2.53829392	-3.49887340
H	-4.07465000	2.35250032	-3.00720053
H	-2.10193384	1.21355213	-4.57509980
H	4.07465000	2.35250032	-3.00720053
N	3.44326798	1.98797181	-0.23436625
H	2.10193384	1.21355213	-4.57509980
N	-3.44326798	1.98797181	-0.23436625
H	0.00000000	0.00000000	-4.36971553
H	0.00000000	-4.70500011	-3.00720053
H	0.00000000	-2.42710426	-4.57509980
N	0.00000000	-3.97594309	-0.23436625
B	0.00000000	0.00000000	-3.17015008
O	0.00000000	5.18765527	0.42303329
O	4.49264128	-2.59382790	0.42303329
O	-4.49264128	-2.59382790	0.42303329
O	-4.49264128	2.59382790	-0.42303329
O	4.49264128	2.59382790	-0.42303329
O	0.00000000	-5.18765527	-0.42303329
O	2.98495974	-1.72336731	-0.87057489
O	0.00000000	3.44673462	-0.87057489
O	-2.98495974	-1.72336731	-0.87057489
O	2.98495974	1.72336731	0.87057489
O	-2.98495974	1.72336731	0.87057489
O	0.00000000	-3.44673462	0.87057489

$[Fe(Tb^{3NO2})_2]^+$ ^2E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.67624037	1.14680171
N	0.00000000	1.42932521	2.46232894
N	1.45166707	-0.83812045	1.14680171
N	1.23783237	-0.71466287	2.46232894
N	-1.45166707	-0.83812045	1.14680171

N	-1.23783237	-0.71466287	2.46232894
C	0.00000000	3.03478442	1.05512969
C	0.00000000	3.62483875	2.31543198
C	0.00000000	2.56082894	3.18708216
C	2.62820061	-1.51739248	1.05512969
C	3.13920221	-1.81241938	2.31543198
C	2.21774322	-1.28041473	3.18708216
C	-2.62820061	-1.51739248	1.05512969
C	-3.13920221	-1.81241938	2.31543198
C	-2.21774322	-1.28041473	3.18708216
H	0.00000000	4.68328056	2.53238619
H	0.00000000	2.52421781	4.26826801
H	4.05583986	-2.34164055	2.53238619
N	3.33585770	-1.92595806	-0.15170189
H	2.18603703	-1.26210890	4.26826801
N	0.00000000	3.85191665	-0.15170189
H	0.00000000	0.00000000	4.18719594
H	-4.05583986	-2.34164055	2.53238619
H	-2.18603703	-1.26210890	4.26826801
N	-3.33585770	-1.92595806	-0.15170189
B	0.00000000	0.00000000	2.99013615
N	-1.45166707	0.83812045	-1.14680171
N	-1.23783237	0.71466287	-2.46232894
N	1.45166707	0.83812045	-1.14680171
N	1.23783237	0.71466287	-2.46232894
N	0.00000000	-1.67624037	-1.14680171
N	0.00000000	-1.42932521	-2.46232894
C	-2.62820061	1.51739248	-1.05512969
C	-3.13920221	1.81241938	-2.31543198
C	-2.21774322	1.28041473	-3.18708216
C	2.62820061	1.51739248	-1.05512969
C	3.13920221	1.81241938	-2.31543198
C	2.21774322	1.28041473	-3.18708216
C	0.00000000	-3.03478442	-1.05512969
C	0.00000000	-3.62483875	-2.31543198
C	0.00000000	-2.56082894	-3.18708216
H	-4.05583986	2.34164055	-2.53238619
H	-2.18603703	1.26210890	-4.26826801
H	4.05583986	2.34164055	-2.53238619
N	3.33585770	1.92595806	0.15170189
H	2.18603703	1.26210890	-4.26826801
N	-3.33585770	1.92595806	0.15170189
H	0.00000000	0.00000000	-4.18719594
H	0.00000000	-4.68328056	-2.53238619
H	0.00000000	-2.52421781	-4.26826801
N	0.00000000	-3.85191665	0.15170189
B	0.00000000	0.00000000	-2.99013615
O	0.00000000	5.05860852	0.04810433
O	4.38088328	-2.52930426	0.04810433
O	-4.38088328	-2.52930426	0.04810433
O	-4.38088328	2.52930426	-0.04810433
O	4.38088328	2.52930426	-0.04810433
O	0.00000000	-5.05860852	-0.04810433
O	2.86949009	-1.65670050	-1.24687283
O	0.00000000	3.31340154	-1.24687283
O	-2.86949009	-1.65670050	-1.24687283
O	2.86949009	1.65670050	1.24687283
O	-2.86949009	1.65670050	1.24687283
O	0.00000000	-3.31340154	1.24687283

$[Fe(Tb^{5CH3})_2]^+$ $^6A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.50546376	0.86917998	1.31058895
N	1.25538888	0.72479926	2.63163179
N	0.00000000	-1.73835996	1.31058895
N	0.00000000	-1.44959799	2.63163179
N	-1.50546376	0.86917998	1.31058895
N	-1.25538888	0.72479926	2.63163179
C	2.67786442	1.54606595	1.19814778
C	3.16312049	1.82622826	2.48129201
C	2.23452078	1.29010132	3.35527692
C	0.00000000	-3.09213189	1.19814778
C	0.00000000	-3.65245704	2.48129201
C	0.00000000	-2.58020265	3.35527692
C	-2.67786442	1.54606595	1.19814778
C	-3.16312049	1.82622826	2.48129201
C	-2.23452078	1.29010132	3.35527692
H	4.07558082	2.35303744	2.73470071
H	2.20259023	1.27166585	4.43735232
H	0.00000000	-4.70607487	2.73470071
C	0.00000000	-3.84395729	-0.08654006
H	0.00000000	-2.54333169	4.43735232
C	3.32896464	1.92197865	-0.08654006
H	0.00000000	0.00000000	4.34320427
H	-4.07558082	2.35303744	2.73470071
H	-2.20259023	1.27166585	4.43735232
C	-3.32896464	1.92197865	-0.08654006
B	0.00000000	0.00000000	3.14246511
N	0.00000000	1.73835996	-1.31058895
N	0.00000000	1.44959799	-2.63163179
N	1.50546376	-0.86917998	-1.31058895
N	1.25538888	-0.72479926	-2.63163179
N	-1.50546376	-0.86917998	-1.31058895
N	-1.25538888	-0.72479926	-2.63163179
C	0.00000000	3.09213189	-1.19814778
C	0.00000000	3.65245704	-2.48129201
C	0.00000000	2.58020265	-3.35527692
C	2.67786442	-1.54606595	-1.19814778
C	3.16312049	-1.82622826	-2.48129201
C	2.23452078	-1.29010132	-3.35527692
C	-2.67786442	-1.54606595	-1.19814778
C	-3.16312049	-1.82622826	-2.48129201
C	-2.23452078	-1.29010132	-3.35527692
H	0.00000000	4.70607487	-2.73470071
H	0.00000000	2.54333169	-4.43735232
H	4.07558082	-2.35303744	-2.73470071
C	3.32896464	-1.92197865	0.08654006
H	2.20259023	-1.27166585	-4.43735232
C	0.00000000	3.84395729	0.08654006
H	0.00000000	0.00000000	-4.34320427
H	-4.07558082	-2.35303744	-2.73470071
H	-2.20259023	-1.27166585	-4.43735232
C	-3.32896464	-1.92197865	0.08654006
B	0.00000000	0.00000000	-3.14246511
H	-0.87842788	-3.62062015	-0.69710953
H	0.00000000	-4.91580052	0.12538643
H	0.87842788	-3.62062015	-0.69710953
H	4.25720821	2.45790026	0.12538643
H	2.69633483	2.57105053	-0.69710953

H	3.57476271	1.04956910	-0.69710953
H	-4.25720821	2.45790026	0.12538643
H	-3.57476271	1.04956910	-0.69710953
H	-2.69633483	2.57105053	-0.69710953
H	3.57476271	-1.04956910	0.69710953
H	4.25720821	-2.45790026	-0.12538643
H	2.69633483	-2.57105053	0.69710953
H	-2.69633483	-2.57105053	0.69710953
H	-4.25720821	-2.45790026	-0.12538643
H	-3.57476271	-1.04956910	0.69710953
H	-0.87842788	3.62062015	0.69710953
H	0.00000000	4.91580052	-0.12538643
H	0.87842788	3.62062015	0.69710953

$[Fe(Tb^{5CH3})_2]^+$ ^4E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.47472862	0.85143508	1.22409017
N	1.24840321	0.72076587	2.54834723
N	0.00000000	-1.70286963	1.22409017
N	0.00000000	-1.44153174	2.54834723
N	-1.47472862	0.85143508	1.22409017
N	-1.24840321	0.72076587	2.54834723
C	2.64524329	1.52723200	1.07999414
C	3.15067953	1.81904573	2.35383173
C	2.23867218	1.29249797	3.24963250
C	0.00000000	-3.05446347	1.07999414
C	0.00000000	-3.63809147	2.35383173
C	0.00000000	-2.58499593	3.24963250
C	-2.64524329	1.52723200	1.07999414
C	-3.15067953	1.81904573	2.35383173
C	-2.23867218	1.29249797	3.24963250
H	4.06781991	2.34855689	2.58370209
H	2.22423252	1.28416131	4.33212066
H	0.00000000	-4.69711379	2.58370209
C	0.00000000	-3.79500099	-0.21052206
H	0.00000000	-2.56832209	4.33212066
C	3.28656749	1.89750049	-0.21052206
H	0.00000000	0.00000000	4.26910306
H	-4.06781991	2.34855689	2.58370209
H	-2.22423252	1.28416131	4.33212066
C	-3.28656749	1.89750049	-0.21052206
B	0.00000000	0.00000000	3.06855916
N	0.00000000	1.70286963	-1.22409017
N	0.00000000	1.44153174	-2.54834723
N	1.47472862	-0.85143508	-1.22409017
N	1.24840321	-0.72076587	-2.54834723
N	-1.47472862	-0.85143508	-1.22409017
N	-1.24840321	-0.72076587	-2.54834723
C	0.00000000	3.05446347	-1.07999414
C	0.00000000	3.63809147	-2.35383173
C	0.00000000	2.58499593	-3.24963250
C	2.64524329	-1.52723200	-1.07999414
C	3.15067953	-1.81904573	-2.35383173
C	2.23867218	-1.29249797	-3.24963250
C	-2.64524329	-1.52723200	-1.07999414
C	-3.15067953	-1.81904573	-2.35383173
C	-2.23867218	-1.29249797	-3.24963250
H	0.00000000	4.69711379	-2.58370209
H	0.00000000	2.56832209	-4.33212066
H	4.06781991	-2.34855689	-2.58370209
C	3.28656749	-1.89750049	0.21052206
H	2.22423252	-1.28416131	-4.33212066
C	0.00000000	3.79500099	0.21052206
H	0.00000000	0.00000000	-4.26910306
H	-4.06781991	-2.34855689	-2.58370209
H	-2.22423252	-1.28416131	-4.33212066
C	-3.28656749	-1.89750049	0.21052206
B	0.00000000	0.00000000	-3.06855916
H	-0.87934759	-3.56944871	-0.81870388
H	0.00000000	-4.86793591	-0.00343330
H	0.87934759	-3.56944871	-0.81870388
H	4.21575617	2.43396769	-0.00343330
H	2.65155902	2.54626175	-0.81870388
H	3.53090661	1.02318696	-0.81870388
H	-4.21575617	2.43396769	-0.00343330
H	-3.53090661	1.02318696	-0.81870388
H	-2.65155902	2.54626175	-0.81870388
H	3.53090661	-1.02318696	0.81870388
H	4.21575617	-2.43396769	0.00343330
H	2.65155902	-2.54626175	0.81870388
H	-2.65155902	-2.54626175	0.81870388
H	-4.21575617	-2.43396769	0.00343330
H	-3.53090661	-1.02318696	0.81870388
H	-0.87934759	3.56944871	0.81870388
H	0.00000000	4.86793591	0.00343330
H	0.87934759	3.56944871	0.81870388

$[Fe(Tb^{5CH3})_2]^+$ ^2E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.41899355	0.81925634	1.13652403
N	1.23626600	0.71375851	2.46935430
N	0.00000000	-1.63851268	1.13652403
N	0.00000000	-1.42751701	2.46935430
N	-1.41899355	0.81925634	1.13652403
N	-1.23626600	0.71375851	2.46935430
C	2.58589553	1.49296777	0.94324045
C	3.12811489	1.80601792	2.19762707
C	2.24606743	1.29676790	3.13076818
C	0.00000000	-2.98593501	0.94324045
C	0.00000000	-3.61203637	2.19762707
C	0.00000000	-2.59353580	3.13076818
C	-2.58589553	1.49296777	0.94324045
C	-3.12811489	1.80601792	2.19762707
C	-2.24606743	1.29676790	3.13076818
H	4.05199380	2.33941959	2.38727626
H	2.26275398	1.30640157	4.21307906
H	0.00000000	-4.67883918	2.38727626
C	0.00000000	-3.70164936	-0.36087560
H	0.00000000	-2.61280314	4.21307906
C	3.20572243	1.85082494	-0.36087560
H	0.00000000	0.00000000	4.21248585
H	-4.05199380	2.33941959	2.38727626
H	-2.26275398	1.30640157	4.21307906
C	-3.20572243	1.85082494	-0.36087560
B	0.00000000	0.00000000	3.01279235
N	0.00000000	1.63851268	-1.13652403
N	0.00000000	1.42751701	-2.46935430
N	1.41899355	-0.81925634	-1.13652403

N	1.23626600	-0.71375851	-2.46935430
N	-1.41899355	-0.81925634	-1.13652403
N	-1.23626600	-0.71375851	-2.46935430
C	0.00000000	2.98593501	-0.94324045
C	0.00000000	3.61203637	-2.19762707
C	0.00000000	2.59353580	-3.13076818
C	2.58589553	-1.49296777	-0.94324045
C	3.12811489	-1.80601792	-2.19762707
C	2.24606743	-1.29676790	-3.13076818
C	-2.58589553	-1.49296777	-0.94324045
C	-3.12811489	-1.80601792	-2.19762707
C	-2.24606743	-1.29676790	-3.13076818
H	0.00000000	4.67883918	-2.38727626
H	0.00000000	2.61280314	-4.21307906
H	4.05199380	-2.33941959	-2.38727626
C	3.20572243	-1.85082494	0.36087560
H	2.26275398	-1.30640157	-4.21307906
C	0.00000000	3.70164936	0.36087560
H	0.00000000	0.00000000	-4.21248585
H	-4.05199380	-2.33941959	-2.38727626
H	-2.26275398	-1.30640157	-4.21307906
C	-3.20572243	-1.85082494	0.36087560
B	0.00000000	0.00000000	-3.01279235
H	-0.88092189	-3.46969933	-0.96458006
H	0.00000000	-4.77745400	-0.16815983
H	0.88092189	-3.46969933	-0.96458006
H	4.13739666	2.38872727	-0.16815983
H	2.56438660	2.49774995	-0.96458006
H	3.44530849	0.97194885	-0.96458006
H	-4.13739666	2.38872727	-0.16815983
H	-3.44530849	0.97194885	-0.96458006
H	-2.56438660	2.49774995	-0.96458006
H	3.44530849	-0.97194885	0.96458006
H	4.13739666	-2.38872727	0.16815983
H	2.56438660	-2.49774995	0.96458006
H	-2.56438660	-2.49774995	0.96458006
H	-4.13739666	-2.38872727	0.16815983
H	-3.44530849	-0.97194885	0.96458006
H	-0.88092189	3.46969933	0.96458006
H	0.00000000	4.77745400	0.16815983
H	0.88092189	3.46969933	0.96458006

$[Fe(Tb^{5CF3})_2]^+$ $^6A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.43363483	0.82770942	1.34001385
N	1.26330432	0.72936923	2.67561330
N	0.00000000	-1.65541884	1.34001385
N	0.00000000	-1.45873847	2.67561330
N	-1.43363483	0.82770942	1.34001385
N	-1.26330432	0.72936923	2.67561330
C	2.57817113	1.48850787	1.11553474
C	3.17194082	1.83132106	2.32197897
C	2.30960998	1.33345417	3.29254454
C	0.00000000	-2.97701520	1.11553474
C	0.00000000	-3.66264212	2.32197897
C	0.00000000	-2.66690834	3.29254454
C	-2.57817113	1.48850787	1.11553474
C	-3.17194082	1.83132106	2.32197897
C	-2.30960998	1.33345417	3.29254454
H	4.09893341	2.36652034	2.48200640
C	2.50721323	1.44754002	4.78771316
H	0.00000000	-4.73304069	2.48200640
H	0.00000000	-3.36395278	0.10473635
C	0.00000000	-2.89508004	4.78771316
H	2.91326839	1.68197613	0.10473635
H	0.00000000	0.00000000	4.41006265
H	-4.09893341	2.36652034	2.48200640
C	-2.50721323	1.44754002	4.78771316
H	-2.91326839	1.68197613	0.10473635
B	0.00000000	0.00000000	3.22534803
N	0.00000000	1.65541884	-1.34001385
N	0.00000000	1.45873847	-2.67561330
N	1.43363483	-0.82770942	-1.34001385
N	1.26330432	-0.72936923	-2.67561330
N	-1.43363483	-0.82770942	-1.34001385
N	-1.26330432	-0.72936923	-2.67561330
C	0.00000000	2.97701520	-1.11553474
C	0.00000000	3.66264212	-2.32197897
C	0.00000000	2.66690834	-3.29254454
C	2.57817113	-1.48850787	-1.11553474
C	3.17194082	-1.83132106	-2.32197897
C	2.30960998	-1.33345417	-3.29254454
C	-2.57817113	-1.48850787	-1.11553474
C	-3.17194082	-1.83132106	-2.32197897
C	-2.30960998	-1.33345417	-3.29254454
H	0.00000000	4.73304069	-2.48200640
C	0.00000000	2.89508004	-4.78771316
H	4.09893341	-2.36652034	-2.48200640
H	2.91326839	-1.68197613	-0.10473635
C	2.50721323	-1.44754002	-4.78771316
H	0.00000000	3.36395278	-0.10473635
H	0.00000000	0.00000000	-4.41006265
H	-4.09893341	-2.36652034	-2.48200640
C	-2.50721323	-1.44754002	-4.78771316
H	-2.91326839	-1.68197613	-0.10473635
B	0.00000000	0.00000000	-3.22534803
F	-3.65540085	-2.11044671	-5.03114793
F	-1.50629087	-2.12760793	-5.38025039
F	-2.59570807	-0.24068251	-5.38025039
F	3.65540085	-2.11044671	-5.03114793
F	2.59570807	-0.24068251	-5.38025039
F	1.50629087	-2.12760793	-5.38025039
F	1.08941720	2.36829044	-5.38025039
F	0.00000000	4.22089289	-5.03114793
F	-1.08941720	2.36829044	-5.38025039
F	-2.59570807	0.24068251	5.38025039
F	-3.65540085	2.11044671	5.03114793
F	-1.50629087	2.12760793	5.38025039
F	-1.08941720	-2.36829044	5.38025039
F	1.08941720	-2.36829044	5.38025039
F	0.00000000	-4.22089289	5.03114793
F	2.59570807	0.24068251	5.38025039
F	1.50629087	2.12760793	5.38025039
F	3.65540085	2.11044671	5.03114793

$[Fe(Tb^{5CF3})_2]^+$ ^4E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.40601654	0.81176425	1.24717023

N	1.25529469	0.72474476	2.58415454
N	0.00000000	-1.62352797	1.24717023
N	0.00000000	-1.44948951	2.58415454
N	-1.40601654	0.81176425	1.24717023
N	-1.25529469	0.72474476	2.58415454
C	2.54715711	1.47060157	0.99871940
C	3.15685662	1.82261186	2.19499230
C	2.30852093	1.33282551	3.18169302
C	0.00000000	-2.94120366	0.99871940
C	0.00000000	-3.64522425	2.19499230
C	0.00000000	-2.66565048	3.18169302
C	-2.54715711	1.47060157	0.99871940
C	-3.15685662	1.82261186	2.19499230
C	-2.30852093	1.33282551	3.18169302
H	4.08624850	2.35919653	2.33646255
C	2.51704799	1.45321862	4.67448246
H	0.00000000	-4.71839306	2.33646255
H	0.00000000	-3.31152772	-0.01773220
C	0.00000000	-2.90643672	4.67448246
H	2.86786710	1.65576386	-0.01773220
H	0.00000000	0.00000000	4.32754698
H	-4.08624850	2.35919653	2.33646255
C	-2.51704799	1.45321862	4.67448246
H	-2.86786710	1.65576386	-0.01773220
B	0.00000000	0.00000000	3.14321231
N	0.00000000	1.62352797	-1.24717023
N	0.00000000	1.44948951	-2.58415454
N	1.40601654	-0.81176425	-1.24717023
N	1.25529469	-0.72474476	-2.58415454
N	-1.40601654	-0.81176425	-1.24717023
N	-1.25529469	-0.72474476	-2.58415454
C	0.00000000	2.94120366	-0.99871940
C	0.00000000	3.64522425	-2.19499230
C	0.00000000	2.66565048	-3.18169302
C	2.54715711	-1.47060157	-0.99871940
C	3.15685662	-1.82261186	-2.19499230
C	2.30852093	-1.33282551	-3.18169302
C	-2.54715711	-1.47060157	-0.99871940
C	-3.15685662	-1.82261186	-2.19499230
C	-2.30852093	-1.33282551	-3.18169302
H	0.00000000	4.71839306	-2.33646255
C	0.00000000	2.90643672	-4.67448246
H	4.08624850	-2.35919653	-2.33646255
H	2.86786710	-1.65576386	0.01773220
C	2.51704799	-1.45321862	-4.67448246
H	0.00000000	3.31152772	0.01773220
H	0.00000000	0.00000000	-4.32754698
H	-4.08624850	-2.35919653	-2.33646255
C	-2.51704799	-1.45321862	-4.67448246
H	-2.86786710	-1.65576386	0.01773220
B	0.00000000	0.00000000	-3.14321231
F	-3.66650617	-2.11685822	-4.90763955
F	-1.51905092	-2.13516405	-5.27051332
F	-2.60863163	-0.24795447	-5.27051332
F	3.66650617	-2.11685822	-4.90763955
F	2.60863163	-0.24795447	-5.27051332
F	1.51905092	-2.13516405	-5.27051332
F	1.08958072	2.38311852	-5.27051332
F	0.00000000	4.23371644	-4.90763955
F	-1.08958072	2.38311852	-5.27051332
F	-2.60863163	0.24795447	5.27051332
F	-3.66650617	2.11685822	4.90763955
F	-1.51905092	2.13516405	5.27051332
F	-1.08958072	-2.38311852	5.27051332
F	1.08958072	-2.38311852	5.27051332
F	0.00000000	-4.23371644	4.90763955
F	2.60863163	0.24795447	5.27051332
F	1.51905092	2.13516405	5.27051332
F	3.66650617	2.11685822	4.90763955

$[Fe(Tb^{5CF3})_2]^+$ ^2E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.35967861	0.78501064	1.15826951
N	1.24431426	0.71840521	2.49984814
N	0.00000000	-1.57002180	1.15826951
N	0.00000000	-1.43681042	2.49984814
N	-1.35967861	0.78501064	1.15826951
N	-1.24431426	0.71840521	2.49984814
C	2.49456007	1.44023473	0.87042513
C	3.13320240	1.80895538	2.04698513
C	2.31170181	1.33466175	3.06216511
C	0.00000000	-2.88046946	0.87042513
C	0.00000000	-3.61791023	2.04698513
C	0.00000000	-2.66932350	3.06216511
C	-2.49456007	1.44023473	0.87042513
C	-3.13320240	1.80895538	2.04698513
C	-2.31170181	1.33466175	3.06216511
H	4.06591222	2.34745567	2.15515372
C	2.54882138	1.47156308	4.54825834
H	0.00000000	-4.69491135	2.15515372
H	0.00000000	-3.22353824	-0.15458061
C	0.00000000	-2.94312563	4.54825834
H	2.79166611	1.61176912	-0.15458061
H	0.00000000	0.00000000	4.26341546
H	-4.06591222	2.34745567	2.15515372
C	-2.54882138	1.47156308	4.54825834
H	-2.79166611	1.61176912	-0.15458061
B	0.00000000	0.00000000	3.07930516
N	0.00000000	1.57002180	-1.15826951
N	0.00000000	1.43681042	-2.49984814
N	1.35967861	-0.78501064	-1.15826951
N	1.24431426	-0.71840521	-2.49984814
N	-1.35967861	-0.78501064	-1.15826951
N	-1.24431426	-0.71840521	-2.49984814
C	0.00000000	2.88046946	-0.87042513
C	0.00000000	3.61791023	-2.04698513
C	0.00000000	2.66932350	-3.06216511
C	2.49456007	-1.44023473	-0.87042513
C	3.13320240	-1.80895538	-2.04698513
C	2.31170181	-1.33466175	-3.06216511
C	-2.49456007	-1.44023473	-0.87042513
C	-3.13320240	-1.80895538	-2.04698513
C	-2.31170181	-1.33466175	-3.06216511
H	0.00000000	4.69491135	-2.15515372
C	0.00000000	2.94312563	-4.54825834
H	4.06591222	-2.34745567	-2.15515372
H	2.79166611	-1.61176912	0.15458061
C	2.54882138	-1.47156308	-4.54825834
H	0.00000000	3.22353824	0.15458061

H	0.00000000	0.00000000	-4.26341546
H	-4.06591222	-2.34745567	-2.15515372
C	-2.54882138	-1.47156308	-4.54825834
H	-2.79166611	-1.61176912	0.15458061
B	0.00000000	0.00000000	-3.07930516
F	-3.70180017	-2.13723525	-4.75423159
F	-1.56078342	-2.15912202	-5.15487433
F	-2.65024613	-0.27211723	-5.15487433
F	3.70180017	-2.13723525	-4.75423159
F	2.65024613	-0.27211723	-5.15487433
F	1.56078342	-2.15912202	-5.15487433
F	1.08946271	2.43123925	-5.15487433
F	0.00000000	4.27447050	-4.75423159
F	-1.08946271	2.43123925	-5.15487433
F	-2.65024613	0.27211723	5.15487433
F	-3.70180017	2.13723525	4.75423159
F	-1.56078342	2.15912202	5.15487433
F	-1.08946271	-2.43123925	5.15487433
F	1.08946271	-2.43123925	5.15487433
F	0.00000000	-4.27447050	4.75423159
F	2.65024613	0.27211723	5.15487433
F	1.56078342	2.15912202	5.15487433
F	3.70180017	2.13723525	4.75423159

$[Fe(Tb^{5NH2})_2]^+$ $^6A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.66889222	-1.33685942
N	0.00000000	1.45115854	-2.68427223
N	-1.44530319	-0.83444637	-1.33685942
N	-1.25674040	-0.72557927	-2.68427223
N	1.44530319	-0.83444637	-1.33685942
N	1.25674040	-0.72557927	-2.68427223
C	0.00000000	2.99388061	-1.15922573
C	0.00000000	3.66103077	-2.37658635
C	0.00000000	2.63934720	-3.33655357
C	-2.59277696	-1.49694030	-1.15922573
C	-3.17054538	-1.83051512	-2.37658635
C	-2.28574197	-1.31967386	-3.33655357
C	2.59277696	-1.49694030	-1.15922573
C	3.17054538	-1.83051512	-2.37658635
C	2.28574197	-1.31967386	-3.33655357
H	0.00000000	4.72963543	-2.55503127
N	0.00000000	2.75310390	-4.69014346
H	-4.09598431	-2.36481798	-2.55503127
H	-2.95019068	-1.70329350	-0.15863093
N	-2.38425784	-1.37655195	-4.69014346
H	0.00000000	3.40658647	-0.15863093
H	0.00000000	0.00000000	-4.41105485
H	4.09598431	-2.36481798	-2.55503127
N	2.38425784	-1.37655195	-4.69014346
H	2.95019068	-1.70329350	-0.15863093
B	0.00000000	0.00000000	-3.20166735
N	1.44530319	0.83444637	1.33685942
N	1.25674040	0.72557927	2.68427223
N	-1.44530319	0.83444637	1.33685942
N	-1.25674040	0.72557927	2.68427223
N	0.00000000	-1.66889222	1.33685942
N	0.00000000	-1.45115854	2.68427223
C	2.59277696	1.49694030	1.15922573
C	3.17054538	1.83051512	2.37658635
C	2.28574197	1.31967386	3.33655357
C	-2.59277696	1.49694030	1.15922573
C	-3.17054538	1.83051512	2.37658635
C	-2.28574197	1.31967386	3.33655357
C	0.00000000	-2.99388061	1.15922573
C	0.00000000	-3.66103077	2.37658635
C	0.00000000	-2.63934720	3.33655357
H	4.09598431	2.36481798	2.55503127
N	2.38425784	1.37655195	4.69014346
H	-4.09598431	2.36481798	2.55503127
H	-2.95019068	1.70329350	0.15863093
N	-2.38425784	1.37655195	4.69014346
H	2.95019068	1.70329350	0.15863093
H	0.00000000	0.00000000	4.41105485
H	0.00000000	-4.72963543	2.55503127
N	0.00000000	-2.75310390	4.69014346
H	0.00000000	-3.40658647	0.15863093
B	0.00000000	0.00000000	3.20166735
H	0.00000000	3.66296280	-5.11154001
H	0.00000000	1.94725797	-5.28518052
H	-3.17221863	-1.83148140	-5.11154001
H	-1.68637465	-0.97362899	-5.28518052
H	3.17221863	-1.83148140	-5.11154001
H	1.68637465	-0.97362899	-5.28518052
H	3.17221863	1.83148140	5.11154001
H	1.68637465	0.97362899	5.28518052
H	-3.17221863	1.83148140	5.11154001
H	-1.68637465	0.97362899	5.28518052
H	0.00000000	-3.66296280	5.11154001
H	0.00000000	-1.94725797	5.28518052

$[Fe(Tb^{5NH2})_2]^+$ ^4E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.62247279	-1.23483776
N	0.00000000	1.44202917	-2.58636650
N	-1.40510265	-0.81123613	-1.23483776
N	-1.24883396	-0.72101458	-2.58636650
N	1.40510265	-0.81123613	-1.23483776
N	1.24883396	-0.72101458	-2.58636650
C	0.00000000	2.94158096	-1.01684160
C	0.00000000	3.64082943	-2.21607366
C	0.00000000	2.64650432	-3.20481119
C	-2.54748362	-1.47079048	-1.01684160
C	-3.15305078	-1.82041471	-2.21607366
C	-2.29194022	-1.32325216	-3.20481119
C	2.54748362	-1.47079048	-1.01684160
C	3.15305078	-1.82041471	-2.21607366
C	2.29194022	-1.32325216	-3.20481119
H	0.00000000	4.71422632	-2.36352943
N	0.00000000	2.79407016	-4.55516199
H	-4.08263951	-2.35711316	-2.36352943
H	-2.87914069	-1.66227274	-0.00508910
N	-2.41973547	-1.39703482	-4.55516199
H	0.00000000	3.32454548	-0.00508910
H	0.00000000	0.00000000	-4.32725329
H	4.08263951	-2.35711316	-2.36352943
N	2.41973547	-1.39703482	-4.55516199
H	2.87914069	-1.66227274	-0.00508910

B	0.00000000	0.00000000	-3.11824467
N	1.40510265	0.81123613	1.23483776
N	1.24883396	0.72101458	2.58636650
N	-1.40510265	0.81123613	1.23483776
N	-1.24883396	0.72101458	2.58636650
N	0.00000000	-1.62247279	1.23483776
N	0.00000000	-1.44202917	2.58636650
C	2.54748362	1.47079048	1.01684160
C	3.15305078	1.82041471	2.21607366
C	2.29194022	1.32325216	3.20481119
C	-2.54748362	1.47079048	1.01684160
C	-3.15305078	1.82041471	2.21607366
C	-2.29194022	1.32325216	3.20481119
C	0.00000000	-2.94158096	1.01684160
C	0.00000000	-3.64082943	2.21607366
C	0.00000000	-2.64650432	3.20481119
H	4.08263951	2.35711316	2.36352943
N	2.41973547	1.39703482	4.55516199
H	-4.08263951	2.35711316	2.36352943
H	-2.87914069	1.66227274	0.00508910
N	-2.41973547	1.39703482	4.55516199
H	2.87914069	1.66227274	0.00508910
H	0.00000000	0.00000000	4.32725329
H	0.00000000	-4.71422632	2.36352943
N	0.00000000	-2.79407016	4.55516199
H	0.00000000	-3.32454548	0.00508910
B	0.00000000	0.00000000	3.11824467
H	0.00000000	3.71405909	-4.95381079
H	0.00000000	2.00354021	-5.17053586
H	-3.21646949	-1.85702955	-4.95381079
H	-1.73511663	-1.00177010	-5.17053586
H	3.21646949	-1.85702955	-4.95381079
H	1.73511663	-1.00177010	-5.17053586
H	3.21646949	1.85702955	4.95381079
H	1.73511663	1.00177010	5.17053586
H	-3.21646949	1.85702955	4.95381079
H	-1.73511663	1.00177010	5.17053586
H	0.00000000	-3.71405909	4.95381079
H	0.00000000	-2.00354021	5.17053586

$[Fe(Tb^{5NH2})_2]^+$ ^2E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.57083673	-1.14731819
N	0.00000000	1.43105721	-2.50339310
N	-1.36038453	-0.78541863	-1.14731819
N	-1.23933206	-0.71552860	-2.50339310
N	1.36038453	-0.78541863	-1.14731819
N	1.23933206	-0.71552860	-2.50339310
C	0.00000000	2.88176118	-0.88760858
C	0.00000000	3.61583110	-2.06785800
C	0.00000000	2.65346935	-3.08509965
C	-2.49567822	-1.44088033	-0.88760858
C	-3.13140161	-1.80791555	-2.06785800
C	-2.29797178	-1.32673468	-3.08509965
C	2.49567822	-1.44088033	-0.88760858
C	3.13140161	-1.80791555	-2.06785800
C	2.29797178	-1.32673468	-3.08509965
H	0.00000000	4.69321904	-2.18032774
N	0.00000000	2.83420508	-4.43195259
H	-4.06444693	-2.34660952	-2.18032774
H	-2.80283651	-1.61821820	0.13327647
N	-2.45449394	-1.41710280	-4.43195259
H	0.00000000	3.23643641	0.13327647
H	0.00000000	0.00000000	-4.26346891
H	4.06444693	-2.34660952	-2.18032774
N	2.45449394	-1.41710280	-4.43195259
H	2.80283651	-1.61821820	0.13327647
B	0.00000000	0.00000000	-3.05533396
N	1.36038453	0.78541863	1.14731819
N	1.23933206	0.71552860	2.50339310
N	-1.36038453	0.78541863	1.14731819
N	-1.23933206	0.71552860	2.50339310
N	0.00000000	-1.57083673	1.14731819
N	0.00000000	-1.43105721	2.50339310
C	2.49567822	1.44088033	0.88760858
C	3.13140161	1.80791555	2.06785800
C	2.29797178	1.32673468	3.08509965
C	-2.49567822	1.44088033	0.88760858
C	-3.13140161	1.80791555	2.06785800
C	-2.29797178	1.32673468	3.08509965
C	0.00000000	-2.88176118	0.88760858
C	0.00000000	-3.61583110	2.06785800
C	0.00000000	-2.65346935	3.08509965
H	4.06444693	2.34660952	2.18032774
N	2.45449394	1.41710280	4.43195259
H	-4.06444693	2.34660952	2.18032774
H	-2.80283651	1.61821820	-0.13327647
N	-2.45449394	1.41710280	4.43195259
H	2.80283651	1.61821820	-0.13327647
H	0.00000000	0.00000000	4.26346891
H	0.00000000	-4.69321904	2.18032774
N	0.00000000	-2.83420508	4.43195259
H	0.00000000	-3.23643641	-0.13327647
B	0.00000000	0.00000000	3.05533396
H	0.00000000	3.76366311	-4.80781978
H	0.00000000	2.05917420	-5.06687162
H	-3.25942810	-1.88183156	-4.80781978
H	-1.78329716	-1.02958683	-5.06687162
H	3.25942810	-1.88183156	-4.80781978
H	1.78329716	-1.02958683	-5.06687162
H	3.25942810	1.88183156	4.80781978
H	1.78329716	1.02958683	5.06687162
H	-3.25942810	1.88183156	4.80781978
H	-1.78329716	1.02958683	5.06687162
H	0.00000000	-3.76366311	4.80781978
H	0.00000000	-2.05917420	5.06687162

$[Fe(Tb^{5NO2})_2]^+$ $^6A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	-1.43315963	-0.82743478	-1.30744034
N	-1.26783725	-0.73198602	-2.64169463
N	1.43315963	-0.82743478	-1.30744034
N	1.26783725	-0.73198602	-2.64169463
N	0.00000000	1.65487008	-1.30744034
N	0.00000000	1.46397203	-2.64169463
C	-2.57599410	-1.48725107	-1.05915938
C	-3.18539726	-1.83908991	-2.24990185
C	-2.32991874	-1.34517915	-3.22546815

C	2.57599410	-1.48725107	-1.05915938
C	3.18539726	-1.83908991	-2.24990185
C	2.32991874	-1.34517915	-3.22546815
C	0.00000000	2.97450214	-1.05915938
C	0.00000000	3.67817982	-2.24990185
C	0.00000000	2.69035830	-3.22546815
H	-4.11114471	-2.37357057	-2.41367109
N	-2.58523935	-1.49258888	-4.66337821
H	4.11114471	-2.37357057	-2.41367109
H	2.89501972	-1.67144074	-0.04152877
N	2.58523935	-1.49258888	-4.66337821
H	-2.89501972	-1.67144074	-0.04152877
H	0.00000000	0.00000000	-4.36300080
H	0.00000000	4.74714061	-2.41367109
N	0.00000000	2.98517723	-4.66337821
H	0.00000000	3.34288094	-0.04152877
B	0.00000000	0.00000000	-3.19590196
N	-1.43315963	0.82743478	1.30744034
N	-1.26783725	0.73198602	2.64169463
N	0.00000000	-1.65487008	1.30744034
N	0.00000000	-1.46397203	2.64169463
N	1.43315963	0.82743478	1.30744034
N	1.26783725	0.73198602	2.64169463
C	-2.57599410	1.48725107	1.05915938
C	-3.18539726	1.83908991	2.24990185
C	-2.32991874	1.34517915	3.22546815
C	0.00000000	-2.97450214	1.05915938
C	0.00000000	-3.67817982	2.24990185
C	0.00000000	-2.69035830	3.22546815
C	2.57599410	1.48725107	1.05915938
C	3.18539726	1.83908991	2.24990185
C	2.32991874	1.34517915	3.22546815
H	-4.11114471	2.37357057	2.41367109
N	-2.58523935	1.49258888	4.66337821
H	0.00000000	-4.74714061	2.41367109
H	0.00000000	-3.34288094	0.04152877
N	0.00000000	-2.98517723	4.66337821
H	-2.89501972	1.67144074	0.04152877
H	0.00000000	0.00000000	4.36300080
H	4.11114471	2.37357057	2.41367109
N	2.58523935	1.49258888	4.66337821
H	2.89501972	1.67144074	0.04152877
B	0.00000000	0.00000000	3.19590196
O	-3.62040530	-2.09024219	-4.92042500
O	-1.78950177	-1.03316936	-5.45999264
O	3.62040530	-2.09024219	-4.92042500
O	1.78950177	-1.03316936	-5.45999264
O	0.00000000	4.18048386	-4.92042500
O	0.00000000	2.06633820	-5.45999264
O	-3.62040530	2.09024219	4.92042500
O	-1.78950177	1.03316936	5.45999264
O	0.00000000	-4.18048386	4.92042500
O	0.00000000	-2.06633820	5.45999264
O	3.62040530	2.09024219	4.92042500
O	1.78950177	1.03316936	5.45999264

$[Fe(Tb^{5NO2})_2]^+$ ^4E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	-1.40673305	-0.81217754	-1.22265980
N	-1.26096588	-0.72801877	-2.55799625
N	1.40673305	-0.81217754	-1.22265980
N	1.26096588	-0.72801877	-2.55799625
N	0.00000000	1.62435507	-1.22265980
N	0.00000000	1.45603755	-2.55799625
C	-2.54588180	-1.46986548	-0.95046637
C	-3.17143916	-1.83103160	-2.13031996
C	-2.33032938	-1.34541622	-3.12168962
C	2.54588180	-1.46986548	-0.95046637
C	3.17143916	-1.83103160	-2.13031996
C	2.33032938	-1.34541622	-3.12168962
C	0.00000000	2.93973149	-0.95046637
C	0.00000000	3.66206267	-2.13031996
C	0.00000000	2.69083297	-3.12168962
H	-4.09970178	-2.36696379	-2.27539761
N	-2.60046273	-1.50137799	-4.55475241
H	4.09970178	-2.36696379	-2.27539761
H	2.85160284	-1.64637361	0.07187074
N	2.60046273	-1.50137799	-4.55475241
H	-2.85160284	-1.64637361	0.07187074
H	0.00000000	0.00000000	-4.28859742
H	0.00000000	4.73392812	-2.27539761
N	0.00000000	3.00275544	-4.55475241
H	0.00000000	3.29274722	0.07187074
B	0.00000000	0.00000000	-3.12136470
N	-1.40673305	0.81217754	1.22265980
N	-1.26096588	0.72801877	2.55799625
N	0.00000000	-1.62435507	1.22265980
N	0.00000000	-1.45603755	2.55799625
N	1.40673305	0.81217754	1.22265980
N	1.26096588	0.72801877	2.55799625
C	-2.54588180	1.46986548	0.95046637
C	-3.17143916	1.83103160	2.13031996
C	-2.33032938	1.34541622	3.12168962
C	0.00000000	-2.93973149	0.95046637
C	0.00000000	-3.66206267	2.13031996
C	0.00000000	-2.69083297	3.12168962
C	2.54588180	1.46986548	0.95046637
C	3.17143916	1.83103160	2.13031996
C	2.33032938	1.34541622	3.12168962
H	-4.09970178	2.36696379	2.27539761
N	-2.60046273	1.50137799	4.55475241
H	0.00000000	-4.73392812	2.27539761
H	0.00000000	-3.29274722	-0.07187074
N	0.00000000	-3.00275544	4.55475241
H	-2.85160284	1.64637361	-0.07187074
H	0.00000000	0.00000000	4.28859742
H	4.09970178	2.36696379	2.27539761
N	2.60046273	1.50137799	4.55475241
H	2.85160284	1.64637361	-0.07187074
B	0.00000000	0.00000000	3.12136470
O	-3.63826345	-2.10055215	-4.79762624
O	-1.81241885	-1.04640038	-5.36146725
O	3.63826345	-2.10055215	-4.79762624
O	1.81241885	-1.04640038	-5.36146725
O	0.00000000	4.20110484	-4.79762624
O	0.00000000	2.09280077	-5.36146725
O	-3.63826345	2.10055215	4.79762624
O	-1.81241885	1.04640038	5.36146725
O	0.00000000	-4.20110484	4.79762624

O	0.00000000	-2.09280077	5.36146725
O	3.63826345	2.10055215	4.79762624
O	1.81241885	1.04640038	5.36146725

$[Fe(Tb^{5NO2})_2]^+$ ^2E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	-1.35748622	-0.78374484	-1.13500635
N	-1.24911337	-0.72117598	-2.47479318
N	1.35748622	-0.78374484	-1.13500635
N	1.24911337	-0.72117598	-2.47479318
N	0.00000000	1.56749022	-1.13500635
N	0.00000000	1.44235197	-2.47479318
C	-2.48968159	-1.43741845	-0.82084387
C	-3.14509089	-1.81581934	-1.97917953
C	-2.33227623	-1.34654019	-3.00067207
C	2.48968159	-1.43741845	-0.82084387
C	3.14509089	-1.81581934	-1.97917953
C	2.33227623	-1.34654019	-3.00067207
C	0.00000000	2.87483637	-0.82084387
C	0.00000000	3.63163815	-1.97917953
C	0.00000000	2.69308039	-3.00067207
H	-4.07698261	-2.35384708	-2.08872187
N	-2.62870703	-1.51768458	-4.42413558
H	4.07698261	-2.35384708	-2.08872187
H	2.77018204	-1.59936521	0.21028551
N	2.62870703	-1.51768458	-4.42413558
H	-2.77018204	-1.59936521	0.21028551
H	0.00000000	0.00000000	-4.22816908
H	0.00000000	4.70769416	-2.08872187
N	0.00000000	3.03536969	-4.42413558
H	0.00000000	3.19873041	0.21028551
B	0.00000000	0.00000000	-3.06113322
N	-1.35748622	0.78374484	1.13500635
N	-1.24911337	0.72117598	2.47479318
N	0.00000000	-1.56749022	1.13500635
N	0.00000000	-1.44235197	2.47479318
N	1.35748622	0.78374484	1.13500635
N	1.24911337	0.72117598	2.47479318
C	-2.48968159	1.43741845	0.82084387
C	-3.14509089	1.81581934	1.97917953
C	-2.33227623	1.34654019	3.00067207
C	0.00000000	-2.87483637	0.82084387
C	0.00000000	-3.63163815	1.97917953
C	0.00000000	-2.69308039	3.00067207
C	2.48968159	1.43741845	0.82084387
C	3.14509089	1.81581934	1.97917953
C	2.33227623	1.34654019	3.00067207
H	-4.07698261	2.35384708	2.08872187
N	-2.62870703	1.51768458	4.42413558
H	0.00000000	-4.70769416	2.08872187
H	0.00000000	-3.19873041	-0.21028551
N	0.00000000	-3.03536969	4.42413558
H	-2.77018204	1.59936521	-0.21028551
H	0.00000000	0.00000000	4.22816908
H	4.07698261	2.35384708	2.08872187
N	2.62870703	1.51768458	4.42413558
H	2.77018204	1.59936521	-0.21028551
B	0.00000000	0.00000000	3.06113322
O	-3.66997651	-2.11886222	-4.64470672
O	-1.85212778	-1.06932646	-5.24656593
O	3.66997651	-2.11886222	-4.64470672
O	1.85212778	-1.06932646	-5.24656593
O	0.00000000	4.23772390	-4.64470672
O	0.00000000	2.13865292	-5.24656593
O	-3.66997651	2.11886222	4.64470672
O	-1.85212778	1.06932646	5.24656593
O	0.00000000	-4.23772390	4.64470672
O	0.00000000	-2.13865292	5.24656593
O	3.66997651	2.11886222	4.64470672
O	1.85212778	1.06932646	5.24656593

$[Fe(Tb^{3,5\text{-}CH3})_2]^+$ $^6A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.49680000	0.86420000	1.31590000
N	1.26330000	0.72940000	2.64550000
N	0.00000000	-1.72830000	1.31590000
N	0.00000000	-1.45880000	2.64550000
N	-1.49680000	0.86420000	1.31590000
N	-1.26330000	0.72940000	2.64550000
C	2.66420000	1.53820000	1.17850000
C	3.16560000	1.82770000	2.44850000
C	2.25830000	1.30380000	3.36080000
C	0.00000000	-3.07630000	1.17850000
C	0.00000000	-3.65530000	2.44850000
C	0.00000000	-2.60770000	3.36080000
C	-2.66420000	1.53820000	1.17850000
C	-3.16560000	1.82770000	2.44850000
C	-2.25830000	1.30380000	3.36080000
H	4.08280000	2.35720000	2.67950000
C	2.32450000	1.34210000	4.84680000
H	0.00000000	-4.71440000	2.67950000
C	0.00000000	-3.81190000	-0.11540000
C	0.00000000	-2.68420000	4.84680000
C	3.30120000	1.90600000	-0.11540000
H	0.00000000	0.00000000	4.34420000
H	-4.08280000	2.35720000	2.67950000
C	-2.32450000	1.34210000	4.84680000
C	-3.30120000	1.90600000	-0.11540000
B	0.00000000	0.00000000	3.14970000
N	0.00000000	1.72830000	-1.31590000
N	0.00000000	1.45880000	-2.64550000
N	1.49680000	-0.86420000	-1.31590000
N	1.26330000	-0.72940000	-2.64550000
N	-1.49680000	-0.86420000	-1.31590000
N	-1.26330000	-0.72940000	-2.64550000
C	0.00000000	3.07630000	-1.17850000
C	0.00000000	3.65530000	-2.44850000
C	0.00000000	2.60770000	-3.36080000
C	2.66420000	-1.53820000	-1.17850000
C	3.16560000	-1.82770000	-2.44850000
C	2.25830000	-1.30380000	-3.36080000
C	-2.66420000	-1.53820000	-1.17850000
C	-3.16560000	-1.82770000	-2.44850000
C	-2.25830000	-1.30380000	-3.36080000
H	0.00000000	4.71440000	-2.67950000
C	0.00000000	2.68420000	-4.84680000
H	4.08280000	-2.35720000	-2.67950000
C	3.30120000	-1.90600000	0.11540000

C	2.32450000	-1.34210000	-4.84680000
C	0.00000000	3.81190000	0.11540000
H	0.00000000	0.00000000	-4.34420000
H	-4.08280000	-2.35720000	-2.67950000
C	-2.32450000	-1.34210000	-4.84680000
C	-3.30120000	-1.90600000	0.11540000
B	0.00000000	0.00000000	-3.14970000
H	-0.87810000	-3.58200000	-0.72360000
H	0.00000000	-4.88610000	0.08520000
H	0.87810000	-3.58200000	-0.72360000
H	4.23150000	2.44310000	0.08520000
H	2.66310000	2.55150000	-0.72360000
H	3.54120000	1.03050000	-0.72360000
H	-4.23150000	2.44310000	0.08520000
H	-3.54120000	1.03050000	-0.72360000
H	-2.66310000	2.55150000	-0.72360000
H	3.54120000	-1.03050000	0.72360000
H	4.23150000	-2.44310000	-0.08520000
H	2.66310000	-2.55150000	0.72360000
H	-2.66310000	-2.55150000	0.72360000
H	-4.23150000	-2.44310000	-0.08520000
H	-3.54120000	-1.03050000	0.72360000
H	-0.87810000	3.58200000	0.72360000
H	0.00000000	4.88610000	-0.08520000
H	0.87810000	3.58200000	0.72360000
H	-3.23270000	-1.86640000	-5.15370000
H	-1.47000000	-1.86930000	-5.28310000
H	-2.35390000	-0.33840000	-5.28310000
H	3.23270000	-1.86640000	-5.15370000
H	2.35390000	-0.33840000	-5.28310000
H	1.47000000	-1.86930000	-5.28310000
H	0.88390000	2.20770000	-5.28310000
H	0.00000000	3.73280000	-5.15370000
H	-0.88390000	2.20770000	-5.28310000
H	-2.35390000	0.33840000	5.28310000
H	-3.23270000	1.86640000	5.15370000
H	-1.47000000	1.86930000	5.28310000
H	-0.88390000	-2.20770000	5.28310000
H	0.88390000	-2.20770000	5.28310000
H	0.00000000	-3.73280000	5.15370000
H	2.35390000	0.33840000	5.28310000
H	1.47000000	1.86930000	5.28310000
H	3.23270000	1.86640000	5.15370000

$[Fe(Tb^{3,5\text{-}CH3})_2]^+$ ^4E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.46550000	0.84610000	1.22520000
N	1.25560000	0.72490000	2.55780000
N	0.00000000	-1.69220000	1.22520000
N	0.00000000	-1.44980000	2.55780000
N	-1.46550000	0.84610000	1.22520000
N	-1.25560000	0.72490000	2.55780000
C	2.63060000	1.51880000	1.05740000
C	3.15150000	1.81950000	2.31830000
C	2.26080000	1.30530000	3.25110000
C	0.00000000	-3.03760000	1.05740000
C	0.00000000	-3.63900000	2.31830000
C	0.00000000	-2.61050000	3.25110000
C	-2.63060000	1.51880000	1.05740000
C	-3.15150000	1.81950000	2.31830000
C	-2.26080000	1.30530000	3.25110000
H	4.07290000	2.35150000	2.52640000
C	2.34680000	1.35490000	4.73590000
H	0.00000000	-4.70300000	2.52640000
C	0.00000000	-3.76160000	-0.24210000
C	0.00000000	-2.70980000	4.73590000
C	3.25760000	1.88080000	-0.24210000
H	0.00000000	0.00000000	4.26650000
H	-4.07290000	2.35150000	2.52640000
C	-2.34680000	1.35490000	4.73590000
C	-3.25760000	1.88080000	-0.24210000
B	0.00000000	0.00000000	3.07170000
N	0.00000000	1.69220000	-1.22520000
N	0.00000000	1.44980000	-2.55780000
N	1.46550000	-0.84610000	-1.22520000
N	1.25560000	-0.72490000	-2.55780000
N	-1.46550000	-0.84610000	-1.22520000
N	-1.25560000	-0.72490000	-2.55780000
C	0.00000000	3.03760000	-1.05740000
C	0.00000000	3.63900000	-2.31830000
C	0.00000000	2.61050000	-3.25110000
C	2.63060000	-1.51880000	-1.05740000
C	3.15150000	-1.81950000	-2.31830000
C	2.26080000	-1.30530000	-3.25110000
C	-2.63060000	-1.51880000	-1.05740000
C	-3.15150000	-1.81950000	-2.31830000
C	-2.26080000	-1.30530000	-3.25110000
H	0.00000000	4.70300000	-2.52640000
C	0.00000000	2.70980000	-4.73590000
H	4.07290000	-2.35150000	-2.52640000
C	3.25760000	-1.88080000	0.24210000
C	2.34680000	-1.35490000	-4.73590000
C	0.00000000	3.76160000	0.24210000
H	0.00000000	0.00000000	-4.26650000
H	-4.07290000	-2.35150000	-2.52640000
C	-2.34680000	-1.35490000	-4.73590000
C	-3.25760000	-1.88080000	0.24210000
B	0.00000000	0.00000000	-3.07170000
H	-0.87930000	-3.52870000	-0.84760000
H	0.00000000	-4.83690000	-0.04700000
H	0.87930000	-3.52870000	-0.84760000
H	4.18890000	2.41850000	-0.04700000
H	2.61630000	2.52580000	-0.84760000
H	3.49560000	1.00290000	-0.84760000
H	-4.18890000	2.41850000	-0.04700000
H	-3.49560000	1.00290000	-0.84760000
H	-2.61630000	2.52580000	-0.84760000
H	3.49560000	-1.00290000	0.84760000
H	4.18890000	-2.41850000	0.04700000
H	2.61630000	-2.52580000	0.84760000
H	-2.61630000	-2.52580000	0.84760000
H	-4.18890000	-2.41850000	0.04700000
H	-3.49560000	-1.00290000	0.84760000
H	-0.87930000	3.52870000	0.84760000
H	0.00000000	4.83690000	0.04700000
H	0.87930000	3.52870000	0.84760000
H	-3.25900000	-1.88160000	-5.02660000
H	-1.49770000	-1.88550000	-5.17910000
H	-2.38180000	-0.35430000	-5.17910000

H	3.25900000	-1.88160000	-5.02660000
H	2.38180000	-0.35430000	-5.17910000
H	1.49770000	-1.88550000	-5.17910000
H	0.88400000	2.23980000	-5.17910000
H	0.00000000	3.76310000	-5.02660000
H	-0.88400000	2.23980000	-5.17910000
H	-2.38180000	0.35430000	5.17910000
H	-3.25900000	1.88160000	5.02660000
H	-1.49770000	1.88550000	5.17910000
H	-0.88400000	-2.23980000	5.17910000
H	0.88400000	-2.23980000	5.17910000
H	0.00000000	-3.76310000	5.02660000
H	2.38180000	0.35430000	5.17910000
H	1.49770000	1.88550000	5.17910000
H	3.25900000	1.88160000	5.02660000

$[Fe(Tb^{3,5\text{-}CH3})_2]^+$ ^2E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.41360000	0.81620000	1.13710000
N	1.24300000	0.71770000	2.47670000
N	0.00000000	-1.63230000	1.13710000
N	0.00000000	-1.43530000	2.47670000
N	-1.41360000	0.81620000	1.13710000
N	-1.24300000	0.71770000	2.47670000
C	2.57520000	1.48680000	0.92660000
C	3.12790000	1.80590000	2.17070000
C	2.26440000	1.30730000	3.13520000
C	0.00000000	-2.97360000	0.92660000
C	0.00000000	-3.61170000	2.17070000
C	0.00000000	-2.61470000	3.13520000
C	-2.57520000	1.48680000	0.92660000
C	-3.12790000	1.80590000	2.17070000
C	-2.26440000	1.30730000	3.13520000
H	4.05470000	2.34100000	2.34290000
C	2.38040000	1.37430000	4.61720000
H	0.00000000	-4.68190000	2.34290000
C	0.00000000	-3.67780000	-0.38360000
C	0.00000000	-2.74870000	4.61720000
C	3.18500000	1.83890000	-0.38360000
H	0.00000000	0.00000000	4.20680000
H	-4.05470000	2.34100000	2.34290000
C	-2.38040000	1.37430000	4.61720000
C	-3.18500000	1.83890000	-0.38360000
B	0.00000000	0.00000000	3.01240000
N	0.00000000	1.63230000	-1.13710000
N	0.00000000	1.43530000	-2.47670000
N	1.41360000	-0.81620000	-1.13710000
N	1.24300000	-0.71770000	-2.47670000
N	-1.41360000	-0.81620000	-1.13710000
N	-1.24300000	-0.71770000	-2.47670000
C	0.00000000	2.97360000	-0.92660000
C	0.00000000	3.61170000	-2.17070000
C	0.00000000	2.61470000	-3.13520000
C	2.57520000	-1.48680000	-0.92660000
C	3.12790000	-1.80590000	-2.17070000
C	2.26440000	-1.30730000	-3.13520000
C	-2.57520000	-1.48680000	-0.92660000
C	-3.12790000	-1.80590000	-2.17070000
C	-2.26440000	-1.30730000	-3.13520000
H	0.00000000	4.68190000	-2.34290000
C	0.00000000	2.74870000	-4.61720000
H	4.05470000	-2.34100000	-2.34290000
C	3.18500000	-1.83890000	0.38360000
C	2.38040000	-1.37430000	-4.61720000
C	0.00000000	3.67780000	0.38360000
H	0.00000000	0.00000000	-4.20680000
H	-4.05470000	-2.34100000	-2.34290000
C	-2.38040000	-1.37430000	-4.61720000
C	-3.18500000	-1.83890000	0.38360000
B	0.00000000	0.00000000	-3.01240000
H	-0.88090000	-3.44070000	-0.98530000
H	0.00000000	-4.75520000	-0.19890000
H	0.88090000	-3.44070000	-0.98530000
H	4.11810000	2.37760000	-0.19890000
H	2.53930000	2.48320000	-0.98530000
H	3.42020000	0.95750000	-0.98530000
H	-4.11810000	2.37760000	-0.19890000
H	-3.42020000	0.95750000	-0.98530000
H	-2.53930000	2.48320000	-0.98530000
H	3.42020000	-0.95750000	0.98530000
H	4.11810000	-2.37760000	0.19890000
H	2.53930000	-2.48320000	0.98530000
H	-2.53930000	-2.48320000	0.98530000
H	-4.11810000	-2.37760000	0.19890000
H	-3.42020000	-0.95750000	0.98530000
H	-0.88090000	3.44070000	0.98530000
H	0.00000000	4.75520000	0.19890000
H	0.88090000	3.44070000	0.98530000
H	-3.29790000	-1.90400000	-4.88440000
H	-1.53920000	-1.90950000	-5.07080000
H	-2.42330000	-0.37820000	-5.07080000
H	3.29790000	-1.90400000	-4.88440000
H	2.42330000	-0.37820000	-5.07080000
H	1.53920000	-1.90950000	-5.07080000
H	0.88410000	2.28770000	-5.07080000
H	0.00000000	3.80810000	-4.88440000
H	-0.88410000	2.28770000	-5.07080000
H	-2.42330000	0.37820000	5.07080000
H	-3.29790000	1.90400000	4.88440000
H	-1.53920000	1.90950000	5.07080000
H	-0.88410000	-2.28770000	5.07080000
H	0.88410000	-2.28770000	5.07080000
H	0.00000000	-3.80810000	4.88440000
H	2.42330000	0.37820000	5.07080000
H	1.53920000	1.90950000	5.07080000
H	3.29790000	1.90400000	4.88440000

$[Fe(Tb^{3,5\text{-}CF3})_2]^+$ $^6A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.55306696	0.89666386	1.24217480
N	1.28908901	0.74425605	2.56308535
N	0.00000000	-1.79332772	1.24217480
N	0.00000000	-1.48851210	2.56308535
N	-1.55306696	0.89666386	1.24217480
N	-1.28908901	0.74425605	2.56308535
C	2.72771927	1.57484948	1.14283553
C	3.20840748	1.85237490	2.41485910
C	2.28166942	1.31732220	3.28956316

C	0.00000000	-3.14969897	1.14283553
C	0.00000000	-3.70474981	2.41485910
C	0.00000000	-2.63464493	3.28956316
C	-2.72771927	1.57484948	1.14283553
C	-3.20840748	1.85237490	2.41485910
C	-2.28166942	1.31732220	3.28956316
H	4.11617983	2.37647734	2.67582709
C	2.40904238	1.39086143	4.79831153
H	0.00000000	-4.75295469	2.67582709
C	0.00000000	-4.05056502	-0.09875982
C	0.00000000	-2.78172287	4.79831153
C	3.50789217	2.02528251	-0.09875982
H	0.00000000	0.00000000	4.24137999
H	-4.11617983	2.37647734	2.67582709
C	-2.40904238	1.39086143	4.79831153
C	-3.50789217	2.02528251	-0.09875982
B	0.00000000	0.00000000	3.05616795
N	0.00000000	1.79332772	-1.24217480
N	0.00000000	1.48851210	-2.56308535
N	1.55306696	-0.89666386	-1.24217480
N	1.28908901	-0.74425605	-2.56308535
N	-1.55306696	-0.89666386	-1.24217480
N	-1.28908901	-0.74425605	-2.56308535
C	0.00000000	3.14969897	-1.14283553
C	0.00000000	3.70474981	-2.41485910
C	0.00000000	2.63464493	-3.28956316
C	2.72771927	-1.57484948	-1.14283553
C	3.20840748	-1.85237490	-2.41485910
C	2.28166942	-1.31732220	-3.28956316
C	-2.72771927	-1.57484948	-1.14283553
C	-3.20840748	-1.85237490	-2.41485910
C	-2.28166942	-1.31732220	-3.28956316
H	0.00000000	4.75295469	-2.67582709
C	0.00000000	2.78172287	-4.79831153
H	4.11617983	-2.37647734	-2.67582709
C	3.50789217	-2.02528251	0.09875982
C	2.40904238	-1.39086143	-4.79831153
C	0.00000000	4.05056502	0.09875982
H	0.00000000	0.00000000	-4.24137999
H	-4.11617983	-2.37647734	-2.67582709
C	-2.40904238	-1.39086143	-4.79831153
C	-3.50789217	-2.02528251	0.09875982
B	0.00000000	0.00000000	-3.05616795
F	-1.07725830	-3.89498903	-0.88545483
F	0.00000000	-5.33226777	0.32399142
F	1.07725830	-3.89498903	-0.88545483
F	4.61787902	2.66613362	0.32399142
F	2.83453052	2.88042765	-0.88545483
F	3.91178882	1.01456190	-0.88545483
F	-4.61787902	2.66613362	0.32399142
F	-3.91178882	1.01456190	-0.88545483
F	-2.83453052	2.88042765	-0.88545483
F	3.91178882	-1.01456190	0.88545483
F	4.61787902	-2.66613362	-0.32399142
F	2.83453052	-2.88042765	0.88545483
F	-2.83453052	-2.88042765	0.88545483
F	-4.61787902	-2.66613362	-0.32399142
F	-3.91178882	-1.01456190	0.88545483
F	-1.07725830	3.89498903	0.88545483
F	0.00000000	5.33226777	-0.32399142
F	1.07725830	3.89498903	0.88545483
F	-3.54592467	-2.04724019	-5.10183225
F	-1.38770912	-2.05860110	-5.36197526
F	-2.47665536	-0.17249062	-5.36197526
F	3.54592467	-2.04724019	-5.10183225
F	2.47665536	-0.17249062	-5.36197526
F	1.38770912	-2.05860110	-5.36197526
F	1.08894623	2.23109171	-5.36197526
F	0.00000000	4.09448091	-5.10183225
F	-1.08894623	2.23109171	-5.36197526
F	-2.47665536	0.17249062	5.36197526
F	-3.54592467	2.04724019	5.10183225
F	-1.38770912	2.05860110	5.36197526
F	-1.08894623	-2.23109171	5.36197526
F	1.08894623	-2.23109171	5.36197526
F	0.00000000	-4.09448091	5.10183225
F	2.47665536	0.17249062	5.36197526
F	1.38770912	2.05860110	5.36197526
F	3.54592467	2.04724019	5.10183225

$[Fe(Tb^{3,5\text{-}CF3})_2]^+$ ^4E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.52256148	0.87905125	1.17693042
N	1.27933786	0.73862613	2.50023920
N	0.00000000	-1.75810251	1.17693042
N	0.00000000	-1.47725227	2.50023920
N	-1.52256148	0.87905125	1.17693042
N	-1.27933786	0.73862613	2.50023920
C	2.69796099	1.55766869	1.05298335
C	3.19309468	1.84353394	2.31820487
C	2.27983846	1.31626543	3.20872763
C	0.00000000	-3.11533684	1.05298335
C	0.00000000	-3.68706788	2.31820487
C	0.00000000	-2.63253034	3.20872763
C	-2.69796099	1.55766869	1.05298335
C	-3.19309468	1.84353394	2.31820487
C	-2.27983846	1.31626543	3.20872763
H	4.10448395	2.36972504	2.56138934
C	2.42406731	1.39953624	4.71525769
H	0.00000000	-4.73944955	2.56138934
C	0.00000000	-4.01598964	-0.18868820
C	0.00000000	-2.79907194	4.71525769
C	3.47794920	2.00799482	-0.18868820
H	0.00000000	0.00000000	4.18535388
H	-4.10448395	2.36972504	2.56138934
C	-2.42406731	1.39953624	4.71525769
C	-3.47794920	2.00799482	-0.18868820
B	0.00000000	0.00000000	2.99996509
N	0.00000000	1.75810251	-1.17693042
N	0.00000000	1.47725227	-2.50023920
N	1.52256148	-0.87905125	-1.17693042
N	1.27933786	-0.73862613	-2.50023920
N	-1.52256148	-0.87905125	-1.17693042
N	-1.27933786	-0.73862613	-2.50023920
C	0.00000000	3.11533684	-1.05298335
C	0.00000000	3.68706788	-2.31820487
C	0.00000000	2.63253034	-3.20872763
C	2.69796099	-1.55766869	-1.05298335
C	3.19309468	-1.84353394	-2.31820487

C	2.27983846	-1.31626543	-3.20872763
C	-2.69796099	-1.55766869	-1.05298335
C	-3.19309468	-1.84353394	-2.31820487
C	-2.27983846	-1.31626543	-3.20872763
H	0.00000000	4.73944955	-2.56138934
C	0.00000000	2.79907194	-4.71525769
H	4.10448395	-2.36972504	-2.56138934
C	3.47794920	-2.00799482	0.18868820
C	2.42406731	-1.39953624	-4.71525769
C	0.00000000	4.01598964	0.18868820
H	0.00000000	0.00000000	-4.18535388
H	-4.10448395	-2.36972504	-2.56138934
C	-2.42406731	-1.39953624	-4.71525769
C	-3.47794920	-2.00799482	0.18868820
B	0.00000000	0.00000000	-2.99996509
F	-1.07888128	-3.86229857	-0.97320617
F	0.00000000	-5.29760561	0.23396831
F	1.07888128	-3.86229857	-0.97320617
F	4.58786144	2.64880307	0.23396831
F	2.80540778	2.86548792	-0.97320617
F	3.88428906	0.99681065	-0.97320617
F	-4.58786144	2.64880307	0.23396831
F	-3.88428906	0.99681065	-0.97320617
F	-2.80540778	2.86548792	-0.97320617
F	3.88428906	-0.99681065	0.97320617
F	4.58786144	-2.64880307	-0.23396831
F	2.80540778	-2.86548792	0.97320617
F	-2.80540778	-2.86548792	0.97320617
F	-4.58786144	-2.64880307	-0.23396831
F	-3.88428906	-0.99681065	0.97320617
F	-1.07888128	3.86229857	0.97320617
F	0.00000000	5.29760561	-0.23396831
F	1.07888128	3.86229857	0.97320617
F	-3.56452577	-2.05797984	-5.00008099
F	-1.40926569	-2.07109497	-5.28595365
F	-2.49825373	-0.18491252	-5.28595365
F	3.56452577	-2.05797984	-5.00008099
F	2.49825373	-0.18491252	-5.28595365
F	1.40926569	-2.07109497	-5.28595365
F	1.08898804	2.25600750	-5.28595365
F	0.00000000	4.11595969	-5.00008099
F	-1.08898804	2.25600750	-5.28595365
F	-2.49825373	0.18491252	5.28595365
F	-3.56452577	2.05797984	5.00008099
F	-1.40926569	2.07109497	5.28595365
F	-1.08898804	-2.25600750	5.28595365
F	1.08898804	-2.25600750	5.28595365
F	0.00000000	-4.11595969	5.00008099
F	2.49825373	0.18491252	5.28595365
F	1.40926569	2.07109497	5.28595365
F	3.56452577	2.05797984	5.00008099

$[Fe(Tb^{3,5\text{-}CF3})_2]^+$ ^2E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.47109264	0.84933583	1.10753676
N	1.26446956	0.73004182	2.43850168
N	0.00000000	-1.69867114	1.10753676
N	0.00000000	-1.46008417	2.43850168
N	-1.47109264	0.84933583	1.10753676
N	-1.26446956	0.73004182	2.43850168
C	2.64858240	1.52915979	0.94783318
C	3.16836887	1.82925833	2.20062592
C	2.27791385	1.31515416	3.11765887
C	0.00000000	-3.05831958	0.94783318
C	0.00000000	-3.65851718	2.20062592
C	0.00000000	-2.63030832	3.11765887
C	-2.64858240	1.52915979	0.94783318
C	-3.16836887	1.82925833	2.20062592
C	-2.27791385	1.31515416	3.11765887
H	4.08424927	2.35804239	2.41760553
C	2.45059444	1.41485168	4.61982745
H	0.00000000	-4.71608532	2.41760553
C	0.00000000	-3.96376990	-0.29435537
C	0.00000000	-2.82970284	4.61982745
C	3.43272518	1.98188469	-0.29435537
H	0.00000000	0.00000000	4.14264028
H	-4.08424927	2.35804239	2.41760553
C	-2.45059444	1.41485168	4.61982745
C	-3.43272518	1.98188469	-0.29435537
B	0.00000000	0.00000000	2.95798122
N	0.00000000	1.69867114	-1.10753676
N	0.00000000	1.46008417	-2.43850168
N	1.47109264	-0.84933583	-1.10753676
N	1.26446956	-0.73004182	-2.43850168
N	-1.47109264	-0.84933583	-1.10753676
N	-1.26446956	-0.73004182	-2.43850168
C	0.00000000	3.05831958	-0.94783318
C	0.00000000	3.65851718	-2.20062592
C	0.00000000	2.63030832	-3.11765887
C	2.64858240	-1.52915979	-0.94783318
C	3.16836887	-1.82925833	-2.20062592
C	2.27791385	-1.31515416	-3.11765887
C	-2.64858240	-1.52915979	-0.94783318
C	-3.16836887	-1.82925833	-2.20062592
C	-2.27791385	-1.31515416	-3.11765887
H	0.00000000	4.71608532	-2.41760553
C	0.00000000	2.82970284	-4.61982745
H	4.08424927	-2.35804239	-2.41760553
C	3.43272518	-1.98188469	0.29435537
C	2.45059444	-1.41485168	-4.61982745
C	0.00000000	3.96376990	0.29435537
H	0.00000000	0.00000000	-4.14264028
H	-4.08424927	-2.35804239	-2.41760553
C	-2.45059444	-1.41485168	-4.61982745
C	-3.43272518	-1.98188469	0.29435537
B	0.00000000	0.00000000	-2.95798122
F	-1.07919350	-3.81961567	-1.07933955
F	0.00000000	-5.24373695	0.13476504
F	1.07919350	-3.81961567	-1.07933955
F	4.54120970	2.62186847	0.13476504
F	2.76828706	2.84441714	-1.07933955
F	3.84748108	0.97519853	-1.07933955
F	-4.54120970	2.62186847	0.13476504
F	-3.84748108	0.97519853	-1.07933955
F	-2.76828706	2.84441714	-1.07933955
F	3.84748108	-0.97519853	1.07933955
F	4.54120970	-2.62186847	-0.13476504
F	2.76828706	-2.84441714	1.07933955
F	-2.76828706	-2.84441714	1.07933955

F	-4.54120970	-2.62186847	-0.13476504
F	-3.84748108	-0.97519853	1.07933955
F	-1.07919350	3.81961567	1.07933955
F	0.00000000	5.24373695	-0.13476504
F	1.07919350	3.81961567	1.07933955
F	-3.59568691	-2.07597081	-4.87650064
F	-1.44583237	-2.09222290	-5.20174726
F	-2.53483416	-0.20601611	-5.20174726
F	3.59568691	-2.07597081	-4.87650064
F	2.53483416	-0.20601611	-5.20174726
F	1.44583237	-2.09222290	-5.20174726
F	1.08900233	2.29823902	-5.20174726
F	0.00000000	4.15194163	-4.87650064
F	-1.08900233	2.29823902	-5.20174726
F	-2.53483416	0.20601611	5.20174726
F	-3.59568691	2.07597081	4.87650064
F	-1.44583237	2.09222290	5.20174726
F	-1.08900233	-2.29823902	5.20174726
F	1.08900233	-2.29823902	5.20174726
F	0.00000000	-4.15194163	4.87650064
F	2.53483416	0.20601611	5.20174726
F	1.44583237	2.09222290	5.20174726
F	3.59568691	2.07597081	4.87650064

$[Fe(Tb^{3,5\text{-}NH2})_2]^+$ $^6A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.69921196	1.33922167
N	0.00000000	1.45263706	2.69874311
N	1.47156096	-0.84960624	1.33922167
N	1.25802101	-0.72631853	2.69874311
N	-1.47156096	-0.84960624	1.33922167
N	-1.25802101	-0.72631853	2.69874311
C	0.00000000	3.04553043	1.19926752
C	0.00000000	3.67284730	2.45318529
C	0.00000000	2.62654270	3.37152054
C	2.63750672	-1.52276521	1.19926752
C	3.18077913	-1.83642338	2.45318529
C	2.27465253	-1.31327135	3.37152054
C	-2.63750672	-1.52276521	1.19926752
C	-3.18077913	-1.83642338	2.45318529
C	-2.27465253	-1.31327135	3.37152054
H	0.00000000	4.73491874	2.66603361
N	0.00000000	2.70490856	4.72991801
H	4.10056010	-2.36745963	2.66603361
N	3.14976300	-1.81851656	-0.01645847
N	2.34251951	-1.35245428	4.72991801
N	0.00000000	3.63703311	-0.01645847
H	0.00000000	0.00000000	4.40797716
H	-4.10056010	-2.36745963	2.66603361
N	-2.34251951	-1.35245428	4.72991801
N	-3.14976300	-1.81851656	-0.01645847
B	0.00000000	0.00000000	3.19659148
N	-1.47156096	0.84960624	-1.33922167
N	-1.25802101	0.72631853	-2.69874311
N	1.47156096	0.84960624	-1.33922167
N	1.25802101	0.72631853	-2.69874311
N	0.00000000	-1.69921196	-1.33922167
N	0.00000000	-1.45263706	-2.69874311
C	-2.63750672	1.52276521	-1.19926752
C	-3.18077913	1.83642338	-2.45318529
C	-2.27465253	1.31327135	-3.37152054
C	2.63750672	1.52276521	-1.19926752
C	3.18077913	1.83642338	-2.45318529
C	2.27465253	1.31327135	-3.37152054
C	0.00000000	-3.04553043	-1.19926752
C	0.00000000	-3.67284730	-2.45318529
C	0.00000000	-2.62654270	-3.37152054
H	-4.10056010	2.36745963	-2.66603361
N	-2.34251951	1.35245428	-4.72991801
H	4.10056010	2.36745963	-2.66603361
N	3.14976300	1.81851656	0.01645847
N	2.34251951	1.35245428	-4.72991801
N	-3.14976300	1.81851656	0.01645847
H	0.00000000	0.00000000	-4.40797716
H	0.00000000	-4.73491874	-2.66603361
N	0.00000000	-2.70490856	-4.72991801
N	0.00000000	-3.63703311	0.01645847
B	0.00000000	0.00000000	-3.19659148
H	0.00000000	3.60208413	5.17635946
H	0.00000000	1.88103514	5.29887775
H	3.11949618	-1.80104206	5.17635946
H	1.62902453	-0.94051784	5.29887775
H	-3.11949618	-1.80104206	5.17635946
H	-1.62902453	-0.94051784	5.29887775
H	-3.11949618	1.80104206	-5.17635946
H	-1.62902453	0.94051784	-5.29887775
H	3.11949618	1.80104206	-5.17635946
H	1.62902453	0.94051784	-5.29887775
H	0.00000000	-3.60208413	-5.17635946
H	0.00000000	-1.88103514	-5.29887775
H	0.00000000	4.63591708	-0.09059144
H	4.01482227	-2.31795881	-0.09059144
H	-4.01482227	-2.31795881	-0.09059144
H	-4.01482227	2.31795881	0.09059144
H	4.01482227	2.31795881	0.09059144
H	0.00000000	-4.63591708	0.09059144
H	2.66962249	-1.54130758	-0.85397566
H	0.00000000	3.08261464	-0.85397566
H	-2.66962249	-1.54130758	-0.85397566
H	2.66962249	1.54130758	0.85397566
H	-2.66962249	1.54130758	0.85397566
H	0.00000000	-3.08261464	0.85397566

$[Fe(Tb^{3,5\text{-}NH2})_2]^+$ ^4E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.65331853	1.24485931
N	0.00000000	1.44256681	2.61041867
N	1.43181605	-0.82665953	1.24485931
N	1.24929964	-0.72128341	2.61041867
N	-1.43181605	-0.82665953	1.24485931
N	-1.24929964	-0.72128341	2.61041867
C	0.00000000	2.99730968	1.06918676
C	0.00000000	3.65309682	2.30964702
C	0.00000000	2.63091952	3.25380612
C	2.59574670	-1.49865484	1.06918676
C	3.16367507	-1.82654841	2.30964702
C	2.27844302	-1.31546003	3.25380612
C	-2.59574670	-1.49865484	1.06918676

C	-3.16367507	-1.82654841	2.30964702
C	-2.27844302	-1.31546003	3.25380612
H	0.00000000	4.72052882	2.49431189
N	0.00000000	2.73893730	4.61047530
H	4.08809798	-2.36026441	2.49431189
N	3.08967439	-1.78382422	-0.15444250
N	2.37198939	-1.36946838	4.61047530
N	0.00000000	3.56764845	-0.15444250
H	0.00000000	0.00000000	4.33185448
H	-4.08809798	-2.36026441	2.49431189
N	-2.37198939	-1.36946838	4.61047530
N	-3.08967439	-1.78382422	-0.15444250
B	0.00000000	0.00000000	3.12093342
N	-1.43181605	0.82665953	-1.24485931
N	-1.24929964	0.72128341	-2.61041867
N	1.43181605	0.82665953	-1.24485931
N	1.24929964	0.72128341	-2.61041867
N	0.00000000	-1.65331853	-1.24485931
N	0.00000000	-1.44256681	-2.61041867
C	-2.59574670	1.49865484	-1.06918676
C	-3.16367507	1.82654841	-2.30964702
C	-2.27844302	1.31546003	-3.25380612
C	2.59574670	1.49865484	-1.06918676
C	3.16367507	1.82654841	-2.30964702
C	2.27844302	1.31546003	-3.25380612
C	0.00000000	-2.99730968	-1.06918676
C	0.00000000	-3.65309682	-2.30964702
C	0.00000000	-2.63091952	-3.25380612
H	-4.08809798	2.36026441	-2.49431189
N	-2.37198939	1.36946838	-4.61047530
H	4.08809798	2.36026441	-2.49431189
N	3.08967439	1.78382422	0.15444250
N	2.37198939	1.36946838	-4.61047530
N	-3.08967439	1.78382422	0.15444250
H	0.00000000	0.00000000	-4.33185448
H	0.00000000	-4.72052882	-2.49431189
N	0.00000000	-2.73893730	-4.61047530
N	0.00000000	-3.56764845	0.15444250
B	0.00000000	0.00000000	-3.12093342
H	0.00000000	3.64567087	5.03707207
H	0.00000000	1.92788056	5.19767419
H	3.15724345	-1.82283517	5.03707207
H	1.66959338	-0.96394028	5.19767419
H	-3.15724345	-1.82283517	5.03707207
H	-1.66959338	-0.96394028	5.19767419
H	-3.15724345	1.82283517	-5.03707207
H	-1.66959338	0.96394028	-5.19767419
H	3.15724345	1.82283517	-5.03707207
H	1.66959338	0.96394028	-5.19767419
H	0.00000000	-3.64567087	-5.03707207
H	0.00000000	-1.92788056	-5.19767419
H	0.00000000	4.56538093	-0.24315165
H	3.95373564	-2.28269020	-0.24315165
H	-3.95373564	-2.28269020	-0.24315165
H	-3.95373564	2.28269020	0.24315165
H	3.95373564	2.28269020	0.24315165
H	0.00000000	-4.56538093	0.24315165
H	2.59669181	-1.49920042	-0.98128936
H	0.00000000	2.99840137	-0.98128936
H	-2.59669181	-1.49920042	-0.98128936
H	2.59669181	1.49920042	0.98128936
H	-2.59669181	1.49920042	0.98128936
H	0.00000000	-2.99840137	0.98128936

$[Fe(Tb^{3,5\text{-}NH2})_2]^+$ ^2E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.60841467	1.16340888
N	0.00000000	1.43273840	2.53481353
N	1.39292787	-0.80420760	1.16340888
N	1.24078782	-0.71636947	2.53481353
N	-1.39292787	-0.80420760	1.16340888
N	-1.24078782	-0.71636947	2.53481353
C	0.00000000	2.94657904	0.95361709
C	0.00000000	3.63157412	2.18040447
C	0.00000000	2.63608588	3.14929044
C	2.55181229	-1.47328979	0.95361709
C	3.14503586	-1.81578706	2.18040447
C	2.28291722	-1.31804294	3.14929044
C	-2.55181229	-1.47328979	0.95361709
C	-3.14503586	-1.81578706	2.18040447
C	-2.28291722	-1.31804294	3.14929044
H	0.00000000	4.70358562	2.33508245
N	0.00000000	2.77178174	4.50428583
H	4.07342442	-2.35179281	2.33508245
N	3.03370543	-1.75151055	-0.27609241
N	2.40043320	-1.38589087	4.50428583
N	0.00000000	3.50302109	-0.27609241
H	0.00000000	0.00000000	4.27160130
H	-4.07342442	-2.35179281	2.33508245
N	-2.40043320	-1.38589087	4.50428583
N	-3.03370543	-1.75151055	-0.27609241
B	0.00000000	0.00000000	3.06188042
N	-1.39292787	0.80420760	-1.16340888
N	-1.24078782	0.71636947	-2.53481353
N	1.39292787	0.80420760	-1.16340888
N	1.24078782	0.71636947	-2.53481353
N	0.00000000	-1.60841467	-1.16340888
N	0.00000000	-1.43273840	-2.53481353
C	-2.55181229	1.47328979	-0.95361709
C	-3.14503586	1.81578706	-2.18040447
C	-2.28291722	1.31804294	-3.14929044
C	2.55181229	1.47328979	-0.95361709
C	3.14503586	1.81578706	-2.18040447
C	2.28291722	1.31804294	-3.14929044
C	0.00000000	-2.94657904	-0.95361709
C	0.00000000	-3.63157412	-2.18040447
C	0.00000000	-2.63608588	-3.14929044
H	-4.07342442	2.35179281	-2.33508245
N	-2.40043320	1.38589087	-4.50428583
H	4.07342442	2.35179281	-2.33508245
N	3.03370543	1.75151055	0.27609241
N	2.40043320	1.38589087	-4.50428583
N	-3.03370543	1.75151055	0.27609241
H	0.00000000	0.00000000	-4.27160130
H	0.00000000	-4.70358562	-2.33508245
N	0.00000000	-2.77178174	-4.50428583
N	0.00000000	-3.50302109	0.27609241
B	0.00000000	0.00000000	-3.06188042
H	0.00000000	3.68723140	4.91168193

H	0.00000000	1.97365439	5.10889465
H	3.19323597	-1.84361543	4.91168193
H	1.70923457	-0.98682720	5.10889465
H	-3.19323597	-1.84361543	4.91168193
H	-1.70923457	-0.98682720	5.10889465
H	-3.19323597	1.84361543	-4.91168193
H	-1.70923457	0.98682720	-5.10889465
H	3.19323597	1.84361543	-4.91168193
H	1.70923457	0.98682720	-5.10889465
H	0.00000000	-3.68723140	-4.91168193
H	0.00000000	-1.97365439	-5.10889465
H	0.00000000	4.50008416	-0.37188407
H	3.89718723	-2.25004208	-0.37188407
H	-3.89718723	-2.25004208	-0.37188407
H	-3.89718723	2.25004208	0.37188407
H	3.89718723	2.25004208	0.37188407
H	0.00000000	-4.50008416	0.37188407
H	2.53548029	-1.46386038	-1.09789145
H	0.00000000	2.92772022	-1.09789145
H	-2.53548029	-1.46386038	-1.09789145
H	2.53548029	1.46386038	1.09789145
H	-2.53548029	1.46386038	1.09789145
H	0.00000000	-2.92772022	1.09789145

$[Fe(Tb^{3,5\text{-}NO2})_2]^+$ $^6A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.77823770	1.41398225
N	0.00000000	1.47438677	2.71976679
N	1.53999946	-0.88911885	1.41398225
N	1.27685655	-0.73719312	2.71976679
N	-1.53999946	-0.88911885	1.41398225
N	-1.27685655	-0.73719312	2.71976679
C	0.00000000	3.12378992	1.34776630
C	0.00000000	3.71034533	2.59937791
C	0.00000000	2.62905470	3.44942655
C	2.70528163	-1.56189470	1.34776630
C	3.21325368	-1.85517266	2.59937791
C	2.27682797	-1.31452709	3.44942655
C	-2.70528163	-1.56189470	1.34776630
C	-3.21325368	-1.85517266	2.59937791
C	-2.27682797	-1.31452709	3.44942655
H	0.00000000	4.75996999	2.85246699
N	0.00000000	2.78197740	4.90768135
H	4.12225478	-2.37998473	2.85246699
N	3.37041986	-1.94591280	0.11642058
N	2.40926305	-1.39098844	4.90768135
N	0.00000000	3.89182561	0.11642058
H	0.00000000	0.00000000	4.37727694
H	-4.12225478	-2.37998473	2.85246699
N	-2.40926305	-1.39098844	4.90768135
N	-3.37041986	-1.94591280	0.11642058
B	0.00000000	0.00000000	3.20210233
N	-1.53999946	0.88911885	-1.41398225
N	-1.27685655	0.73719312	-2.71976679
N	1.53999946	0.88911885	-1.41398225
N	1.27685655	0.73719312	-2.71976679
N	0.00000000	-1.77823770	-1.41398225
N	0.00000000	-1.47438677	-2.71976679
C	-2.70528163	1.56189470	-1.34776630
C	-3.21325368	1.85517266	-2.59937791
C	-2.27682797	1.31452709	-3.44942655
C	2.70528163	1.56189470	-1.34776630
C	3.21325368	1.85517266	-2.59937791
C	2.27682797	1.31452709	-3.44942655
C	0.00000000	-3.12378992	-1.34776630
C	0.00000000	-3.71034533	-2.59937791
C	0.00000000	-2.62905470	-3.44942655
H	-4.12225478	2.37998473	-2.85246699
N	-2.40926305	1.39098844	-4.90768135
H	4.12225478	2.37998473	-2.85246699
N	3.37041986	1.94591280	-0.11642058
N	2.40926305	1.39098844	-4.90768135
N	-3.37041986	1.94591280	-0.11642058
H	0.00000000	0.00000000	-4.37727694
H	0.00000000	-4.75996999	-2.85246699
N	0.00000000	-2.78197740	-4.90768135
N	0.00000000	-3.89182561	-0.11642058
B	0.00000000	0.00000000	-3.20210233
O	0.00000000	3.94004530	5.29079615
O	0.00000000	1.79123218	5.61708367
O	3.41217935	-1.97002265	5.29079615
O	1.55125241	-0.89561609	5.61708367
O	-3.41217935	-1.97002265	5.29079615
O	-1.55125241	-0.89561609	5.61708367
O	-3.41217935	1.97002265	-5.29079615
O	-1.55125241	0.89561609	-5.61708367
O	3.41217935	1.97002265	-5.29079615
O	1.55125241	0.89561609	-5.61708367
O	0.00000000	-3.94004530	-5.29079615
O	0.00000000	-1.79123218	-5.61708367
O	0.00000000	5.10352403	0.24606901
O	4.41978151	-2.55176201	0.24606901
O	-4.41978151	-2.55176201	0.24606901
O	-4.41978151	2.55176201	-0.24606901
O	4.41978151	2.55176201	-0.24606901
O	0.00000000	-5.10352403	-0.24606901
O	2.83686261	-1.63786338	-0.94098298
O	0.00000000	3.27572623	-0.94098298
O	-2.83686261	-1.63786338	-0.94098298
O	2.83686261	1.63786338	0.94098298
O	-2.83686261	1.63786338	0.94098298
O	0.00000000	-3.27572623	0.94098298

$[Fe(Tb^{3,5\text{-}NO2})_2]^+$ ^4E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.79094801	1.41417698
N	0.00000000	1.47779573	2.71638324
N	1.55100634	-0.89547374	1.41417698
N	1.27980883	-0.73889813	2.71638324
N	-1.55100634	-0.89547374	1.41417698
N	-1.27980883	-0.73889813	2.71638324
C	0.00000000	3.13480845	1.35496893
C	0.00000000	3.71643192	2.61107961
C	0.00000000	2.63107510	3.45478182
C	2.71482375	-1.56740449	1.35496893
C	3.21852429	-1.85821596	2.61107961
C	2.27857796	-1.31553781	3.45478182
C	-2.71482375	-1.56740449	1.35496893

C	-3.21852429	-1.85821596	2.61107961
C	-2.27857796	-1.31553781	3.45478182
H	0.00000000	4.76514005	2.86770359
N	0.00000000	2.78987961	4.90752736
H	4.12673215	-2.38256976	2.86770359
N	3.39239817	-1.95860194	0.13161009
N	2.41610690	-1.39493980	4.90752736
N	0.00000000	3.91720389	0.13161009
H	0.00000000	0.00000000	4.35903885
H	-4.12673215	-2.38256976	2.86770359
N	-2.41610690	-1.39493980	4.90752736
N	-3.39239817	-1.95860194	0.13161009
B	0.00000000	0.00000000	3.19404137
N	-1.55100634	0.89547374	-1.41417698
N	-1.27980883	0.73889813	-2.71638324
N	1.55100634	0.89547374	-1.41417698
N	1.27980883	0.73889813	-2.71638324
N	0.00000000	-1.79094801	-1.41417698
N	0.00000000	-1.47779573	-2.71638324
C	-2.71482375	1.56740449	-1.35496893
C	-3.21852429	1.85821596	-2.61107961
C	-2.27857796	1.31553781	-3.45478182
C	2.71482375	1.56740449	-1.35496893
C	3.21852429	1.85821596	-2.61107961
C	2.27857796	1.31553781	-3.45478182
C	0.00000000	-3.13480845	-1.35496893
C	0.00000000	-3.71643192	-2.61107961
C	0.00000000	-2.63107510	-3.45478182
H	-4.12673215	2.38256976	-2.86770359
N	-2.41610690	1.39493980	-4.90752736
H	4.12673215	2.38256976	-2.86770359
N	3.39239817	1.95860194	-0.13161009
N	2.41610690	1.39493980	-4.90752736
N	-3.39239817	1.95860194	-0.13161009
H	0.00000000	0.00000000	-4.35903885
H	0.00000000	-4.76514005	-2.86770359
N	0.00000000	-2.78987961	-4.90752736
N	0.00000000	-3.91720389	-0.13161009
B	0.00000000	0.00000000	-3.19404137
O	0.00000000	3.95552849	5.28399252
O	0.00000000	1.81998608	5.64261647
O	3.42558817	-1.97776398	5.28399252
O	1.57615443	-0.90999331	5.64261647
O	-3.42558817	-1.97776398	5.28399252
O	-1.57615443	-0.90999331	5.64261647
O	-3.42558817	1.97776398	-5.28399252
O	-1.57615443	0.90999331	-5.64261647
O	3.42558817	1.97776398	-5.28399252
O	1.57615443	0.90999331	-5.64261647
O	0.00000000	-3.95552849	-5.28399252
O	0.00000000	-1.81998608	-5.64261647
O	0.00000000	5.12794291	0.27852874
O	4.44092902	-2.56397119	0.27852874
O	-4.44092902	-2.56397119	0.27852874
O	-4.44092902	2.56397119	-0.27852874
O	4.44092902	2.56397119	-0.27852874
O	0.00000000	-5.12794291	-0.27852874
O	2.87648211	-1.66073760	-0.93679031
O	0.00000000	3.32147519	-0.93679031
O	-2.87648211	-1.66073760	-0.93679031
O	2.87648211	1.66073760	0.93679031
O	-2.87648211	1.66073760	0.93679031
O	0.00000000	-3.32147519	0.93679031

$[Fe(Tb^{3,5\text{-}NO2})_2]^+$ ^2E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.66486783	1.13205090
N	0.00000000	1.44840999	2.45606507
N	1.44181803	-0.83243391	1.13205090
N	1.25436016	-0.72420499	2.45606507
N	-1.44181803	-0.83243391	1.13205090
N	-1.25436016	-0.72420499	2.45606507
C	0.00000000	3.01699031	0.97263625
C	0.00000000	3.66185100	2.19515370
C	0.00000000	2.63736490	3.11101611
C	2.61279044	-1.50849542	0.97263625
C	3.17125553	-1.83092523	2.19515370
C	2.28402479	-1.31868219	3.11101611
C	-2.61279044	-1.50849542	0.97263625
C	-3.17125553	-1.83092523	2.19515370
C	-2.28402479	-1.31868219	3.11101611
H	0.00000000	4.72433202	2.38613324
N	0.00000000	2.87691974	4.56582385
H	4.09139158	-2.36216574	2.38613324
N	3.28781000	-1.89821806	-0.26819338
N	2.49148555	-1.43845987	4.56582385
N	0.00000000	3.79643559	-0.26819338
H	0.00000000	0.00000000	4.15285287
H	-4.09139158	-2.36216574	2.38613324
N	-2.49148555	-1.43845987	4.56582385
N	-3.28781000	-1.89821806	-0.26819338
B	0.00000000	0.00000000	2.98770141
N	-1.44181803	0.83243391	-1.13205090
N	-1.25436016	0.72420499	-2.45606507
N	1.44181803	0.83243391	-1.13205090
N	1.25436016	0.72420499	-2.45606507
N	0.00000000	-1.66486783	-1.13205090
N	0.00000000	-1.44840999	-2.45606507
C	-2.61279044	1.50849542	-0.97263625
C	-3.17125553	1.83092523	-2.19515370
C	-2.28402479	1.31868219	-3.11101611
C	2.61279044	1.50849542	-0.97263625
C	3.17125553	1.83092523	-2.19515370
C	2.28402479	1.31868219	-3.11101611
C	0.00000000	-3.01699031	-0.97263625
C	0.00000000	-3.66185100	-2.19515370
C	0.00000000	-2.63736490	-3.11101611
H	-4.09139158	2.36216574	-2.38613324
N	-2.49148555	1.43845987	-4.56582385
H	4.09139158	2.36216574	-2.38613324
N	3.28781000	1.89821806	0.26819338
N	2.49148555	1.43845987	-4.56582385
N	-3.28781000	1.89821806	0.26819338
H	0.00000000	0.00000000	-4.15285287
H	0.00000000	-4.72433202	-2.38613324
N	0.00000000	-2.87691974	-4.56582385
N	0.00000000	-3.79643559	0.26819338
B	0.00000000	0.00000000	-2.98770141
O	0.00000000	4.06170897	4.85676656

O	0.00000000	1.93314270	5.32934407
O	3.51754277	-2.03085422	4.85676656
O	1.67415065	-0.96657135	5.32934407
O	-3.51754277	-2.03085422	4.85676656
O	-1.67415065	-0.96657135	5.32934407
O	-3.51754277	2.03085422	-4.85676656
O	-1.67415065	0.96657135	-5.32934407
O	3.51754277	2.03085422	-4.85676656
O	1.67415065	0.96657135	-5.32934407
O	0.00000000	-4.06170897	-4.85676656
O	0.00000000	-1.93314270	-5.32934407
O	0.00000000	5.00403553	-0.10670118
O	4.33362193	-2.50201777	-0.10670118
O	-4.33362193	-2.50201777	-0.10670118
O	-4.33362193	2.50201777	0.10670118
O	4.33362193	2.50201777	0.10670118
O	0.00000000	-5.00403553	0.10670118
O	2.78524401	-1.60806118	-1.34142887
O	0.00000000	3.21612235	-1.34142887
O	-2.78524401	-1.60806118	-1.34142887
O	2.78524401	1.60806118	1.34142887
O	-2.78524401	1.60806118	1.34142887
O	0.00000000	-3.21612235	1.34142887

$[Fe(Tb^{3CH3})_2]$ $^5A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.54819059	0.89384811	1.37709912
N	1.26601106	0.73093190	2.68686361
N	0.00000000	-1.78769674	1.37709912
N	0.00000000	-1.46186326	2.68686361
N	-1.54819059	0.89384811	1.37709912
N	-1.26601106	0.73093190	2.68686361
C	2.71518306	1.56761193	1.31278927
C	3.17631817	1.83384841	2.61338153
C	2.22451986	1.28432694	3.45205550
C	0.00000000	-3.13522332	1.31278927
C	0.00000000	-3.66769629	2.61338153
C	0.00000000	-2.56865441	3.45205550
C	-2.71518306	1.56761193	1.31278927
C	-3.17631817	1.83384841	2.61338153
C	-2.22451986	1.28432694	3.45205550
H	4.08234212	2.35694118	2.89838422
H	2.16046401	1.24734433	4.53220046
H	0.00000000	-4.71388235	2.89838422
C	0.00000000	-3.90598163	0.03599569
H	0.00000000	-2.49468919	4.53220046
C	3.38267931	1.95299108	0.03599569
H	0.00000000	0.00000000	4.37541371
H	-4.08234212	2.35694118	2.89838422
H	-2.16046401	1.24734433	4.53220046
C	-3.38267931	1.95299108	0.03599569
B	0.00000000	0.00000000	3.16816725
N	0.00000000	1.78769674	-1.37709912
N	0.00000000	1.46186326	-2.68686361
N	1.54819059	-0.89384811	-1.37709912
N	1.26601106	-0.73093190	-2.68686361
N	-1.54819059	-0.89384811	-1.37709912
N	-1.26601106	-0.73093190	-2.68686361
C	0.00000000	3.13522332	-1.31278927
C	0.00000000	3.66769629	-2.61338153
C	0.00000000	2.56865441	-3.45205550
C	2.71518306	-1.56761193	-1.31278927
C	3.17631817	-1.83384841	-2.61338153
C	2.22451986	-1.28432694	-3.45205550
C	-2.71518306	-1.56761193	-1.31278927
C	-3.17631817	-1.83384841	-2.61338153
C	-2.22451986	-1.28432694	-3.45205550
H	0.00000000	4.71388235	-2.89838422
H	0.00000000	2.49468919	-4.53220046
H	4.08234212	-2.35694118	-2.89838422
C	3.38267931	-1.95299108	-0.03599569
H	2.16046401	-1.24734433	-4.53220046
C	0.00000000	3.90598163	-0.03599569
H	0.00000000	0.00000000	-4.37541371
H	-4.08234212	-2.35694118	-2.89838422
H	-2.16046401	-1.24734433	-4.53220046
C	-3.38267931	-1.95299108	-0.03599569
B	0.00000000	0.00000000	-3.16816725
H	-0.87676468	-3.68356737	-0.57795310
H	0.00000000	-4.97763488	0.25476339
H	0.87676468	-3.68356737	-0.57795310
H	4.31075830	2.48881744	0.25476339
H	2.75168042	2.60108398	-0.57795310
H	3.62844509	1.08248339	-0.57795310
H	-4.31075830	2.48881744	0.25476339
H	-3.62844509	1.08248339	-0.57795310
H	-2.75168042	2.60108398	-0.57795310
H	3.62844509	-1.08248339	0.57795310
H	4.31075830	-2.48881744	-0.25476339
H	2.75168042	-2.60108398	0.57795310
H	-2.75168042	-2.60108398	0.57795310
H	-4.31075830	-2.48881744	-0.25476339
H	-3.62844509	-1.08248339	0.57795310
H	-0.87676468	3.68356737	0.57795310
H	0.00000000	4.97763488	-0.25476339
H	0.87676468	3.68356737	0.57795310

$[Fe(Tb^{3CH3})_2]$ ^3E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.49119397	0.86094122	1.27235007
N	1.25380929	0.72388696	2.59299551
N	0.00000000	-1.72188244	1.27235007
N	0.00000000	-1.44777392	2.59299551
N	-1.49119397	0.86094122	1.27235007
N	-1.25380929	0.72388696	2.59299551
C	2.65824782	1.53473996	1.15618244
C	3.15720376	1.82281242	2.43861969
C	2.23473986	1.29022780	3.31830966
C	0.00000000	-3.06948046	1.15618244
C	0.00000000	-3.64562483	2.43861969
C	0.00000000	-2.58045559	3.31830966
C	-2.65824782	1.53473996	1.15618244
C	-3.15720376	1.82281242	2.43861969
C	-2.23473986	1.29022780	3.31830966
H	4.07225759	2.35111917	2.68218992
H	2.20301727	1.27191244	4.40031097
H	0.00000000	-4.70223781	2.68218992
C	0.00000000	-3.81763813	-0.13302246

H	0.00000000	-2.54382541	4.40031097
C	3.30617192	1.90881907	-0.13302246
H	0.00000000	0.00000000	4.30431133
H	-4.07225759	2.35111917	2.68218992
H	-2.20301727	1.27191244	4.40031097
C	-3.30617192	1.90881907	-0.13302246
B	0.00000000	0.00000000	3.09763639
N	0.00000000	1.72188244	-1.27235007
N	0.00000000	1.44777392	-2.59299551
N	1.49119397	-0.86094122	-1.27235007
N	1.25380929	-0.72388696	-2.59299551
N	-1.49119397	-0.86094122	-1.27235007
N	-1.25380929	-0.72388696	-2.59299551
C	0.00000000	3.06948046	-1.15618244
C	0.00000000	3.64562483	-2.43861969
C	0.00000000	2.58045559	-3.31830966
C	2.65824782	-1.53473996	-1.15618244
C	3.15720376	-1.82281242	-2.43861969
C	2.23473986	-1.29022780	-3.31830966
C	-2.65824782	-1.53473996	-1.15618244
C	-3.15720376	-1.82281242	-2.43861969
C	-2.23473986	-1.29022780	-3.31830966
H	0.00000000	4.70223781	-2.68218992
H	0.00000000	2.54382541	-4.40031097
H	4.07225759	-2.35111917	-2.68218992
C	3.30617192	-1.90881907	0.13302246
H	2.20301727	-1.27191244	-4.40031097
C	0.00000000	3.81763813	0.13302246
H	0.00000000	0.00000000	-4.30431133
H	-4.07225759	-2.35111917	-2.68218992
H	-2.20301727	-1.27191244	-4.40031097
C	-3.30617192	-1.90881907	0.13302246
B	0.00000000	0.00000000	-3.09763639
H	-0.87746213	-3.58988765	-0.74330512
H	0.00000000	-4.89165945	0.07497172
H	0.87746213	-3.58988765	-0.74330512
H	4.23630147	2.44582973	0.07497172
H	2.67020300	2.55484871	-0.74330512
H	3.54766513	1.03503948	-0.74330512
H	-4.23630147	2.44582973	0.07497172
H	-3.54766513	1.03503948	-0.74330512
H	-2.67020300	2.55484871	-0.74330512
H	3.54766513	-1.03503948	0.74330512
H	4.23630147	-2.44582973	-0.07497172
H	2.67020300	-2.55484871	0.74330512
H	-2.67020300	-2.55484871	0.74330512
H	-4.23630147	-2.44582973	-0.07497172
H	-3.54766513	-1.03503948	0.74330512
H	-0.87746213	3.58988765	0.74330512
H	0.00000000	4.89165945	-0.07497172
H	0.87746213	3.58988765	0.74330512

$[Fe(Tb^{3CH3})_2]$ $^1A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.42835100	0.82465871	1.15119230
N	1.24042058	0.71615727	2.48323621
N	0.00000000	-1.64931795	1.15119230
N	0.00000000	-1.43231400	2.48323621
N	-1.42835100	0.82465871	1.15119230
N	-1.24042058	0.71615727	2.48323621
C	2.59281294	1.49696147	0.97861648
C	3.13326960	1.80899401	2.23944742
C	2.24500484	1.29615405	3.16274054
C	0.00000000	-2.99392241	0.97861648
C	0.00000000	-3.61798802	2.23944742
C	0.00000000	-2.59230863	3.16274054
C	-2.59281294	1.49696147	0.97861648
C	-3.13326960	1.80899401	2.23944742
C	-2.24500484	1.29615405	3.16274054
H	4.05652779	2.34203743	2.43627755
H	2.24922662	1.29859144	4.24514561
H	0.00000000	-4.68407486	2.43627755
C	0.00000000	-3.71548840	-0.32525880
H	0.00000000	-2.59718341	4.24514561
C	3.21770777	1.85774447	-0.32525880
H	0.00000000	0.00000000	4.21955354
H	-4.05652779	2.34203743	2.43627755
H	-2.24922662	1.29859144	4.24514561
C	-3.21770777	1.85774447	-0.32525880
B	0.00000000	0.00000000	3.01409042
N	0.00000000	1.64931795	-1.15119230
N	0.00000000	1.43231400	-2.48323621
N	1.42835100	-0.82465871	-1.15119230
N	1.24042058	-0.71615727	-2.48323621
N	-1.42835100	-0.82465871	-1.15119230
N	-1.24042058	-0.71615727	-2.48323621
C	0.00000000	2.99392241	-0.97861648
C	0.00000000	3.61798802	-2.23944742
C	0.00000000	2.59230863	-3.16274054
C	2.59281294	-1.49696147	-0.97861648
C	3.13326960	-1.80899401	-2.23944742
C	2.24500484	-1.29615405	-3.16274054
C	-2.59281294	-1.49696147	-0.97861648
C	-3.13326960	-1.80899401	-2.23944742
C	-2.24500484	-1.29615405	-3.16274054
H	0.00000000	4.68407486	-2.43627755
H	0.00000000	2.59718341	-4.24514561
H	4.05652779	-2.34203743	-2.43627755
C	3.21770777	-1.85774447	0.32525880
H	2.24922662	-1.29859144	-4.24514561
C	0.00000000	3.71548840	0.32525880
H	0.00000000	0.00000000	-4.21955354
H	-4.05652779	-2.34203743	-2.43627755
H	-2.24922662	-1.29859144	-4.24514561
C	-3.21770777	-1.85774447	0.32525880
B	0.00000000	0.00000000	-3.01409042
H	-0.87966192	-3.48206779	-0.93042113
H	0.00000000	-4.79239374	-0.13105180
H	0.87966192	-3.48206779	-0.93042113
H	4.15033451	2.39619660	-0.13105180
H	2.57572792	2.50284328	-0.93042113
H	3.45538985	0.97922451	-0.93042113
H	-4.15033451	2.39619660	-0.13105180
H	-3.45538985	0.97922451	-0.93042113
H	-2.57572792	2.50284328	-0.93042113
H	3.45538985	-0.97922451	0.93042113
H	4.15033451	-2.39619660	0.13105180
H	2.57572792	-2.50284328	0.93042113
H	-2.57572792	-2.50284328	0.93042113

H	-4.15033451	-2.39619660	0.13105180
H	-3.45538985	-0.97922451	0.93042113
H	-0.87966192	3.48206779	0.93042113
H	0.00000000	4.79239374	0.13105180
H	0.87966192	3.48206779	0.93042113

$[Fe(Tb^{3CF3})_2]$ $^5A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.64157715	0.94776492	1.26368003
N	1.28559750	0.74223988	2.54587333
N	0.00000000	-1.89552984	1.26368003
N	0.00000000	-1.48447977	2.54587333
N	-1.64157715	0.94776492	1.26368003
N	-1.28559750	0.74223988	2.54587333
C	2.81374656	1.62451753	1.31142611
C	3.19425781	1.84420547	2.64147396
C	2.19305922	1.26616346	3.39155519
C	0.00000000	-3.24903453	1.31142611
C	0.00000000	-3.68841093	2.64147396
C	0.00000000	-2.53232692	3.39155519
C	-2.81374656	1.62451753	1.31142611
C	-3.19425781	1.84420547	2.64147396
C	-2.19305922	1.26616346	3.39155519
H	4.07683444	2.35376135	3.00278666
H	2.06356584	1.19140024	4.46283643
H	0.00000000	-4.70752323	3.00278666
C	0.00000000	-4.22549038	0.14249632
H	0.00000000	-2.38280101	4.46283643
C	3.65938238	2.11274546	0.14249632
H	0.00000000	0.00000000	4.18686468
H	-4.07683444	2.35376135	3.00278666
H	-2.06356584	1.19140024	4.46283643
C	-3.65938238	2.11274546	0.14249632
B	0.00000000	0.00000000	2.98236677
N	0.00000000	1.89552984	-1.26368003
N	0.00000000	1.48447977	-2.54587333
N	1.64157715	-0.94776492	-1.26368003
N	1.28559750	-0.74223988	-2.54587333
N	-1.64157715	-0.94776492	-1.26368003
N	-1.28559750	-0.74223988	-2.54587333
C	0.00000000	3.24903453	-1.31142611
C	0.00000000	3.68841093	-2.64147396
C	0.00000000	2.53232692	-3.39155519
C	2.81374656	-1.62451753	-1.31142611
C	3.19425781	-1.84420547	-2.64147396
C	2.19305922	-1.26616346	-3.39155519
C	-2.81374656	-1.62451753	-1.31142611
C	-3.19425781	-1.84420547	-2.64147396
C	-2.19305922	-1.26616346	-3.39155519
H	0.00000000	4.70752323	-3.00278666
H	0.00000000	2.38280101	-4.46283643
H	4.07683444	-2.35376135	-3.00278666
C	3.65938238	-2.11274546	-0.14249632
H	2.06356584	-1.19140024	-4.46283643
C	0.00000000	4.22549038	-0.14249632
H	0.00000000	0.00000000	-4.18686468
H	-4.07683444	-2.35376135	-3.00278666
H	-2.06356584	-1.19140024	-4.46283643
C	-3.65938238	-2.11274546	-0.14249632
B	0.00000000	0.00000000	-2.98236677
F	-1.07371387	-4.13713948	-0.66320515
F	0.00000000	-5.49043356	0.65111027
F	1.07371387	-4.13713948	-0.66320515
F	4.75485496	2.74521652	0.65111027
F	3.04601092	2.99843312	-0.66320515
F	4.11972479	1.13870636	-0.66320515
F	-4.75485496	2.74521652	0.65111027
F	-4.11972479	1.13870636	-0.66320515
F	-3.04601092	2.99843312	-0.66320515
F	4.11972479	-1.13870636	0.66320515
F	4.75485496	-2.74521652	-0.65111027
F	3.04601092	-2.99843312	0.66320515
F	-3.04601092	-2.99843312	0.66320515
F	-4.75485496	-2.74521652	-0.65111027
F	-4.11972479	-1.13870636	0.66320515
F	-1.07371387	4.13713948	0.66320515
F	0.00000000	5.49043356	-0.65111027
F	1.07371387	4.13713948	0.66320515

$[Fe(Tb^{3CF3})_2]$ ^3E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.56944500	0.90611973	1.19604695
N	1.27027041	0.73339098	2.49491938
N	0.00000000	-1.81223893	1.19604695
N	0.00000000	-1.46678196	2.49491938
N	-1.56944500	0.90611973	1.19604695
N	-1.27027041	0.73339098	2.49491938
C	2.74615316	1.58549230	1.17780303
C	3.17694207	1.83420825	2.48743047
C	2.20899116	1.27536162	3.29188519
C	0.00000000	-3.17098459	1.17780303
C	0.00000000	-3.66841703	2.48743047
C	0.00000000	-2.55072324	3.29188519
C	-2.74615316	1.58549230	1.17780303
C	-3.17694207	1.83420825	2.48743047
C	-2.20899116	1.27536162	3.29188519
H	4.07339849	2.35177799	2.79931113
H	2.12046192	1.22424945	4.36869474
H	0.00000000	-4.70355546	2.79931113
C	0.00000000	-4.11261106	-0.01900699
H	0.00000000	-2.44849837	4.36869474
C	3.56162588	2.05630553	-0.01900699
H	0.00000000	0.00000000	4.16562403
H	-4.07339849	2.35177799	2.79931113
H	-2.12046192	1.22424945	4.36869474
C	-3.56162588	2.05630553	-0.01900699
B	0.00000000	0.00000000	2.96135632
N	0.00000000	1.81223893	-1.19604695
N	0.00000000	1.46678196	-2.49491938
N	1.56944500	-0.90611973	-1.19604695
N	1.27027041	-0.73339098	-2.49491938
N	-1.56944500	-0.90611973	-1.19604695
N	-1.27027041	-0.73339098	-2.49491938
C	0.00000000	3.17098459	-1.17780303
C	0.00000000	3.66841703	-2.48743047
C	0.00000000	2.55072324	-3.29188519
C	2.74615316	-1.58549230	-1.17780303
C	3.17694207	-1.83420825	-2.48743047

C	2.20899116	-1.27536162	-3.29188519
C	-2.74615316	-1.58549230	-1.17780303
C	-3.17694207	-1.83420825	-2.48743047
C	-2.20899116	-1.27536162	-3.29188519
H	0.00000000	4.70355546	-2.79931113
H	0.00000000	2.44849837	-4.36869474
H	4.07339849	-2.35177799	-2.79931113
C	3.56162588	-2.05630553	0.01900699
H	2.12046192	-1.22424945	-4.36869474
C	0.00000000	4.11261106	0.01900699
H	0.00000000	0.00000000	-4.16562403
H	-4.07339849	-2.35177799	-2.79931113
H	-2.12046192	-1.22424945	-4.36869474
C	-3.56162588	-2.05630553	0.01900699
B	0.00000000	0.00000000	-2.96135632
F	-1.07572844	-4.00445569	-0.82043376
F	0.00000000	-5.39249397	0.45142312
F	1.07572844	-4.00445569	-0.82043376
F	4.67003684	2.69624698	0.45142312
F	2.93009623	2.93383593	-0.82043376
F	4.00582467	1.07061977	-0.82043376
F	-4.67003684	2.69624698	0.45142312
F	-4.00582467	1.07061977	-0.82043376
F	-2.93009623	2.93383593	-0.82043376
F	4.00582467	-1.07061977	0.82043376
F	4.67003684	-2.69624698	-0.45142312
F	2.93009623	-2.93383593	0.82043376
F	-2.93009623	-2.93383593	0.82043376
F	-4.67003684	-2.69624698	-0.45142312
F	-4.00582467	-1.07061977	0.82043376
F	-1.07572844	4.00445569	0.82043376
F	0.00000000	5.39249397	-0.45142312
F	1.07572844	4.00445569	0.82043376

$[Fe(Tb^{3CF3})_2]$ $^1A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.49587454	0.86364373	1.11509764
N	1.25305415	0.72345092	2.42926648
N	0.00000000	-1.72728746	1.11509764
N	0.00000000	-1.44690236	2.42926648
N	-1.49587454	0.86364373	1.11509764
N	-1.25305415	0.72345092	2.42926648
C	2.67605570	1.54502135	1.03591421
C	3.15248826	1.82008980	2.32526886
C	2.21930165	1.28131433	3.17834862
C	0.00000000	-3.09004270	1.03591421
C	0.00000000	-3.64018013	2.32526886
C	0.00000000	-2.56262867	3.17834862
C	-2.67605570	1.54502135	1.03591421
C	-3.15248826	1.82008980	2.32526886
C	-2.21930165	1.28131433	3.17834862
H	4.05964200	2.34383557	2.59046022
H	2.16927270	1.25243025	4.25830890
H	0.00000000	-4.68767115	2.59046022
C	0.00000000	-4.01335698	-0.17577363
H	0.00000000	-2.50485998	4.25830890
C	3.47566898	2.00667823	-0.17577363
H	0.00000000	0.00000000	4.12985535
H	-4.05964200	2.34383557	2.59046022
H	-2.16927270	1.25243025	4.25830890
C	-3.47566898	2.00667823	-0.17577363
B	0.00000000	0.00000000	2.92657826
N	0.00000000	1.72728746	-1.11509764
N	0.00000000	1.44690236	-2.42926648
N	1.49587454	-0.86364373	-1.11509764
N	1.25305415	-0.72345092	-2.42926648
N	-1.49587454	-0.86364373	-1.11509764
N	-1.25305415	-0.72345092	-2.42926648
C	0.00000000	3.09004270	-1.03591421
C	0.00000000	3.64018013	-2.32526886
C	0.00000000	2.56262867	-3.17834862
C	2.67605570	-1.54502135	-1.03591421
C	3.15248826	-1.82008980	-2.32526886
C	2.21930165	-1.28131433	-3.17834862
C	-2.67605570	-1.54502135	-1.03591421
C	-3.15248826	-1.82008980	-2.32526886
C	-2.21930165	-1.28131433	-3.17834862
H	0.00000000	4.68767115	-2.59046022
H	0.00000000	2.50485998	-4.25830890
H	4.05964200	-2.34383557	-2.59046022
C	3.47566898	-2.00667823	0.17577363
H	2.16927270	-1.25243025	-4.25830890
C	0.00000000	4.01335698	0.17577363
H	0.00000000	0.00000000	-4.12985535
H	-4.05964200	-2.34383557	-2.59046022
H	-2.16927270	-1.25243025	-4.25830890
C	-3.47566898	-2.00667823	0.17577363
B	0.00000000	0.00000000	-2.92657826
F	-1.07751283	-3.90002256	-0.97453653
F	0.00000000	-5.30039014	0.27629085
F	1.07751283	-3.90002256	-0.97453653
F	4.59027290	2.65019533	0.27629085
F	2.83876235	2.88316509	-0.97453653
F	3.91627518	1.01685748	-0.97453653
F	-4.59027290	2.65019533	0.27629085
F	-3.91627518	1.01685748	-0.97453653
F	-2.83876235	2.88316509	-0.97453653
F	3.91627518	-1.01685748	0.97453653
F	4.59027290	-2.65019533	-0.27629085
F	2.83876235	-2.88316509	0.97453653
F	-2.83876235	-2.88316509	0.97453653
F	-4.59027290	-2.65019533	-0.27629085
F	-3.91627518	-1.01685748	0.97453653
F	-1.07751283	3.90002256	0.97453653
F	0.00000000	5.30039014	-0.27629085
F	1.07751283	3.90002256	0.97453653

$[Fe(Tb^{3NH2})_2]$ $^5A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.74988174	1.38718577
N	0.00000000	1.45537079	2.71989380
N	1.51544193	-0.87494113	1.38718577
N	1.26038802	-0.72768539	2.71989380
N	-1.51544193	-0.87494113	1.38718577
N	-1.26038802	-0.72768539	2.71989380
C	0.00000000	3.09615999	1.29984718
C	0.00000000	3.67048981	2.58949235
C	0.00000000	2.58396668	3.44550640

C	2.68135329	-1.54807999	1.29984718
C	3.17873704	-1.83524491	2.58949235
C	2.23778104	-1.29198361	3.44550640
C	-2.68135329	-1.54807999	1.29984718
C	-3.17873704	-1.83524491	2.58949235
C	-2.23778104	-1.29198361	3.44550640
H	0.00000000	4.72202586	2.85289139
H	0.00000000	2.54371376	4.52777389
H	4.08939446	-2.36101320	2.85289139
N	3.23743550	-1.86913395	0.10243972
H	2.20292043	-1.27185688	4.52777389
N	0.00000000	3.73826842	0.10243972
H	0.00000000	0.00000000	4.42074250
H	-4.08939446	-2.36101320	2.85289139
H	-2.20292043	-1.27185688	4.52777389
N	-3.23743550	-1.86913395	0.10243972
B	0.00000000	0.00000000	3.21164975
N	-1.51544193	0.87494113	-1.38718577
N	-1.26038802	0.72768539	-2.71989380
N	1.51544193	0.87494113	-1.38718577
N	1.26038802	0.72768539	-2.71989380
N	0.00000000	-1.74988174	-1.38718577
N	0.00000000	-1.45537079	-2.71989380
C	-2.68135329	1.54807999	-1.29984718
C	-3.17873704	1.83524491	-2.58949235
C	-2.23778104	1.29198361	-3.44550640
C	2.68135329	1.54807999	-1.29984718
C	3.17873704	1.83524491	-2.58949235
C	2.23778104	1.29198361	-3.44550640
C	0.00000000	-3.09615999	-1.29984718
C	0.00000000	-3.67048981	-2.58949235
C	0.00000000	-2.58396668	-3.44550640
H	-4.08939446	2.36101320	-2.85289139
H	-2.20292043	1.27185688	-4.52777389
H	4.08939446	2.36101320	-2.85289139
N	3.23743550	1.86913395	-0.10243972
H	2.20292043	1.27185688	-4.52777389
N	-3.23743550	1.86913395	-0.10243972
H	0.00000000	0.00000000	-4.42074250
H	0.00000000	-4.72202586	-2.85289139
H	0.00000000	-2.54371376	-4.52777389
N	0.00000000	-3.73826842	-0.10243972
B	0.00000000	0.00000000	-3.21164975
H	0.00000000	4.73812926	0.06597623
H	4.10334040	-2.36906463	0.06597623
H	-4.10334040	-2.36906463	0.06597623
H	-4.10334040	2.36906463	-0.06597623
H	4.10334040	2.36906463	-0.06597623
H	0.00000000	-4.73812926	-0.06597623
H	2.78407294	-1.60738542	-0.75454326
H	0.00000000	3.21477031	-0.75454326
H	-2.78407294	-1.60738542	-0.75454326
H	2.78407294	1.60738542	0.75454326
H	-2.78407294	1.60738542	0.75454326
H	0.00000000	-3.21477031	0.75454326

$[Fe(Tb^{3NH2})_2]$ ^3E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.68160517	1.29865547
N	0.00000000	1.44213342	2.64241061
N	1.45631272	-0.84080285	1.29865547
N	1.24892392	-0.72106644	2.64241061
N	-1.45631272	-0.84080285	1.29865547
N	-1.24892392	-0.72106644	2.64241061
C	0.00000000	3.02529998	1.15594642
C	0.00000000	3.64794581	2.42339578
C	0.00000000	2.59838147	3.32350935
C	2.61998672	-1.51264999	1.15594642
C	3.15921357	-1.82397290	2.42339578
C	2.25026434	-1.29919047	3.32350935
C	-2.61998672	-1.51264999	1.15594642
C	-3.15921357	-1.82397290	2.42339578
C	-2.25026434	-1.29919047	3.32350935
H	0.00000000	4.70965052	2.64231800
H	0.00000000	2.59996159	4.40648170
H	4.07867704	-2.35482500	2.64231800
N	3.13732204	-1.81133403	-0.06178885
H	2.25163279	-1.29998106	4.40648170
N	0.00000000	3.62266754	-0.06178885
H	0.00000000	0.00000000	4.36683416
H	-4.07867704	-2.35482500	2.64231800
H	-2.25163279	-1.29998106	4.40648170
N	-3.13732204	-1.81133403	-0.06178885
B	0.00000000	0.00000000	3.15833091
N	-1.45631272	0.84080285	-1.29865547
N	-1.24892392	0.72106644	-2.64241061
N	1.45631272	0.84080285	-1.29865547
N	1.24892392	0.72106644	-2.64241061
N	0.00000000	-1.68160517	-1.29865547
N	0.00000000	-1.44213342	-2.64241061
C	-2.61998672	1.51264999	-1.15594642
C	-3.15921357	1.82397290	-2.42339578
C	-2.25026434	1.29919047	-3.32350935
C	2.61998672	1.51264999	-1.15594642
C	3.15921357	1.82397290	-2.42339578
C	2.25026434	1.29919047	-3.32350935
C	0.00000000	-3.02529998	-1.15594642
C	0.00000000	-3.64794581	-2.42339578
C	0.00000000	-2.59838147	-3.32350935
H	-4.07867704	2.35482500	-2.64231800
H	-2.25163279	1.29998106	-4.40648170
H	4.07867704	2.35482500	-2.64231800
N	3.13732204	1.81133403	0.06178885
H	2.25163279	1.29998106	-4.40648170
N	-3.13732204	1.81133403	0.06178885
H	0.00000000	0.00000000	-4.36683416
H	0.00000000	-4.70965052	-2.64231800
H	0.00000000	-2.59996159	-4.40648170
N	0.00000000	-3.62266754	0.06178885
B	0.00000000	0.00000000	-3.15833091
H	0.00000000	4.62051961	-0.13443589
H	4.00148701	-2.31025981	-0.13443589
H	-4.00148701	-2.31025981	-0.13443589
H	-4.00148701	2.31025981	0.13443589
H	4.00148701	2.31025981	0.13443589
H	0.00000000	-4.62051961	0.13443589
H	2.65331060	-1.53188982	-0.89612092
H	0.00000000	3.06377963	-0.89612092
H	-2.65331060	-1.53188982	-0.89612092

H	2.65331060	1.53188982	0.89612092
H	-2.65331060	1.53188982	0.89612092
H	0.00000000	-3.06377963	0.89612092

$[Fe(Tb^{3NH2})_2]$ $^1A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.62743700	1.19134785
N	0.00000000	1.43047723	2.54370106
N	1.40940169	-0.81371850	1.19134785
N	1.23882987	-0.71523861	2.54370106
N	-1.40940169	-0.81371850	1.19134785
N	-1.23882987	-0.71523861	2.54370106
C	0.00000000	2.96773184	1.00876053
C	0.00000000	3.62511128	2.25919103
C	0.00000000	2.60601750	3.19132246
C	2.57013134	-1.48386592	1.00876053
C	3.13943822	-1.81255537	2.25919103
C	2.25687746	-1.30300901	3.19132246
C	-2.57013134	-1.48386592	1.00876053
C	-3.13943822	-1.81255537	2.25919103
C	-2.25687746	-1.30300901	3.19132246
H	0.00000000	4.69335186	2.44249062
H	0.00000000	2.63746439	4.27353915
H	4.06456176	-2.34667567	2.44249062
N	3.07246714	-1.77388945	-0.21693833
H	2.28411104	-1.31873193	4.27353915
N	0.00000000	3.54777943	-0.21693833
H	0.00000000	0.00000000	4.28613410
H	-4.06456176	-2.34667567	2.44249062
H	-2.28411104	-1.31873193	4.27353915
N	-3.07246714	-1.77388945	-0.21693833
B	0.00000000	0.00000000	3.07835000
N	-1.40940169	0.81371850	-1.19134785
N	-1.23882987	0.71523861	-2.54370106
N	1.40940169	0.81371850	-1.19134785
N	1.23882987	0.71523861	-2.54370106
N	0.00000000	-1.62743700	-1.19134785
N	0.00000000	-1.43047723	-2.54370106
C	-2.57013134	1.48386592	-1.00876053
C	-3.13943822	1.81255537	-2.25919103
C	-2.25687746	1.30300901	-3.19132246
C	2.57013134	1.48386592	-1.00876053
C	3.13943822	1.81255537	-2.25919103
C	2.25687746	1.30300901	-3.19132246
C	0.00000000	-2.96773184	-1.00876053
C	0.00000000	-3.62511128	-2.25919103
C	0.00000000	-2.60601750	-3.19132246
H	-4.06456176	2.34667567	-2.44249062
H	-2.28411104	1.31873193	-4.27353915
H	4.06456176	2.34667567	-2.44249062
N	3.07246714	1.77388945	0.21693833
H	2.28411104	1.31873193	-4.27353915
N	-3.07246714	1.77388945	0.21693833
H	0.00000000	0.00000000	-4.28613410
H	0.00000000	-4.69335186	-2.44249062
H	0.00000000	-2.63746439	-4.27353915
N	0.00000000	-3.54777943	0.21693833
B	0.00000000	0.00000000	-3.07835000
H	0.00000000	4.54491341	-0.29842369
H	3.93601032	-2.27245697	-0.29842369
H	-3.93601032	-2.27245697	-0.29842369
H	-3.93601032	2.27245697	0.29842369
H	3.93601032	2.27245697	0.29842369
H	0.00000000	-4.54491341	0.29842369
H	2.58177430	-1.49058806	-1.04492715
H	0.00000000	2.98117612	-1.04492715
H	-2.58177430	-1.49058806	-1.04492715
H	2.58177430	1.49058806	1.04492715
H	-2.58177430	1.49058806	1.04492715
H	0.00000000	-2.98117612	1.04492715

$[Fe(Tb^{3NO2})_2]$ $^5A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.83035425	1.47017187
N	0.00000000	1.46108220	2.75599956
N	1.58513351	-0.91517713	1.47017187
N	1.26533424	-0.73054136	2.75599956
N	-1.58513351	-0.91517713	1.47017187
N	-1.26533424	-0.73054136	2.75599956
C	0.00000000	3.17390248	1.51368982
C	0.00000000	3.66912189	2.81900129
C	0.00000000	2.52880472	3.58617812
C	2.74868051	-1.58695124	1.51368982
C	3.17755274	-1.83456068	2.81900129
C	2.19000904	-1.26440236	3.58617812
C	-2.74868051	-1.58695124	1.51368982
C	-3.17755274	-1.83456068	2.81900129
C	-2.19000904	-1.26440236	3.58617812
H	0.00000000	4.70356657	3.13015275
H	0.00000000	2.39349092	4.65943054
H	4.07340802	-2.35178329	3.13015275
N	3.47647174	-2.00714179	0.33854273
H	2.07282380	-1.19674546	4.65943054
N	0.00000000	4.01428410	0.33854273
H	0.00000000	0.00000000	4.42375034
H	-4.07340802	-2.35178329	3.13015275
H	-2.07282380	-1.19674546	4.65943054
N	-3.47647174	-2.00714179	0.33854273
B	0.00000000	0.00000000	3.22043250
N	-1.58513351	0.91517713	-1.47017187
N	-1.26533424	0.73054136	-2.75599956
N	1.58513351	0.91517713	-1.47017187
N	1.26533424	0.73054136	-2.75599956
N	0.00000000	-1.83035425	-1.47017187
N	0.00000000	-1.46108220	-2.75599956
C	-2.74868051	1.58695124	-1.51368982
C	-3.17755274	1.83456068	-2.81900129
C	-2.19000904	1.26440236	-3.58617812
C	2.74868051	1.58695124	-1.51368982
C	3.17755274	1.83456068	-2.81900129
C	2.19000904	1.26440236	-3.58617812
C	0.00000000	-3.17390248	-1.51368982
C	0.00000000	-3.66912189	-2.81900129
C	0.00000000	-2.52880472	-3.58617812
H	-4.07340802	2.35178329	-3.13015275
H	-2.07282380	1.19674546	-4.65943054
H	4.07340802	2.35178329	-3.13015275
N	3.47647174	2.00714179	-0.33854273

H	2.07282380	1.19674546	-4.65943054
N	-3.47647174	2.00714179	-0.33854273
H	0.00000000	0.00000000	-4.42375034
H	0.00000000	-4.70356657	-3.13015275
H	0.00000000	-2.39349092	-4.65943054
N	0.00000000	-4.01428410	-0.33854273
B	0.00000000	0.00000000	-3.22043250
O	0.00000000	5.22510462	0.54861605
O	4.52507350	-2.61255231	0.54861605
O	-4.52507350	-2.61255231	0.54861605
O	-4.52507350	2.61255231	-0.54861605
O	4.52507350	2.61255231	-0.54861605
O	0.00000000	-5.22510462	-0.54861605
O	3.01762903	-1.74222878	-0.76261162
O	0.00000000	3.48445755	-0.76261162
O	-3.01762903	-1.74222878	-0.76261162
O	3.01762903	1.74222878	0.76261162
O	-3.01762903	1.74222878	0.76261162
O	0.00000000	-3.48445755	0.76261162

$[Fe(Tb^{3NO2})_2]$ ^3E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.77498432	1.31076940
N	0.00000000	1.44884709	2.60727112
N	1.53718159	-0.88749216	1.31076940
N	1.25473799	-0.72442354	2.60727112
N	-1.53718159	-0.88749216	1.31076940
N	-1.25473799	-0.72442354	2.60727112
C	0.00000000	3.12581349	1.31134567
C	0.00000000	3.65260892	2.60494592
C	0.00000000	2.53799071	3.40596416
C	2.70703373	-1.56290648	1.31134567
C	3.16325173	-1.82630446	2.60494592
C	2.19796416	-1.26899509	3.40596416
C	-2.70703373	-1.56290648	1.31134567
C	-3.16325173	-1.82630446	2.60494592
C	-2.19796416	-1.26899509	3.40596416
H	0.00000000	4.69581201	2.88430123
H	0.00000000	2.43155729	4.48229216
H	4.06669223	-2.34790600	2.88430123
N	3.43624157	-1.98391461	0.13580911
H	2.10579048	-1.21577838	4.48229216
N	0.00000000	3.96782975	0.13580911
H	0.00000000	0.00000000	4.29409557
H	-4.06669223	-2.34790600	2.88430123
H	-2.10579048	-1.21577838	4.48229216
N	-3.43624157	-1.98391461	0.13580911
B	0.00000000	0.00000000	3.09137728
N	-1.53718159	0.88749216	-1.31076940
N	-1.25473799	0.72442354	-2.60727112
N	1.53718159	0.88749216	-1.31076940
N	1.25473799	0.72442354	-2.60727112
N	0.00000000	-1.77498432	-1.31076940
N	0.00000000	-1.44884709	-2.60727112
C	-2.70703373	1.56290648	-1.31134567
C	-3.16325173	1.82630446	-2.60494592
C	-2.19796416	1.26899509	-3.40596416
C	2.70703373	1.56290648	-1.31134567
C	3.16325173	1.82630446	-2.60494592
C	2.19796416	1.26899509	-3.40596416
C	0.00000000	-3.12581349	-1.31134567
C	0.00000000	-3.65260892	-2.60494592
C	0.00000000	-2.53799071	-3.40596416
H	-4.06669223	2.34790600	-2.88430123
H	-2.10579048	1.21577838	-4.48229216
H	4.06669223	2.34790600	-2.88430123
N	3.43624157	1.98391461	-0.13580911
H	2.10579048	1.21577838	-4.48229216
N	-3.43624157	1.98391461	-0.13580911
H	0.00000000	0.00000000	-4.29409557
H	0.00000000	-4.69581201	-2.88430123
H	0.00000000	-2.43155729	-4.48229216
N	0.00000000	-3.96782975	-0.13580911
B	0.00000000	0.00000000	-3.09137728
O	0.00000000	5.17792688	0.35603469
O	4.48421625	-2.58896370	0.35603469
O	-4.48421625	-2.58896370	0.35603469
O	-4.48421625	2.58896370	-0.35603469
O	4.48421625	2.58896370	-0.35603469
O	0.00000000	-5.17792688	-0.35603469
O	2.99012028	-1.72634658	-0.97133500
O	0.00000000	3.45269369	-0.97133500
O	-2.99012028	-1.72634658	-0.97133500
O	2.99012028	1.72634658	0.97133500
O	-2.99012028	1.72634658	0.97133500
O	0.00000000	-3.45269369	0.97133500

$[Fe(Tb^{3NO2})_2]$ $^1A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	1.69191778	1.15800069
N	0.00000000	1.43289028	2.46921989
N	1.46524365	-0.84595862	1.15800069
N	1.24091959	-0.71644514	2.46921989
N	-1.46524365	-0.84595862	1.15800069
N	-1.24091959	-0.71644514	2.46921989
C	0.00000000	3.04883725	1.09128996
C	0.00000000	3.62810325	2.36379455
C	0.00000000	2.55572555	3.21648696
C	2.64037063	-1.52441889	1.09128996
C	3.14202960	-1.81405136	2.36379455
C	2.21332300	-1.27786251	3.21648696
C	-2.64037063	-1.52441889	1.09128996
C	-3.14202960	-1.81405136	2.36379455
C	-2.21332300	-1.27786251	3.21648696
H	0.00000000	4.68333189	2.59167574
H	0.00000000	2.49756315	4.29622604
H	4.05588431	-2.34166595	2.59167574
N	3.35803340	-1.93876150	-0.09735644
H	2.16295326	-1.24878158	4.29622604
N	0.00000000	3.87752300	-0.09735644
H	0.00000000	0.00000000	4.18447333
H	-4.05588431	-2.34166595	2.59167574
H	-2.16295326	-1.24878158	4.29622604
N	-3.35803340	-1.93876150	-0.09735644
B	0.00000000	0.00000000	2.98285626
N	-1.46524365	0.84595862	-1.15800069
N	-1.24091959	0.71644514	-2.46921989
N	1.46524365	0.84595862	-1.15800069

N	1.24091959	0.71644514	-2.46921989
N	0.00000000	-1.69191778	-1.15800069
N	0.00000000	-1.43289028	-2.46921989
C	-2.64037063	1.52441889	-1.09128996
C	-3.14202960	1.81405136	-2.36379455
C	-2.21332300	1.27786251	-3.21648696
C	2.64037063	1.52441889	-1.09128996
C	3.14202960	1.81405136	-2.36379455
C	2.21332300	1.27786251	-3.21648696
C	0.00000000	-3.04883725	-1.09128996
C	0.00000000	-3.62810325	-2.36379455
C	0.00000000	-2.55572555	-3.21648696
H	-4.05588431	2.34166595	-2.59167574
H	-2.16295326	1.24878158	-4.29622604
H	4.05588431	2.34166595	-2.59167574
N	3.35803340	1.93876150	0.09735644
H	2.16295326	1.24878158	-4.29622604
N	-3.35803340	1.93876150	0.09735644
H	0.00000000	0.00000000	-4.18447333
H	0.00000000	-4.68333189	-2.59167574
H	0.00000000	-2.49756315	-4.29622604
N	0.00000000	-3.87752300	0.09735644
B	0.00000000	0.00000000	-2.98285626
O	0.00000000	5.08919708	0.11690425
O	4.40737390	-2.54459854	0.11690425
O	-4.40737390	-2.54459854	0.11690425
O	-4.40737390	2.54459854	-0.11690425
O	4.40737390	2.54459854	-0.11690425
O	0.00000000	-5.08919708	-0.11690425
O	2.91431034	-1.68257780	-1.20513557
O	0.00000000	3.36515560	-1.20513557
O	-2.91431034	-1.68257780	-1.20513557
O	2.91431034	1.68257780	1.20513557
O	-2.91431034	1.68257780	1.20513557
O	0.00000000	-3.36515560	1.20513557

$[Fe(Tb^{5CH3})_2]$ $^5A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.54819059	0.89384811	1.37709912
N	1.26601106	0.73093190	2.68686361
N	0.00000000	-1.78769674	1.37709912
N	0.00000000	-1.46186326	2.68686361
N	-1.54819059	0.89384811	1.37709912
N	-1.26601106	0.73093190	2.68686361
C	2.71518306	1.56761193	1.31278927
C	3.17631817	1.83384841	2.61338153
C	2.22451986	1.28432694	3.45205550
C	0.00000000	-3.13522332	1.31278927
C	0.00000000	-3.66769629	2.61338153
C	0.00000000	-2.56865441	3.45205550
C	-2.71518306	1.56761193	1.31278927
C	-3.17631817	1.83384841	2.61338153
C	-2.22451986	1.28432694	3.45205550
H	4.08234212	2.35694118	2.89838422
H	2.16046401	1.24734433	4.53220046
H	0.00000000	-4.71388235	2.89838422
C	0.00000000	-3.90598163	0.03599569
H	0.00000000	-2.49468919	4.53220046
C	3.38267931	1.95299108	0.03599569
H	0.00000000	0.00000000	4.37541371
H	-4.08234212	2.35694118	2.89838422
H	-2.16046401	1.24734433	4.53220046
C	-3.38267931	1.95299108	0.03599569
B	0.00000000	0.00000000	3.16816725
N	0.00000000	1.78769674	-1.37709912
N	0.00000000	1.46186326	-2.68686361
N	1.54819059	-0.89384811	-1.37709912
N	1.26601106	-0.73093190	-2.68686361
N	-1.54819059	-0.89384811	-1.37709912
N	-1.26601106	-0.73093190	-2.68686361
C	0.00000000	3.13522332	-1.31278927
C	0.00000000	3.66769629	-2.61338153
C	0.00000000	2.56865441	-3.45205550
C	2.71518306	-1.56761193	-1.31278927
C	3.17631817	-1.83384841	-2.61338153
C	2.22451986	-1.28432694	-3.45205550
C	-2.71518306	-1.56761193	-1.31278927
C	-3.17631817	-1.83384841	-2.61338153
C	-2.22451986	-1.28432694	-3.45205550
H	0.00000000	4.71388235	-2.89838422
H	0.00000000	2.49468919	-4.53220046
H	4.08234212	-2.35694118	-2.89838422
C	3.38267931	-1.95299108	-0.03599569
H	2.16046401	-1.24734433	-4.53220046
C	0.00000000	3.90598163	-0.03599569
H	0.00000000	0.00000000	-4.37541371
H	-4.08234212	-2.35694118	-2.89838422
H	-2.16046401	-1.24734433	-4.53220046
C	-3.38267931	-1.95299108	-0.03599569
B	0.00000000	0.00000000	-3.16816725
H	-0.87676468	-3.68356737	-0.57795310
H	0.00000000	-4.97763488	0.25476339
H	0.87676468	-3.68356737	-0.57795310
H	4.31075830	2.48881744	0.25476339
H	2.75168042	2.60108398	-0.57795310
H	3.62844509	1.08248339	-0.57795310
H	-4.31075830	2.48881744	0.25476339
H	-3.62844509	1.08248339	-0.57795310
H	-2.75168042	2.60108398	-0.57795310
H	3.62844509	-1.08248339	0.57795310
H	4.31075830	-2.48881744	-0.25476339
H	2.75168042	-2.60108398	0.57795310
H	-2.75168042	-2.60108398	0.57795310
H	-4.31075830	-2.48881744	-0.25476339
H	-3.62844509	-1.08248339	0.57795310
H	-0.87676468	3.68356737	0.57795310
H	0.00000000	4.97763488	-0.25476339
H	0.87676468	3.68356737	0.57795310

$[Fe(Tb^{5CH3})_2]$ ^3E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.49119397	0.86094122	1.27235007
N	1.25380929	0.72388696	2.59299551
N	0.00000000	-1.72188244	1.27235007
N	0.00000000	-1.44777392	2.59299551
N	-1.49119397	0.86094122	1.27235007
N	-1.25380929	0.72388696	2.59299551
C	2.65824782	1.53473996	1.15618244

C	3.15720376	1.82281242	2.43861969
C	2.23473986	1.29022780	3.31830966
C	0.00000000	-3.06948046	1.15618244
C	0.00000000	-3.64562483	2.43861969
C	0.00000000	-2.58045559	3.31830966
C	-2.65824782	1.53473996	1.15618244
C	-3.15720376	1.82281242	2.43861969
C	-2.23473986	1.29022780	3.31830966
H	4.07225759	2.35111917	2.68218992
H	2.20301727	1.27191244	4.40031097
H	0.00000000	-4.70223781	2.68218992
C	0.00000000	-3.81763813	-0.13302246
H	0.00000000	-2.54382541	4.40031097
C	3.30617192	1.90881907	-0.13302246
H	0.00000000	0.00000000	4.30431133
H	-4.07225759	2.35111917	2.68218992
H	-2.20301727	1.27191244	4.40031097
C	-3.30617192	1.90881907	-0.13302246
B	0.00000000	0.00000000	3.09763639
N	0.00000000	1.72188244	-1.27235007
N	0.00000000	1.44777392	-2.59299551
N	1.49119397	-0.86094122	-1.27235007
N	1.25380929	-0.72388696	-2.59299551
N	-1.49119397	-0.86094122	-1.27235007
N	-1.25380929	-0.72388696	-2.59299551
C	0.00000000	3.06948046	-1.15618244
C	0.00000000	3.64562483	-2.43861969
C	0.00000000	2.58045559	-3.31830966
C	2.65824782	-1.53473996	-1.15618244
C	3.15720376	-1.82281242	-2.43861969
C	2.23473986	-1.29022780	-3.31830966
C	-2.65824782	-1.53473996	-1.15618244
C	-3.15720376	-1.82281242	-2.43861969
C	-2.23473986	-1.29022780	-3.31830966
H	0.00000000	4.70223781	-2.68218992
H	0.00000000	2.54382541	-4.40031097
H	4.07225759	-2.35111917	-2.68218992
C	3.30617192	-1.90881907	0.13302246
H	2.20301727	-1.27191244	-4.40031097
C	0.00000000	3.81763813	0.13302246
H	0.00000000	0.00000000	-4.30431133
H	-4.07225759	-2.35111917	-2.68218992
H	-2.20301727	-1.27191244	-4.40031097
C	-3.30617192	-1.90881907	0.13302246
B	0.00000000	0.00000000	-3.09763639
H	-0.87746213	-3.58988765	-0.74330512
H	0.00000000	-4.89165945	0.07497172
H	0.87746213	-3.58988765	-0.74330512
H	4.23630147	2.44582973	0.07497172
H	2.67020300	2.55484871	-0.74330512
H	3.54766513	1.03503948	-0.74330512
H	-4.23630147	2.44582973	0.07497172
H	-3.54766513	1.03503948	-0.74330512
H	-2.67020300	2.55484871	-0.74330512
H	3.54766513	-1.03503948	0.74330512
H	4.23630147	-2.44582973	-0.07497172
H	2.67020300	-2.55484871	0.74330512
H	-2.67020300	-2.55484871	0.74330512
H	-4.23630147	-2.44582973	-0.07497172
H	-3.54766513	-1.03503948	0.74330512
H	-0.87746213	3.58988765	0.74330512
H	0.00000000	4.89165945	-0.07497172
H	0.87746213	3.58988765	0.74330512

$[Fe(Tb^{5CH3})_2]$ $^1A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.42835100	0.82465871	1.15119230
N	1.24042058	0.71615727	2.48323621
N	0.00000000	-1.64931795	1.15119230
N	0.00000000	-1.43231400	2.48323621
N	-1.42835100	0.82465871	1.15119230
N	-1.24042058	0.71615727	2.48323621
C	2.59281294	1.49696147	0.97861648
C	3.13326960	1.80899401	2.23944742
C	2.24500484	1.29615405	3.16274054
C	0.00000000	-2.99392241	0.97861648
C	0.00000000	-3.61798802	2.23944742
C	0.00000000	-2.59230863	3.16274054
C	-2.59281294	1.49696147	0.97861648
C	-3.13326960	1.80899401	2.23944742
C	-2.24500484	1.29615405	3.16274054
H	4.05652779	2.34203743	2.43627755
H	2.24922662	1.29859144	4.24514561
H	0.00000000	-4.68407486	2.43627755
C	0.00000000	-3.71548840	-0.32525880
H	0.00000000	-2.59718341	4.24514561
C	3.21770777	1.85774447	-0.32525880
H	0.00000000	0.00000000	4.21955354
H	-4.05652779	2.34203743	2.43627755
H	-2.24922662	1.29859144	4.24514561
C	-3.21770777	1.85774447	-0.32525880
B	0.00000000	0.00000000	3.01409042
N	0.00000000	1.64931795	-1.15119230
N	0.00000000	1.43231400	-2.48323621
N	1.42835100	-0.82465871	-1.15119230
N	1.24042058	-0.71615727	-2.48323621
N	-1.42835100	-0.82465871	-1.15119230
N	-1.24042058	-0.71615727	-2.48323621
C	0.00000000	2.99392241	-0.97861648
C	0.00000000	3.61798802	-2.23944742
C	0.00000000	2.59230863	-3.16274054
C	2.59281294	-1.49696147	-0.97861648
C	3.13326960	-1.80899401	-2.23944742
C	2.24500484	-1.29615405	-3.16274054
C	-2.59281294	-1.49696147	-0.97861648
C	-3.13326960	-1.80899401	-2.23944742
C	-2.24500484	-1.29615405	-3.16274054
H	0.00000000	4.68407486	-2.43627755
H	0.00000000	2.59718341	-4.24514561
H	4.05652779	-2.34203743	-2.43627755
C	3.21770777	-1.85774447	0.32525880
H	2.24922662	-1.29859144	-4.24514561
C	0.00000000	3.71548840	0.32525880
H	0.00000000	0.00000000	-4.21955354
H	-4.05652779	-2.34203743	-2.43627755
H	-2.24922662	-1.29859144	-4.24514561
C	-3.21770777	-1.85774447	0.32525880
B	0.00000000	0.00000000	-3.01409042
H	-0.87966192	-3.48206779	-0.93042113

H	0.00000000	-4.79239374	-0.13105180
H	0.87966192	-3.48206779	-0.93042113
H	4.15033451	2.39619660	-0.13105180
H	2.57572792	2.50284328	-0.93042113
H	3.45538985	0.97922451	-0.93042113
H	-4.15033451	2.39619660	-0.13105180
H	-3.45538985	0.97922451	-0.93042113
H	-2.57572792	2.50284328	-0.93042113
H	3.45538985	-0.97922451	0.93042113
H	4.15033451	-2.39619660	0.13105180
H	2.57572792	-2.50284328	0.93042113
H	-2.57572792	-2.50284328	0.93042113
H	-4.15033451	-2.39619660	0.13105180
H	-3.45538985	-0.97922451	0.93042113
H	-0.87966192	3.48206779	0.93042113
H	0.00000000	4.79239374	0.13105180
H	0.87966192	3.48206779	0.93042113

$[Fe(Tb^{5CF3})_2]$ $^5A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.46371327	0.84507543	1.39489853
N	1.27325020	0.73511134	2.72434100
N	0.00000000	-1.69015086	1.39489853
N	0.00000000	-1.47022267	2.72434100
N	-1.46371327	0.84507543	1.39489853
N	-1.27325020	0.73511134	2.72434100
C	2.60756111	1.50547593	1.20255583
C	3.18759917	1.84036152	2.42299626
C	2.31081597	1.33415004	3.37143217
C	0.00000000	-3.01095187	1.20255583
C	0.00000000	-3.68072251	2.42299626
C	0.00000000	-2.66830007	3.37143217
C	-2.60756111	1.50547593	1.20255583
C	-3.18759917	1.84036152	2.42299626
C	-2.31081597	1.33415004	3.37143217
H	4.11143311	2.37373726	2.60410876
C	2.49507708	1.44053371	4.86015224
H	0.00000000	-4.74747453	2.60410876
H	0.00000000	-3.41466595	0.19790171
C	0.00000000	-2.88106690	4.86015224
H	2.95718746	1.70733271	0.19790171
H	0.00000000	0.00000000	4.43994687
H	-4.11143311	2.37373726	2.60410876
C	-2.49507708	1.44053371	4.86015224
H	-2.95718746	1.70733271	0.19790171
B	0.00000000	0.00000000	3.25165078
N	0.00000000	1.69015086	-1.39489853
N	0.00000000	1.47022267	-2.72434100
N	1.46371327	-0.84507543	-1.39489853
N	1.27325020	-0.73511134	-2.72434100
N	-1.46371327	-0.84507543	-1.39489853
N	-1.27325020	-0.73511134	-2.72434100
C	0.00000000	3.01095187	-1.20255583
C	0.00000000	3.68072251	-2.42299626
C	0.00000000	2.66830007	-3.37143217
C	2.60756111	-1.50547593	-1.20255583
C	3.18759917	-1.84036152	-2.42299626
C	2.31081597	-1.33415004	-3.37143217
C	-2.60756111	-1.50547593	-1.20255583
C	-3.18759917	-1.84036152	-2.42299626
C	-2.31081597	-1.33415004	-3.37143217
H	0.00000000	4.74747453	-2.60410876
C	0.00000000	2.88106690	-4.86015224
H	4.11143311	-2.37373726	-2.60410876
H	2.95718746	-1.70733271	-0.19790171
C	2.49507708	-1.44053371	-4.86015224
H	0.00000000	3.41466595	-0.19790171
H	0.00000000	0.00000000	-4.43994687
H	-4.11143311	-2.37373726	-2.60410876
C	-2.49507708	-1.44053371	-4.86015224
H	-2.95718746	-1.70733271	-0.19790171
B	0.00000000	0.00000000	-3.25165078
F	-3.64770238	-2.10600215	-5.12324276
F	-1.49840560	-2.12187323	-5.46724237
F	-2.58679884	-0.23672056	-5.46724237
F	3.64770238	-2.10600215	-5.12324276
F	2.58679884	-0.23672056	-5.46724237
F	1.49840560	-2.12187323	-5.46724237
F	1.08839377	2.35859380	-5.46724237
F	0.00000000	4.21200430	-5.12324276
F	-1.08839377	2.35859380	-5.46724237
F	-2.58679884	0.23672056	5.46724237
F	-3.64770238	2.10600215	5.12324276
F	-1.49840560	2.12187323	5.46724237
F	-1.08839377	-2.35859380	5.46724237
F	1.08839377	-2.35859380	5.46724237
F	0.00000000	-4.21200430	5.12324276
F	2.58679884	0.23672056	5.46724237
F	1.49840560	2.12187323	5.46724237
F	3.64770238	2.10600215	5.12324276

$[Fe(Tb^{5CF3})_2]$ ^3E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.40983403	0.81396827	1.27137162
N	1.25847716	0.72658206	2.60661018
N	0.00000000	-1.62793602	1.27137162
N	0.00000000	-1.45316412	2.60661018
N	-1.40983403	0.81396827	1.27137162
N	-1.25847716	0.72658206	2.60661018
C	2.54937331	1.47188112	1.03435895
C	3.16082756	1.82490478	2.23474092
C	2.31129223	1.33442521	3.21601758
C	0.00000000	-2.94376223	1.03435895
C	0.00000000	-3.64980957	2.23474092
C	0.00000000	-2.66885042	3.21601758
C	-2.54937331	1.47188112	1.03435895
C	-3.16082756	1.82490478	2.23474092
C	-2.31129223	1.33442521	3.21601758
H	4.08953575	2.36109469	2.38031176
C	2.51645055	1.45287360	4.69943687
H	0.00000000	-4.72218938	2.38031176
H	0.00000000	-3.31408417	0.01788990
C	0.00000000	-2.90574667	4.69943687
H	2.87008065	1.65704182	0.01788990
H	0.00000000	0.00000000	4.34409276
H	-4.08953575	2.36109469	2.38031176
C	-2.51645055	1.45287360	4.69943687
H	-2.87008065	1.65704182	0.01788990

B	0.00000000	0.00000000	3.15659944
N	0.00000000	1.62793602	-1.27137162
N	0.00000000	1.45316412	-2.60661018
N	1.40983403	-0.81396827	-1.27137162
N	1.25847716	-0.72658206	-2.60661018
N	-1.40983403	-0.81396827	-1.27137162
N	-1.25847716	-0.72658206	-2.60661018
C	0.00000000	2.94376223	-1.03435895
C	0.00000000	3.64980957	-2.23474092
C	0.00000000	2.66885042	-3.21601758
C	2.54937331	-1.47188112	-1.03435895
C	3.16082756	-1.82490478	-2.23474092
C	2.31129223	-1.33442521	-3.21601758
C	-2.54937331	-1.47188112	-1.03435895
C	-3.16082756	-1.82490478	-2.23474092
C	-2.31129223	-1.33442521	-3.21601758
H	0.00000000	4.72218938	-2.38031176
C	0.00000000	2.90574667	-4.69943687
H	4.08953575	-2.36109469	-2.38031176
H	2.87008065	-1.65704182	-0.01788990
C	2.51645055	-1.45287360	-4.69943687
H	0.00000000	3.31408417	-0.01788990
H	0.00000000	0.00000000	-4.34409276
H	-4.08953575	-2.36109469	-2.38031176
C	-2.51645055	-1.45287360	-4.69943687
H	-2.87008065	-1.65704182	-0.01788990
B	0.00000000	0.00000000	-3.15659944
F	-3.67152647	-2.11975705	-4.94372202
F	-1.52503432	-2.13746438	-5.31400005
F	-2.61361596	-0.25198627	-5.31400005
F	3.67152647	-2.11975705	-4.94372202
F	2.61361596	-0.25198627	-5.31400005
F	1.52503432	-2.13746438	-5.31400005
F	1.08858163	2.38945065	-5.31400005
F	0.00000000	4.23951358	-4.94372202
F	-1.08858163	2.38945065	-5.31400005
F	-2.61361596	0.25198627	5.31400005
F	-3.67152647	2.11975705	4.94372202
F	-1.52503432	2.13746438	5.31400005
F	-1.08858163	-2.38945065	5.31400005
F	1.08858163	-2.38945065	5.31400005
F	0.00000000	-4.23951358	4.94372202
F	2.61361596	0.25198627	5.31400005
F	1.52503432	2.13746438	5.31400005
F	3.67152647	2.11975705	4.94372202

$[Fe(Tb^{5CF3})_2]$ $^1A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.35976645	0.78506144	1.15679152
N	1.24716388	0.72005042	2.49850615
N	0.00000000	-1.57012340	1.15679152
N	0.00000000	-1.44010085	2.49850615
N	-1.35976645	0.78506144	1.15679152
N	-1.24716388	0.72005042	2.49850615
C	2.49326094	1.43948488	0.87539728
C	3.13627321	1.81072813	2.05390571
C	2.31722590	1.33785110	3.06736375
C	0.00000000	-2.87896977	0.87539728
C	0.00000000	-3.62145678	2.05390571
C	0.00000000	-2.67570221	3.06736375
C	-2.49326094	1.43948488	0.87539728
C	-3.13627321	1.81072813	2.05390571
C	-2.31722590	1.33785110	3.06736375
H	4.06871527	2.34907390	2.16179490
C	2.55781104	1.47675272	4.54209766
H	0.00000000	-4.69814780	2.16179490
H	0.00000000	-3.21902754	-0.15028740
C	0.00000000	-2.95350597	4.54209766
H	2.78775972	1.60951377	-0.15028740
H	0.00000000	0.00000000	4.25832213
H	-4.06871527	2.34907390	2.16179490
C	-2.55781104	1.47675272	4.54209766
H	-2.78775972	1.60951377	-0.15028740
B	0.00000000	0.00000000	3.07074678
N	0.00000000	1.57012340	-1.15679152
N	0.00000000	1.44010085	-2.49850615
N	1.35976645	-0.78506144	-1.15679152
N	1.24716388	-0.72005042	-2.49850615
N	-1.35976645	-0.78506144	-1.15679152
N	-1.24716388	-0.72005042	-2.49850615
C	0.00000000	2.87896977	-0.87539728
C	0.00000000	3.62145678	-2.05390571
C	0.00000000	2.67570221	-3.06736375
C	2.49326094	-1.43948488	-0.87539728
C	3.13627321	-1.81072813	-2.05390571
C	2.31722590	-1.33785110	-3.06736375
C	-2.49326094	-1.43948488	-0.87539728
C	-3.13627321	-1.81072813	-2.05390571
C	-2.31722590	-1.33785110	-3.06736375
H	0.00000000	4.69814780	-2.16179490
C	0.00000000	2.95350597	-4.54209766
H	4.06871527	-2.34907390	-2.16179490
H	2.78775972	-1.60951377	0.15028740
C	2.55781104	-1.47675272	-4.54209766
H	0.00000000	3.21902754	0.15028740
H	0.00000000	0.00000000	-4.25832213
H	-4.06871527	-2.34907390	-2.16179490
C	-2.55781104	-1.47675272	-4.54209766
H	-2.78775972	-1.60951377	0.15028740
B	0.00000000	0.00000000	-3.07074678
F	-3.71777445	-2.14645775	-4.75124174
F	-1.58034605	-2.16893879	-5.17105340
F	-2.66852921	-0.28415019	-5.17105340
F	3.71777445	-2.14645775	-4.75124174
F	2.66852921	-0.28415019	-5.17105340
F	1.58034605	-2.16893879	-5.17105340
F	1.08818316	2.45308898	-5.17105340
F	0.00000000	4.29291603	-4.75124174
F	-1.08818316	2.45308898	-5.17105340
F	-2.66852921	0.28415019	5.17105340
F	-3.71777445	2.14645775	4.75124174
F	-1.58034605	2.16893879	5.17105340
F	-1.08818316	-2.45308898	5.17105340
F	1.08818316	-2.45308898	5.17105340
F	0.00000000	-4.29291603	4.75124174
F	2.66852921	0.28415019	5.17105340
F	1.58034605	2.16893879	5.17105340
F	3.71777445	2.14645775	4.75124174

$[Fe(Tb^{5NH2})_2]$ $^5A_{1g}$ D_{3d} OPBE

Fe	0.000000	0.000000	0.000000
N	0.000000	1.713298	-1.375431
N	0.000000	1.461094	-2.716487
N	-1.483760	-0.856649	-1.375431
N	-1.265345	-0.730547	-2.716487
N	1.483760	-0.856649	-1.375431
N	1.265345	-0.730547	-2.716487
C	0.000000	3.037157	-1.242162
C	0.000000	3.675676	-2.484420
C	0.000000	2.627611	-3.406791
C	-2.630255	-1.518578	-1.242162
C	-3.183228	-1.837838	-2.484420
C	-2.275578	-1.313806	-3.406791
C	2.630255	-1.518578	-1.242162
C	3.183228	-1.837838	-2.484420
C	2.275578	-1.313806	-3.406791
H	0.000000	4.738676	-2.697401
N	0.000000	2.690986	-4.774142
H	-4.103814	-2.369338	-2.697401
H	-3.010786	-1.738278	-0.252031
N	-2.330462	-1.345493	-4.774142
H	0.000000	3.476557	-0.252031
H	0.000000	0.000000	-4.422884
H	4.103814	-2.369338	-2.697401
N	2.330462	-1.345493	-4.774142
H	3.010786	-1.738278	-0.252031
B	0.000000	0.000000	-3.206972
N	1.483760	0.856649	1.375431
N	1.265345	0.730547	2.716487
N	-1.483760	0.856649	1.375431
N	-1.265345	0.730547	2.716487
N	0.000000	-1.713298	1.375431
N	0.000000	-1.461094	2.716487
C	2.630255	1.518578	1.242162
C	3.183228	1.837838	2.484420
C	2.275578	1.313806	3.406791
C	-2.630255	1.518578	1.242162
C	-3.183228	1.837838	2.484420
C	-2.275578	1.313806	3.406791
C	0.000000	-3.037157	1.242162
C	0.000000	-3.675676	2.484420
C	0.000000	-2.627611	3.406791
H	4.103814	2.369338	2.697401
N	2.330462	1.345493	4.774142
H	-4.103814	2.369338	2.697401
H	-3.010786	1.738278	0.252031
N	-2.330462	1.345493	4.774142
H	3.010786	1.738278	0.252031
H	0.000000	0.000000	4.422884
H	0.000000	-4.738676	2.697401
N	0.000000	-2.690986	4.774142
H	0.000000	-3.476557	0.252031
B	0.000000	0.000000	3.206972
H	0.000000	3.581788	-5.230783
H	0.000000	1.857670	-5.328693
H	-3.101919	-1.790894	-5.230783
H	-1.608789	-0.928835	-5.328693
H	3.101919	-1.790894	-5.230783
H	1.608789	-0.928835	-5.328693
H	3.101919	1.790894	5.230783
H	1.608789	0.928835	5.328693
H	-3.101919	1.790894	5.230783
H	-1.608789	0.928835	5.328693
H	0.000000	-3.581788	5.230783
H	0.000000	-1.857670	5.328693

$[Fe(Tb^{5NH2})_2]$ ^3E_g D_{3d} OPBE

Fe	0.000000	0.000000	0.000000
N	0.000000	1.641308	-1.261792
N	0.000000	1.447060	-2.611587
N	-1.421414	-0.820654	-1.261792
N	-1.253191	-0.723530	-2.611587
N	1.421414	-0.820654	-1.261792
N	1.253191	-0.723530	-2.611587
C	0.000000	2.958424	-1.068502
C	0.000000	3.647581	-2.285109
C	0.000000	2.640960	-3.251657
C	-2.562071	-1.479212	-1.068502
C	-3.158898	-1.823791	-2.285109
C	-2.287139	-1.320480	-3.251657
C	2.562071	-1.479212	-1.068502
C	3.158898	-1.823791	-2.285109
C	2.287139	-1.320480	-3.251657
H	0.000000	4.719060	-2.450299
N	0.000000	2.753975	-4.616471
H	-4.086826	-2.359530	-2.450299
H	-2.904249	-1.676769	-0.061068
N	-2.385012	-1.376987	-4.616471
H	0.000000	3.353538	-0.061068
H	0.000000	0.000000	-4.344017
H	4.086826	-2.359530	-2.450299
N	2.385012	-1.376987	-4.616471
H	2.904249	-1.676769	-0.061068
B	0.000000	0.000000	-3.129326
N	1.421414	0.820654	1.261792
N	1.253191	0.723530	2.611587
N	-1.421414	0.820654	1.261792
N	-1.253191	0.723530	2.611587
N	0.000000	-1.641308	1.261792
N	0.000000	-1.447060	2.611587
C	2.562071	1.479212	1.068502
C	3.158898	1.823791	2.285109
C	2.287139	1.320480	3.251657
C	-2.562071	1.479212	1.068502
C	-3.158898	1.823791	2.285109
C	-2.287139	1.320480	3.251657
C	0.000000	-2.958424	1.068502
C	0.000000	-3.647581	2.285109
C	0.000000	-2.640960	3.251657
H	4.086826	2.359530	2.450299
N	2.385012	1.376987	4.616471
H	-4.086826	2.359530	2.450299
H	-2.904249	1.676769	0.061068
N	-2.385012	1.376987	4.616471
H	2.904249	1.676769	0.061068
H	0.000000	0.000000	4.344017
H	0.000000	-4.719060	2.450299

N	0.000000	-2.753975	4.616471
H	0.000000	-3.353538	0.061068
B	0.000000	0.000000	3.129326
H	0.000000	3.660765	-5.040413
H	0.000000	1.941521	-5.201255
H	-3.170316	-1.830383	-5.040413
H	-1.681406	-0.970760	-5.201255
H	3.170316	-1.830383	-5.040413
H	1.681406	-0.970760	-5.201255
H	3.170316	1.830383	5.040413
H	1.681406	0.970760	5.201255
H	-3.170316	1.830383	5.040413
H	-1.681406	0.970760	5.201255
H	0.000000	-3.660765	5.040413
H	0.000000	-1.941521	5.201255

$[Fe(Tb^{5NH2})_2]$ $^1A_{1g}$ D_{3d} OPBE

Fe	0.000000	0.000000	0.000000
N	1.370331	-0.791161	-1.159497
N	1.235910	-0.713553	-2.487024
N	0.000000	1.582322	-1.159497
N	0.000000	1.427106	-2.487024
N	-1.370331	-0.791161	-1.159497
N	-1.235910	-0.713553	-2.487024
C	2.514877	-1.451965	-0.914805
C	3.135459	-1.810258	-2.124227
C	2.281301	-1.317110	-3.106318
C	0.000000	2.903930	-0.914805
C	0.000000	3.620517	-2.124227
C	0.000000	2.634219	-3.106318
C	-2.514877	-1.451965	-0.914805
C	-3.135459	-1.810258	-2.124227
C	-2.281301	-1.317110	-3.106318
N	4.322713	-2.495720	-2.287527
H	2.341151	-1.351664	-4.186708
N	0.000000	4.991439	-2.287527
H	0.000000	3.272126	0.101889
H	0.000000	2.703328	-4.186708
H	2.833744	-1.636063	0.101889
H	0.000000	0.000000	-4.252956
N	-4.322713	-2.495720	-2.287527
H	-2.341151	-1.351664	-4.186708
H	-2.833744	-1.636063	0.101889
B	0.000000	0.000000	-3.047965
N	0.000000	-1.582322	1.159497
N	0.000000	-1.427106	2.487024
N	1.370331	0.791161	1.159497
N	1.235910	0.713553	2.487024
N	-1.370331	0.791161	1.159497
N	-1.235910	0.713553	2.487024
C	0.000000	-2.903930	0.914805
C	0.000000	-3.620517	2.124227
C	0.000000	-2.634219	3.106318
C	2.514877	1.451965	0.914805
C	3.135459	1.810258	2.124227
C	2.281301	1.317110	3.106318
C	-2.514877	1.451965	0.914805
C	-3.135459	1.810258	2.124227
C	-2.281301	1.317110	3.106318
N	0.000000	-4.991439	2.287527
H	0.000000	-2.703328	4.186708
N	4.322713	2.495720	2.287527
H	2.833744	1.636063	-0.101889
H	2.341151	1.351664	4.186708
H	0.000000	-3.272126	-0.101889
H	0.000000	0.000000	4.252956
N	-4.322713	2.495720	2.287527
H	-2.341151	1.351664	4.186708
H	-2.833744	1.636063	-0.101889
B	0.000000	0.000000	3.047965
H	0.000000	-5.404944	3.199344
H	0.000000	-5.600748	1.492844
H	-4.680819	2.702472	3.199344
H	-4.850390	2.800374	1.492844
H	4.680819	2.702472	3.199344
H	4.850390	2.800374	1.492844
H	0.000000	5.404944	-3.199344
H	0.000000	5.600748	-1.492844
H	-4.680819	-2.702472	-3.199344
H	-4.850390	-2.800374	-1.492844
H	4.680819	-2.702472	-3.199344
H	4.850390	-2.800374	-1.492844

$[Fe(Tb^{5NO2})_2]$ $^5A_{1g}$ D_{3d} OPBE

Fe	0.000000	0.000000	0.000000
N	-1.460551	-0.843249	-1.347671
N	-1.276905	-0.737221	-2.674815
N	1.460551	-0.843249	-1.347671
N	1.276905	-0.737221	-2.674815
N	0.000000	1.686499	-1.347671
N	0.000000	1.474443	-2.674815
C	-2.604015	-1.503429	-1.128975
C	-3.200326	-1.847709	-2.331778
C	-2.331239	-1.345941	-3.288522
C	2.604015	-1.503429	-1.128975
C	3.200326	-1.847709	-2.331778
C	2.331239	-1.345941	-3.288522
C	0.000000	3.006857	-1.128975
C	0.000000	3.695418	-2.331778
C	0.000000	2.691883	-3.288522
H	-4.122564	-2.380164	-2.516227
N	-2.569792	-1.483670	-4.719338
H	4.122564	-2.380164	-2.516227
H	2.935790	-1.694979	-0.116637
N	2.569792	-1.483670	-4.719338
H	-2.935790	-1.694979	-0.116637
H	0.000000	0.000000	-4.375542
H	0.000000	4.760327	-2.516227
N	0.000000	2.967340	-4.719338
H	0.000000	3.389959	-0.116637
B	0.000000	0.000000	-3.207335
N	-1.460551	0.843249	1.347671
N	-1.276905	0.737221	2.674815
N	0.000000	-1.686499	1.347671
N	0.000000	-1.474443	2.674815
N	1.460551	0.843249	1.347671
N	1.276905	0.737221	2.674815
C	-2.604015	1.503429	1.128975
C	-3.200326	1.847709	2.331778

C	-2.331239	1.345941	3.288522
C	0.000000	-3.006857	1.128975
C	0.000000	-3.695418	2.331778
C	0.000000	-2.691883	3.288522
C	2.604015	1.503429	1.128975
C	3.200326	1.847709	2.331778
C	2.331239	1.345941	3.288522
H	-4.122564	2.380164	2.516227
N	-2.569792	1.483670	4.719338
H	0.000000	-4.760327	2.516227
H	0.000000	-3.389959	0.116637
N	0.000000	-2.967340	4.719338
H	-2.935790	1.694979	0.116637
H	0.000000	0.000000	4.375542
H	4.122564	2.380164	2.516227
N	2.569792	1.483670	4.719338
H	2.935790	1.694979	0.116637
B	0.000000	0.000000	3.207335
O	-3.604480	-2.081048	-5.004451
O	-1.770773	-1.022356	-5.515564
O	3.604480	-2.081048	-5.004451
O	1.770773	-1.022356	-5.515564
O	0.000000	4.162095	-5.004451
O	0.000000	2.044713	-5.515564
O	-3.604480	2.081048	5.004451
O	-1.770773	1.022356	5.515564
O	0.000000	-4.162095	5.004451
O	0.000000	-2.044713	5.515564
O	3.604480	2.081048	5.004451
O	1.770773	1.022356	5.515564

$[Fe(Tb^{5NO2})_2]$ ^3E_g D_{3d} OPBE

Fe	0.000000	0.000000	0.000000
N	-1.402151	-0.809532	-1.233111
N	-1.262717	-0.729030	-2.567384
N	1.402151	-0.809532	-1.233111
N	1.262717	-0.729030	-2.567384
N	0.000000	1.619065	-1.233111
N	0.000000	1.458060	-2.567384
C	-2.539817	-1.466364	-0.962137
C	-3.171789	-1.831233	-2.139266
C	-2.335369	-1.348326	-3.134800
C	2.539817	-1.466364	-0.962137
C	3.171789	-1.831233	-2.139266
C	2.335369	-1.348326	-3.134800
C	0.000000	2.932728	-0.962137
C	0.000000	3.662467	-2.139266
C	0.000000	2.696652	-3.134800
H	-4.099736	-2.366984	-2.281704
N	-2.607811	-1.505620	-4.552568
H	4.099736	-2.366984	-2.281704
H	2.839390	-1.639323	0.062383
N	2.607811	-1.505620	-4.552568
H	-2.839390	-1.639323	0.062383
H	0.000000	0.000000	-4.295509
H	0.000000	4.733968	-2.281704
N	0.000000	3.011240	-4.552568
H	0.000000	3.278645	0.062383
B	0.000000	0.000000	-3.127309
N	-1.402151	0.809532	1.233111
N	-1.262717	0.729030	2.567384
N	0.000000	-1.619065	1.233111
N	0.000000	-1.458060	2.567384
N	1.402151	0.809532	1.233111
N	1.262717	0.729030	2.567384
C	-2.539817	1.466364	0.962137
C	-3.171789	1.831233	2.139266
C	-2.335369	1.348326	3.134800
C	0.000000	-2.932728	0.962137
C	0.000000	-3.662467	2.139266
C	0.000000	-2.696652	3.134800
C	2.539817	1.466364	0.962137
C	3.171789	1.831233	2.139266
C	2.335369	1.348326	3.134800
H	-4.099736	2.366984	2.281704
N	-2.607811	1.505620	4.552568
H	0.000000	-4.733968	2.281704
H	0.000000	-3.278645	-0.062383
N	0.000000	-3.011240	4.552568
H	-2.839390	1.639323	-0.062383
H	0.000000	0.000000	4.295509
H	4.099736	2.366984	2.281704
N	2.607811	1.505620	4.552568
H	2.839390	1.639323	-0.062383
B	0.000000	0.000000	3.127309
O	-3.649314	-2.106933	-4.806510
O	-1.824659	-1.053467	-5.371451
O	3.649314	-2.106933	-4.806510
O	1.824659	-1.053467	-5.371451
O	0.000000	4.213865	-4.806510
O	0.000000	2.106935	-5.371451
O	-3.649314	2.106933	4.806510
O	-1.824659	1.053467	5.371451
O	0.000000	-4.213865	4.806510
O	0.000000	-2.106935	5.371451
O	3.649314	2.106933	4.806510
O	1.824659	1.053467	5.371451

$[Fe(Tb^{5NO2})_2]$ $^1A_{1g}$ D_{3d} OPBE

Fe	0.000000	0.000000	0.000000
N	1.368001	-0.789816	1.146654
N	1.233703	-0.712279	2.494859
N	-1.368001	-0.789816	1.146654
N	-1.233703	-0.712279	2.494859
N	0.000000	1.579632	1.146654
N	0.000000	1.424558	2.494859
C	2.502425	-1.444776	0.900036
C	3.098829	-1.789110	2.118613
C	2.261925	-1.305923	3.111706
C	-2.502425	-1.444776	0.900036
C	-3.098829	-1.789110	2.118613
C	-2.261925	-1.305923	3.111706
C	0.000000	2.889552	0.900036
C	0.000000	3.578219	2.118613
C	0.000000	2.611846	3.111706
N	4.328919	-2.499303	2.313589
H	2.343053	-1.352762	4.188581
N	-4.328919	-2.499303	2.313589

H	-2.845814	-1.643031	-0.104171
H	-2.343053	-1.352762	4.188581
H	2.845814	-1.643031	-0.104171
H	0.000000	0.000000	4.261424
N	0.000000	4.998605	2.313589
H	0.000000	2.705525	4.188581
H	0.000000	3.286063	-0.104171
B	0.000000	0.000000	3.062858
N	1.368001	0.789816	-1.146654
N	1.233703	0.712279	-2.494859
N	0.000000	-1.579632	-1.146654
N	0.000000	-1.424558	-2.494859
N	-1.368001	0.789816	-1.146654
N	-1.233703	0.712279	-2.494859
C	2.502425	1.444776	-0.900036
C	3.098829	1.789110	-2.118613
C	2.261925	1.305923	-3.111706
C	0.000000	-2.889552	-0.900036
C	0.000000	-3.578219	-2.118613
C	0.000000	-2.611846	-3.111706
C	-2.502425	1.444776	-0.900036
C	-3.098829	1.789110	-2.118613
C	-2.261925	1.305923	-3.111706
N	4.328919	2.499303	-2.313589
H	2.343053	1.352762	-4.188581
N	0.000000	-4.998605	-2.313589
H	0.000000	-3.286063	0.104171
H	0.000000	-2.705525	-4.188581
H	2.845814	1.643031	0.104171
H	0.000000	0.000000	-4.261424
N	-4.328919	2.499303	-2.313589
H	-2.343053	1.352762	-4.188581
H	-2.845814	1.643031	0.104171
B	0.000000	0.000000	-3.062858
O	4.678768	2.701288	-3.473778
O	4.935816	2.849694	-1.306207
O	-4.678768	2.701288	-3.473778
O	-4.935816	2.849694	-1.306207
O	0.000000	-5.402576	-3.473778
O	0.000000	-5.699389	-1.306207
O	-4.678768	-2.701288	3.473778
O	-4.935816	-2.849694	1.306207
O	0.000000	5.402576	3.473778
O	0.000000	5.699389	1.306207
O	4.678768	-2.701288	3.473778
O	4.935816	-2.849694	1.306207

$[Fe(Tb^{3,5\text{-}CH3})_2]$ $^5A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	-1.78010000	1.37250000
N	0.00000000	-1.47050000	2.69130000
N	-1.54160000	0.89000000	1.37250000
N	-1.27350000	0.73520000	2.69130000
N	1.54160000	0.89000000	1.37250000
N	1.27350000	0.73520000	2.69130000
C	0.00000000	-3.12330000	1.28610000
C	0.00000000	-3.67160000	2.57540000
C	0.00000000	-2.59430000	3.44910000
C	-2.70490000	1.56170000	1.28610000
C	-3.17970000	1.83580000	2.57540000
C	-2.24670000	1.29710000	3.44910000
C	2.70490000	1.56170000	1.28610000
C	3.17970000	1.83580000	2.57540000
C	2.24670000	1.29710000	3.44910000
H	0.00000000	-4.72320000	2.84180000
C	0.00000000	-2.61760000	4.93850000
H	-4.09040000	2.36160000	2.84180000
C	-3.36380000	1.94210000	0.00390000
C	-2.26690000	1.30880000	4.93850000
C	0.00000000	-3.88420000	0.00390000
H	0.00000000	0.00000000	4.36300000
H	4.09040000	2.36160000	2.84180000
C	2.26690000	1.30880000	4.93850000
C	3.36380000	1.94210000	0.00390000
B	0.00000000	0.00000000	3.16470000
N	1.54160000	-0.89000000	-1.37250000
N	1.27350000	-0.73520000	-2.69130000
N	-1.54160000	-0.89000000	-1.37250000
N	-1.27350000	-0.73520000	-2.69130000
N	0.00000000	1.78010000	-1.37250000
N	0.00000000	1.47050000	-2.69130000
C	2.70490000	-1.56170000	-1.28610000
C	3.17970000	-1.83580000	-2.57540000
C	2.24670000	-1.29710000	-3.44910000
C	-2.70490000	-1.56170000	-1.28610000
C	-3.17970000	-1.83580000	-2.57540000
C	-2.24670000	-1.29710000	-3.44910000
C	0.00000000	3.12330000	-1.28610000
C	0.00000000	3.67160000	-2.57540000
C	0.00000000	2.59430000	-3.44910000
H	4.09040000	-2.36160000	-2.84180000
C	2.26690000	-1.30880000	-4.93850000
H	-4.09040000	-2.36160000	-2.84180000
C	-3.36380000	-1.94210000	-0.00390000
C	-2.26690000	-1.30880000	-4.93850000
C	3.36380000	-1.94210000	-0.00390000
H	0.00000000	0.00000000	-4.36300000
H	0.00000000	4.72320000	-2.84180000
C	0.00000000	2.61760000	-4.93850000
C	0.00000000	3.88420000	-0.00390000
B	0.00000000	0.00000000	-3.16470000
H	-2.72980000	2.58820000	-0.60900000
H	-4.29300000	2.47860000	0.21680000
H	-3.60630000	1.06990000	-0.60900000
H	0.00000000	-4.95720000	0.21680000
H	0.87660000	-3.65810000	-0.60900000
H	-0.87660000	-3.65810000	-0.60900000
H	4.29300000	2.47860000	0.21680000
H	2.72980000	2.58820000	-0.60900000
H	3.60630000	1.06990000	-0.60900000
H	-2.72980000	-2.58820000	0.60900000
H	-4.29300000	-2.47860000	-0.21680000
H	-3.60630000	-1.06990000	0.60900000
H	-0.87660000	3.65810000	0.60900000
H	0.00000000	4.95720000	-0.21680000
H	0.87660000	3.65810000	0.60900000
H	3.60630000	-1.06990000	0.60900000
H	4.29300000	-2.47860000	-0.21680000
H	2.72980000	-2.58820000	0.60900000

H	0.00000000	3.65590000	-5.28230000
H	-0.88340000	2.12590000	-5.36070000
H	0.88340000	2.12590000	-5.36070000
H	-3.16610000	-1.82790000	-5.28230000
H	-1.39940000	-1.82800000	-5.36070000
H	-2.28280000	-0.29800000	-5.36070000
H	1.39940000	-1.82800000	-5.36070000
H	3.16610000	-1.82790000	-5.28230000
H	2.28280000	-0.29800000	-5.36070000
H	1.39940000	1.82800000	5.36070000
H	3.16610000	1.82790000	5.28230000
H	2.28280000	0.29800000	5.36070000
H	-1.39940000	1.82800000	5.36070000
H	-2.28280000	0.29800000	5.36070000
H	-3.16610000	1.82790000	5.28230000
H	-0.88340000	-2.12590000	5.36070000
H	0.88340000	-2.12590000	5.36070000
H	0.00000000	-3.65590000	5.28230000

$[Fe(Tb^{3,5\text{-}CH3})_2]$ ^3E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	0.00000000	-1.71300000	1.26790000
N	0.00000000	-1.45650000	2.59740000
N	-1.48350000	0.85650000	1.26790000
N	-1.26140000	0.72830000	2.59740000
N	1.48350000	0.85650000	1.26790000
N	1.26140000	0.72830000	2.59740000
C	0.00000000	-3.05540000	1.12880000
C	0.00000000	-3.64780000	2.39920000
C	0.00000000	-2.60670000	3.31370000
C	-2.64600000	1.52770000	1.12880000
C	-3.15910000	1.82390000	2.39920000
C	-2.25740000	1.30330000	3.31370000
C	2.64600000	1.52770000	1.12880000
C	3.15910000	1.82390000	2.39920000
C	2.25740000	1.30330000	3.31370000
H	0.00000000	-4.70930000	2.62310000
C	0.00000000	-2.68330000	4.80100000
H	-4.07840000	2.35460000	2.62310000
C	-3.28310000	1.89550000	-0.16720000
C	-2.32380000	1.34160000	4.80100000
C	0.00000000	-3.79100000	-0.16720000
H	0.00000000	0.00000000	4.29440000
H	4.07840000	2.35460000	2.62310000
C	2.32380000	1.34160000	4.80100000
C	3.28310000	1.89550000	-0.16720000
B	0.00000000	0.00000000	3.09530000
N	1.48350000	-0.85650000	-1.26790000
N	1.26140000	-0.72830000	-2.59740000
N	-1.48350000	-0.85650000	-1.26790000
N	-1.26140000	-0.72830000	-2.59740000
N	0.00000000	1.71300000	-1.26790000
N	0.00000000	1.45650000	-2.59740000
C	2.64600000	-1.52770000	-1.12880000
C	3.15910000	-1.82390000	-2.39920000
C	2.25740000	-1.30330000	-3.31370000
C	-2.64600000	-1.52770000	-1.12880000
C	-3.15910000	-1.82390000	-2.39920000
C	-2.25740000	-1.30330000	-3.31370000
C	0.00000000	3.05540000	-1.12880000
C	0.00000000	3.64780000	-2.39920000
C	0.00000000	2.60670000	-3.31370000
H	4.07840000	-2.35460000	-2.62310000
C	2.32380000	-1.34160000	-4.80100000
H	-4.07840000	-2.35460000	-2.62310000
C	-3.28310000	-1.89550000	0.16720000
C	-2.32380000	-1.34160000	-4.80100000
C	3.28310000	-1.89550000	0.16720000
H	0.00000000	0.00000000	-4.29440000
H	0.00000000	4.70930000	-2.62310000
C	0.00000000	2.68330000	-4.80100000
C	0.00000000	3.79100000	0.16720000
B	0.00000000	0.00000000	-3.09530000
H	-2.64270000	2.53890000	-0.77570000
H	-4.21480000	2.43340000	0.03250000
H	-3.52010000	1.01920000	-0.77570000
H	0.00000000	-4.86680000	0.03250000
H	0.87740000	-3.55810000	-0.77570000
H	-0.87740000	-3.55810000	-0.77570000
H	4.21480000	2.43340000	0.03250000
H	2.64270000	2.53890000	-0.77570000
H	3.52010000	1.01920000	-0.77570000
H	-2.64270000	-2.53890000	0.77570000
H	-4.21480000	-2.43340000	-0.03250000
H	-3.52010000	-1.01920000	0.77570000
H	-0.87740000	3.55810000	0.77570000
H	0.00000000	4.86680000	-0.03250000
H	0.87740000	3.55810000	0.77570000
H	3.52010000	-1.01920000	0.77570000
H	4.21480000	-2.43340000	-0.03250000
H	2.64270000	-2.53890000	0.77570000
H	0.00000000	3.73360000	-5.10630000
H	-0.88330000	2.20800000	-5.24150000
H	0.88330000	2.20800000	-5.24150000
H	-3.23340000	-1.86680000	-5.10630000
H	-1.47050000	-1.86900000	-5.24150000
H	-2.35380000	-0.33900000	-5.24150000
H	1.47050000	-1.86900000	-5.24150000
H	3.23340000	-1.86680000	-5.10630000
H	2.35380000	-0.33900000	-5.24150000
H	1.47050000	1.86900000	5.24150000
H	3.23340000	1.86680000	5.10630000
H	2.35380000	0.33900000	5.24150000
H	-1.47050000	1.86900000	5.24150000
H	-2.35380000	0.33900000	5.24150000
H	-3.23340000	1.86680000	5.10630000
H	-0.88330000	-2.20800000	5.24150000
H	0.88330000	-2.20800000	5.24150000
H	0.00000000	-3.73360000	5.10630000

$[Fe(Tb^{3,5\text{-}CH3})_2]$ $^1A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	-1.42330000	-0.82170000	1.14720000
N	-1.24770000	-0.72040000	2.48640000
N	0.00000000	1.64350000	1.14720000
N	0.00000000	1.44070000	2.48640000
N	1.42330000	-0.82170000	1.14720000
N	1.24770000	-0.72040000	2.48640000

C	-2.58230000	-1.49090000	0.95520000
C	-3.13420000	-1.80950000	2.20590000
C	-2.26500000	-1.30770000	3.15930000
C	0.00000000	2.98170000	0.95520000
C	0.00000000	3.61910000	2.20590000
C	0.00000000	2.61540000	3.15930000
C	2.58230000	-1.49090000	0.95520000
C	3.13420000	-1.80950000	2.20590000
C	2.26500000	-1.30770000	3.15930000
H	-4.06050000	-2.34430000	2.38620000
C	-2.36820000	-1.36730000	4.64400000
H	0.00000000	4.68860000	2.38620000
C	0.00000000	3.69130000	-0.35500000
C	0.00000000	2.73460000	4.64400000
C	-3.19680000	-1.84570000	-0.35500000
H	0.00000000	0.00000000	4.20900000
H	4.06050000	-2.34430000	2.38620000
C	2.36820000	-1.36730000	4.64400000
C	3.19680000	-1.84570000	-0.35500000
B	0.00000000	0.00000000	3.01010000
N	0.00000000	-1.64350000	-1.14720000
N	0.00000000	-1.44070000	-2.48640000
N	-1.42330000	0.82170000	-1.14720000
N	-1.24770000	0.72040000	-2.48640000
N	1.42330000	0.82170000	-1.14720000
N	1.24770000	0.72040000	-2.48640000
C	0.00000000	-2.98170000	-0.95520000
C	0.00000000	-3.61910000	-2.20590000
C	0.00000000	-2.61540000	-3.15930000
C	-2.58230000	1.49090000	-0.95520000
C	-3.13420000	1.80950000	-2.20590000
C	-2.26500000	1.30770000	-3.15930000
C	2.58230000	1.49090000	-0.95520000
C	3.13420000	1.80950000	-2.20590000
C	2.26500000	1.30770000	-3.15930000
H	0.00000000	-4.68860000	-2.38620000
C	0.00000000	-2.73460000	-4.64400000
H	-4.06050000	2.34430000	-2.38620000
C	-3.19680000	1.84570000	0.35500000
C	-2.36820000	1.36730000	-4.64400000
C	0.00000000	-3.69130000	0.35500000
H	0.00000000	0.00000000	-4.20900000
H	4.06050000	2.34430000	-2.38620000
C	2.36820000	1.36730000	-4.64400000
C	3.19680000	1.84570000	0.35500000
B	0.00000000	0.00000000	-3.01010000
H	0.87980000	3.45320000	-0.95810000
H	0.00000000	4.76980000	-0.16880000
H	-0.87980000	3.45320000	-0.95810000
H	-4.13080000	-2.38490000	-0.16880000
H	-2.55060000	-2.48850000	-0.95810000
H	-3.43050000	-0.96460000	-0.95810000
H	4.13080000	-2.38490000	-0.16880000
H	3.43050000	-0.96460000	-0.95810000
H	2.55060000	-2.48850000	-0.95810000
H	-3.43050000	0.96460000	0.95810000
H	-4.13080000	2.38490000	0.16880000
H	-2.55060000	2.48850000	0.95810000
H	2.55060000	2.48850000	0.95810000
H	4.13080000	2.38490000	0.16880000
H	3.43050000	0.96460000	0.95810000
H	0.87980000	-3.45320000	0.95810000
H	0.00000000	-4.76980000	0.16880000
H	-0.87980000	-3.45320000	0.95810000
H	3.28460000	1.89640000	-4.92060000
H	1.52430000	1.90020000	-5.09720000
H	2.40780000	0.36990000	-5.09720000
H	-3.28460000	1.89640000	-4.92060000
H	-2.40780000	0.36990000	-5.09720000
H	-1.52430000	1.90020000	-5.09720000
H	-0.88350000	-2.27020000	-5.09720000
H	0.00000000	-3.79270000	-4.92060000
H	0.88350000	-2.27020000	-5.09720000
H	2.40780000	-0.36990000	5.09720000
H	3.28460000	-1.89640000	4.92060000
H	1.52430000	-1.90020000	5.09720000
H	0.88350000	2.27020000	5.09720000
H	-0.88350000	2.27020000	5.09720000
H	0.00000000	3.79270000	4.92060000
H	-2.40780000	-0.36990000	5.09720000
H	-1.52430000	-1.90020000	5.09720000
H	-3.28460000	-1.89640000	4.92060000

$Fe(Tb^{3,5\text{-}CF3})_2]$ $^5A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.35976645	0.78506144	1.15679152
N	1.24716388	0.72005042	2.49850615
N	0.00000000	-1.57012340	1.15679152
N	0.00000000	-1.44010085	2.49850615
N	-1.35976645	0.78506144	1.15679152
N	-1.24716388	0.72005042	2.49850615
C	2.49326094	1.43948488	0.87539728
C	3.13627321	1.81072813	2.05390571
C	2.31722590	1.33785110	3.06736375
C	0.00000000	-2.87896977	0.87539728
C	0.00000000	-3.62145678	2.05390571
C	0.00000000	-2.67570221	3.06736375
C	-2.49326094	1.43948488	0.87539728
C	-3.13627321	1.81072813	2.05390571
C	-2.31722590	1.33785110	3.06736375
H	4.06871527	2.34907390	2.16179490
C	2.55781104	1.47675272	4.54209766
H	0.00000000	-4.69814780	2.16179490
H	0.00000000	-3.21902754	-0.15028740
C	0.00000000	-2.95350597	4.54209766
H	2.78775972	1.60951377	-0.15028740
H	0.00000000	0.00000000	4.25832213
H	-4.06871527	2.34907390	2.16179490
C	-2.55781104	1.47675272	4.54209766
H	-2.78775972	1.60951377	-0.15028740
B	0.00000000	0.00000000	3.07074678
N	0.00000000	1.57012340	-1.15679152
N	0.00000000	1.44010085	-2.49850615
N	1.35976645	-0.78506144	-1.15679152
N	1.24716388	-0.72005042	-2.49850615
N	-1.35976645	-0.78506144	-1.15679152
N	-1.24716388	-0.72005042	-2.49850615
C	0.00000000	2.87896977	-0.87539728
C	0.00000000	3.62145678	-2.05390571

C	0.00000000	2.67570221	-3.06736375
C	2.49326094	-1.43948488	-0.87539728
C	3.13627321	-1.81072813	-2.05390571
C	2.31722590	-1.33785110	-3.06736375
C	-2.49326094	-1.43948488	-0.87539728
C	-3.13627321	-1.81072813	-2.05390571
C	-2.31722590	-1.33785110	-3.06736375
H	0.00000000	4.69814780	-2.16179490
C	0.00000000	2.95350597	-4.54209766
H	4.06871527	-2.34907390	-2.16179490
H	2.78775972	-1.60951377	0.15028740
C	2.55781104	-1.47675272	-4.54209766
H	0.00000000	3.21902754	0.15028740
H	0.00000000	0.00000000	-4.25832213
H	-4.06871527	-2.34907390	-2.16179490
C	-2.55781104	-1.47675272	-4.54209766
H	-2.78775972	-1.60951377	0.15028740
B	0.00000000	0.00000000	-3.07074678
F	-3.71777445	-2.14645775	-4.75124174
F	-1.58034605	-2.16893879	-5.17105340
F	-2.66852921	-0.28415019	-5.17105340
F	3.71777445	-2.14645775	-4.75124174
F	2.66852921	-0.28415019	-5.17105340
F	1.58034605	-2.16893879	-5.17105340
F	1.08818316	2.45308898	-5.17105340
F	0.00000000	4.29291603	-4.75124174
F	-1.08818316	2.45308898	-5.17105340
F	-2.66852921	0.28415019	5.17105340
F	-3.71777445	2.14645775	4.75124174
F	-1.58034605	2.16893879	5.17105340
F	-1.08818316	-2.45308898	5.17105340
F	1.08818316	-2.45308898	5.17105340
F	0.00000000	-4.29291603	4.75124174
F	2.66852921	0.28415019	5.17105340
F	1.58034605	2.16893879	5.17105340
F	3.71777445	2.14645775	4.75124174

$[Fe(Tb^{3,5\text{-}CF3})_2]$ ^3E_g D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.53570148	0.88663754	1.20661567
N	1.28520908	0.74201551	2.52480520
N	0.00000000	-1.77327561	1.20661567
N	0.00000000	-1.48403155	2.52480520
N	-1.53570148	0.88663754	1.20661567
N	-1.28520908	0.74201551	2.52480520
C	2.70792434	1.56342084	1.10320809
C	3.20016184	1.84761443	2.37448340
C	2.28157364	1.31726717	3.25226410
C	0.00000000	-3.12684116	1.10320809
C	0.00000000	-3.69522832	2.37448340
C	0.00000000	-2.63453433	3.25226410
C	-2.70792434	1.56342084	1.10320809
C	-3.20016184	1.84761443	2.37448340
C	-2.28157364	1.31726717	3.25226410
H	4.10911319	2.37239792	2.62614158
C	2.41659215	1.39522027	4.75149416
H	0.00000000	-4.74479530	2.62614158
C	0.00000000	-4.02602284	-0.13155135
C	0.00000000	-2.79044053	4.75149416
C	3.48663776	2.01301142	-0.13155135
H	0.00000000	0.00000000	4.19799380
H	-4.10911319	2.37239792	2.62614158
C	-2.41659215	1.39522027	4.75149416
C	-3.48663776	2.01301142	-0.13155135
B	0.00000000	0.00000000	3.00988769
N	0.00000000	1.77327561	-1.20661567
N	0.00000000	1.48403155	-2.52480520
N	1.53570148	-0.88663754	-1.20661567
N	1.28520908	-0.74201551	-2.52480520
N	-1.53570148	-0.88663754	-1.20661567
N	-1.28520908	-0.74201551	-2.52480520
C	0.00000000	3.12684116	-1.10320809
C	0.00000000	3.69522832	-2.37448340
C	0.00000000	2.63453433	-3.25226410
C	2.70792434	-1.56342084	-1.10320809
C	3.20016184	-1.84761443	-2.37448340
C	2.28157364	-1.31726717	-3.25226410
C	-2.70792434	-1.56342084	-1.10320809
C	-3.20016184	-1.84761443	-2.37448340
C	-2.28157364	-1.31726717	-3.25226410
H	0.00000000	4.74479530	-2.62614158
C	0.00000000	2.79044053	-4.75149416
H	4.10911319	-2.37239792	-2.62614158
C	3.48663776	-2.01301142	0.13155135
C	2.41659215	-1.39522027	-4.75149416
C	0.00000000	4.02602284	0.13155135
H	0.00000000	0.00000000	-4.19799380
H	-4.10911319	-2.37239792	-2.62614158
C	-2.41659215	-1.39522027	-4.75149416
C	-3.48663776	-2.01301142	0.13155135
B	0.00000000	0.00000000	-3.00988769
F	-1.07776366	-3.88646822	-0.92253586
F	0.00000000	-5.31697720	0.29303508
F	1.07776366	-3.88646822	-0.92253586
F	4.60463742	2.65848860	0.29303508
F	2.82689820	2.87660435	-0.92253586
F	3.90466186	1.00986334	-0.92253586
F	-4.60463742	2.65848860	0.29303508
F	-3.90466186	1.00986334	-0.92253586
F	-2.82689820	2.87660435	-0.92253586
F	3.90466186	-1.00986334	0.92253586
F	4.60463742	-2.65848860	-0.29303508
F	2.82689820	-2.87660435	0.92253586
F	-2.82689820	-2.87660435	0.92253586
F	-4.60463742	-2.65848860	-0.29303508
F	-3.90466186	-1.00986334	0.92253586
F	-1.07776366	3.88646822	0.92253586
F	0.00000000	5.31697720	-0.29303508
F	1.07776366	3.88646822	0.92253586
F	-3.56031194	-2.05554722	-5.05431742
F	-1.40492432	-2.06761987	-5.33575135
F	-2.49307308	-0.18289001	-5.33575135
F	3.56031194	-2.05554722	-5.05431742
F	2.49307308	-0.18289001	-5.33575135
F	1.40492432	-2.06761987	-5.33575135
F	1.08814929	2.25050987	-5.33575135
F	0.00000000	4.11109390	-5.05431742
F	-1.08814929	2.25050987	-5.33575135
F	-2.49307308	0.18289001	5.33575135

F	-3.56031194	2.05554722	5.05431742
F	-1.40492432	2.06761987	5.33575135
F	-1.08814929	-2.25050987	5.33575135
F	1.08814929	-2.25050987	5.33575135
F	0.00000000	-4.11109390	5.05431742
F	2.49307308	0.18289001	5.33575135
F	1.40492432	2.06761987	5.33575135
F	3.56031194	2.05554722	5.05431742

$[Fe(Tb^{3,5\text{-}CF3})_2]$ $^1A_{1g}$ D_{3d} OPBE

Fe	0.00000000	0.00000000	0.00000000
N	1.47937003	0.85411483	1.11483676
N	1.26914008	0.73273851	2.44277161
N	0.00000000	-1.70822967	1.11483676
N	0.00000000	-1.46547701	2.44277161
N	-1.47937003	0.85411483	1.11483676
N	-1.26914008	0.73273851	2.44277161
C	2.65456263	1.53261267	0.97097516
C	3.17401942	1.83252123	2.22886388
C	2.28102065	1.31694807	3.13657590
C	0.00000000	-3.06522534	0.97097516
C	0.00000000	-3.66504193	2.22886388
C	0.00000000	-2.63389562	3.13657590
C	-2.65456263	1.53261267	0.97097516
C	-3.17401942	1.83252123	2.22886388
C	-2.28102065	1.31694807	3.13657590
H	4.08825567	2.36035543	2.45070504
C	2.44803534	1.41337369	4.63055546
H	0.00000000	-4.72071139	2.45070504
C	0.00000000	-3.96945009	-0.26391710
C	0.00000000	-2.82674738	4.63055546
C	3.43764495	1.98472531	-0.26391710
H	0.00000000	0.00000000	4.13712043
H	-4.08825567	2.36035543	2.45070504
C	-2.44803534	1.41337369	4.63055546
C	-3.43764495	1.98472531	-0.26391710
B	0.00000000	0.00000000	2.94988270
N	0.00000000	1.70822967	-1.11483676
N	0.00000000	1.46547701	-2.44277161
N	1.47937003	-0.85411483	-1.11483676
N	1.26914008	-0.73273851	-2.44277161
N	-1.47937003	-0.85411483	-1.11483676
N	-1.26914008	-0.73273851	-2.44277161
C	0.00000000	3.06522534	-0.97097516
C	0.00000000	3.66504193	-2.22886388
C	0.00000000	2.63389562	-3.13657590
C	2.65456263	-1.53261267	-0.97097516
C	3.17401942	-1.83252123	-2.22886388
C	2.28102065	-1.31694807	-3.13657590
C	-2.65456263	-1.53261267	-0.97097516
C	-3.17401942	-1.83252123	-2.22886388
C	-2.28102065	-1.31694807	-3.13657590
H	0.00000000	4.72071139	-2.45070504
C	0.00000000	2.82674738	-4.63055546
H	4.08825567	-2.36035543	-2.45070504
C	3.43764495	-1.98472531	0.26391710
C	2.44803534	-1.41337369	-4.63055546
C	0.00000000	3.96945009	0.26391710
H	0.00000000	0.00000000	-4.13712043
H	-4.08825567	-2.36035543	-2.45070504
C	-2.44803534	-1.41337369	-4.63055546
C	-3.43764495	-1.98472531	0.26391710
B	0.00000000	0.00000000	-2.94988270
F	-1.07823304	-3.84095262	-1.05573930
F	0.00000000	-5.25855391	0.16798679
F	1.07823304	-3.84095262	-1.05573930
F	4.55404119	2.62927696	0.16798679
F	2.78724589	2.85425349	-1.05573930
F	3.86547893	0.98669913	-1.05573930
F	-4.55404119	2.62927696	0.16798679
F	-3.86547893	0.98669913	-1.05573930
F	-2.78724589	2.85425349	-1.05573930
F	3.86547893	-0.98669913	1.05573930
F	4.55404119	-2.62927696	-0.16798679
F	2.78724589	-2.85425349	1.05573930
F	-2.78724589	-2.85425349	1.05573930
F	-4.55404119	-2.62927696	-0.16798679
F	-3.86547893	-0.98669913	1.05573930
F	-1.07823304	3.84095262	1.05573930
F	0.00000000	5.25855391	-0.16798679
F	1.07823304	3.84095262	1.05573930
F	-3.59748188	-2.07700694	-4.90056021
F	-1.44812952	-2.09252824	-5.22805372
F	-2.53624760	-0.20785236	-5.22805372
F	3.59748188	-2.07700694	-4.90056021
F	2.53624760	-0.20785236	-5.22805372
F	1.44812952	-2.09252824	-5.22805372
F	1.08811807	2.30038113	-5.22805372
F	0.00000000	4.15401441	-4.90056021
F	-1.08811807	2.30038113	-5.22805372
F	-2.53624760	0.20785236	5.22805372
F	-3.59748188	2.07700694	4.90056021
F	-1.44812952	2.09252824	5.22805372
F	-1.08811807	-2.30038113	5.22805372
F	1.08811807	-2.30038113	5.22805372
F	0.00000000	-4.15401441	4.90056021
F	2.53624760	0.20785236	5.22805372
F	1.44812952	2.09252824	5.22805372
F	3.59748188	2.07700694	4.90056021

$[Fe(Tb^{3,5\text{-}NH2})_2]$ $^5A_{1g}$ D_{3d} OPBE

Fe	0.000000	0.000000	0.000000
N	0.000000	1.733051	1.389194
N	0.000000	1.460534	2.744950
N	1.500866	-0.866525	1.389194
N	1.264860	-0.730267	2.744950
N	-1.500866	-0.866525	1.389194
N	-1.264860	-0.730267	2.744950
C	0.000000	3.071410	1.281538
C	0.000000	3.682011	2.550373
C	0.000000	2.615087	3.443783
C	2.659919	-1.535705	1.281538
C	3.188715	-1.841006	2.550373
C	2.264732	-1.307543	3.443783
C	-2.659919	-1.535705	1.281538
C	-3.188715	-1.841006	2.550373
C	-2.264732	-1.307543	3.443783
H	0.000000	4.739960	2.787189

N	0.000000	2.662023	4.812912
H	4.104926	-2.369980	2.787189
N	3.193983	-1.844047	0.070759
N	2.305380	-1.331012	4.812912
N	0.000000	3.688094	0.070759
H	0.000000	0.000000	4.438764
H	-4.104926	-2.369980	2.787189
N	-2.305380	-1.331012	4.812912
N	-3.193983	-1.844047	0.070759
B	0.000000	0.000000	3.220745
N	-1.500866	0.866525	-1.389194
N	-1.264860	0.730267	-2.744950
N	1.500866	0.866525	-1.389194
N	1.264860	0.730267	-2.744950
N	0.000000	-1.733051	-1.389194
N	0.000000	-1.460534	-2.744950
C	-2.659919	1.535705	-1.281538
C	-3.188715	1.841006	-2.550373
C	-2.264732	1.307543	-3.443783
C	2.659919	1.535705	-1.281538
C	3.188715	1.841006	-2.550373
C	2.264732	1.307543	-3.443783
C	0.000000	-3.071410	-1.281538
C	0.000000	-3.682011	-2.550373
C	0.000000	-2.615087	-3.443783
H	-4.104926	2.369980	-2.787189
N	-2.305380	1.331012	-4.812912
H	4.104926	2.369980	-2.787189
N	3.193983	1.844047	-0.070759
N	2.305380	1.331012	-4.812912
N	-3.193983	1.844047	-0.070759
H	0.000000	0.000000	-4.438764
H	0.000000	-4.739960	-2.787189
N	0.000000	-2.662023	-4.812912
N	0.000000	-3.688094	-0.070759
B	0.000000	0.000000	-3.220745
H	0.000000	3.546501	5.280878
H	0.000000	1.819553	5.353011
H	3.071360	-1.773250	5.280878
H	1.575779	-0.909777	5.353011
H	-3.071360	-1.773250	5.280878
H	-1.575779	-0.909777	5.353011
H	-3.071360	1.773250	-5.280878
H	-1.575779	0.909777	-5.353011
H	3.071360	1.773250	-5.280878
H	1.575779	0.909777	-5.353011
H	0.000000	-3.546501	-5.280878
H	0.000000	-1.819553	-5.353011
H	0.000000	4.686318	0.010327
H	4.058470	-2.343159	0.010327
H	-4.058470	-2.343159	0.010327
H	-4.058470	2.343159	-0.010327
H	4.058470	2.343159	-0.010327
H	0.000000	-4.686318	-0.010327
H	2.719128	-1.569889	-0.771211
H	0.000000	3.139778	-0.771211
H	-2.719128	-1.569889	-0.771211
H	2.719128	1.569889	0.771211
H	-2.719128	1.569889	0.771211
H	0.000000	-3.139778	0.771211

$[Fe(Tb^{3,5\text{-}NH2})_2]$ ^3E_g D_{3d} OPBE

Fe	0.000000	0.000000	0.000000
N	0.000000	1.674972	1.300340
N	0.000000	1.448153	2.664638
N	1.450568	-0.837486	1.300340
N	1.254137	-0.724076	2.664638
N	-1.450568	-0.837486	1.300340
N	-1.254137	-0.724076	2.664638
C	0.000000	3.010408	1.148829
C	0.000000	3.659269	2.400257
C	0.000000	2.623138	3.327307
C	2.607090	-1.505204	1.148829
C	3.169020	-1.829635	2.400257
C	2.271704	-1.311569	3.327307
C	-2.607090	-1.505204	1.148829
C	-3.169020	-1.829635	2.400257
C	-2.271704	-1.311569	3.327307
H	0.000000	4.724735	2.600670
N	0.000000	2.705676	4.695457
H	4.091741	-2.362367	2.600670
N	3.111832	-1.796617	-0.076342
N	2.343184	-1.352838	4.695457
N	0.000000	3.593234	-0.076342
H	0.000000	0.000000	4.378838
H	-4.091741	-2.362367	2.600670
N	-2.343184	-1.352838	4.695457
N	-3.111832	-1.796617	-0.076342
B	0.000000	0.000000	3.161432
N	-1.450568	0.837486	-1.300340
N	-1.254137	0.724076	-2.664638
N	1.450568	0.837486	-1.300340
N	1.254137	0.724076	-2.664638
N	0.000000	-1.674972	-1.300340
N	0.000000	-1.448153	-2.664638
C	-2.607090	1.505204	-1.148829
C	-3.169020	1.829635	-2.400257
C	-2.271704	1.311569	-3.327307
C	2.607090	1.505204	-1.148829
C	3.169020	1.829635	-2.400257
C	2.271704	1.311569	-3.327307
C	0.000000	-3.010408	-1.148829
C	0.000000	-3.659269	-2.400257
C	0.000000	-2.623138	-3.327307
H	-4.091741	2.362367	-2.600670
N	-2.343184	1.352838	-4.695457
H	4.091741	2.362367	-2.600670
N	3.111832	1.796617	0.076342
N	2.343184	1.352838	-4.695457
N	-3.111832	1.796617	0.076342
H	0.000000	0.000000	-4.378838
H	0.000000	-4.724735	-2.600670
N	0.000000	-2.705676	-4.695457
N	0.000000	-3.593234	0.076342
B	0.000000	0.000000	-3.161432
H	0.000000	3.601914	5.140479
H	0.000000	1.877678	5.257637
H	3.119349	-1.800957	5.140479
H	1.626117	-0.938839	5.257637
H	-3.119349	-1.800957	5.140479

H	-1.626117	-0.938839	5.257637
H	-3.119349	1.800957	-5.140479
H	-1.626117	0.938839	-5.257637
H	3.119349	1.800957	-5.140479
H	1.626117	0.938839	-5.257637
H	0.000000	-3.601914	-5.140479
H	0.000000	-1.877678	-5.257637
H	0.000000	4.589429	-0.163637
H	3.974562	-2.294714	-0.163637
H	-3.974562	-2.294714	-0.163637
H	-3.974562	2.294714	0.163637
H	3.974562	2.294714	0.163637
H	0.000000	-4.589429	0.163637
H	2.613411	-1.508853	-0.899609
H	0.000000	3.017707	-0.899609
H	-2.613411	-1.508853	-0.899609
H	2.613411	1.508853	0.899609
H	-2.613411	1.508853	0.899609
H	0.000000	-3.017707	0.899609

$[Fe(Tb^{3,5\text{-}NH2})_2]$ $^1A_{1g}$ D_{3d} OPBE

Fe	0.000000	0.000000	0.000000
N	0.000000	1.628716	1.194416
N	0.000000	1.437761	2.566020
N	1.410510	-0.814358	1.194416
N	1.245138	-0.718881	2.566020
N	-1.410510	-0.814358	1.194416
N	-1.245138	-0.718881	2.566020
C	0.000000	2.960155	1.010324
C	0.000000	3.637621	2.248662
C	0.000000	2.627719	3.200695
C	2.563570	-1.480078	1.010324
C	3.150272	-1.818810	2.248662
C	2.275671	-1.313859	3.200695
C	-2.563570	-1.480078	1.010324
C	-3.150272	-1.818810	2.248662
C	-2.275671	-1.313859	3.200695
H	0.000000	4.708118	2.418840
N	0.000000	2.737268	4.567829
H	4.077350	-2.354059	2.418840
N	3.059606	-1.766464	-0.219394
N	2.370544	-1.368634	4.567829
N	0.000000	3.532929	-0.219394
H	0.000000	0.000000	4.295437
H	-4.077350	-2.354059	2.418840
N	-2.370544	-1.368634	4.567829
N	-3.059606	-1.766464	-0.219394
B	0.000000	0.000000	3.079287
N	-1.410510	0.814358	-1.194416
N	-1.245138	0.718881	-2.566020
N	1.410510	0.814358	-1.194416
N	1.245138	0.718881	-2.566020
N	0.000000	-1.628716	-1.194416
N	0.000000	-1.437761	-2.566020
C	-2.563570	1.480078	-1.010324
C	-3.150272	1.818810	-2.248662
C	-2.275671	1.313859	-3.200695
C	2.563570	1.480078	-1.010324
C	3.150272	1.818810	-2.248662
C	2.275671	1.313859	-3.200695
C	0.000000	-2.960155	-1.010324
C	0.000000	-3.637621	-2.248662
C	0.000000	-2.627719	-3.200695
H	-4.077350	2.354059	-2.418840
N	-2.370544	1.368634	-4.567829
H	4.077350	2.354059	-2.418840
N	3.059606	1.766464	0.219394
N	2.370544	1.368634	-4.567829
N	-3.059606	1.766464	0.219394
H	0.000000	0.000000	-4.295437
H	0.000000	-4.708118	-2.418840
N	0.000000	-2.737268	-4.567829
N	0.000000	-3.532929	0.219394
B	0.000000	0.000000	-3.079287
H	0.000000	3.642445	4.994221
H	0.000000	1.921345	5.147322
H	3.154450	-1.821223	4.994221
H	1.663934	-0.960673	5.147322
H	-3.154450	-1.821223	4.994221
H	-1.663934	-0.960673	5.147322
H	-3.154450	1.821223	-4.994221
H	-1.663934	0.960673	-5.147322
H	3.154450	1.821223	-4.994221
H	1.663934	0.960673	-5.147322
H	0.000000	-3.642445	-4.994221
H	0.000000	-1.921345	-5.147322
H	0.000000	4.528819	-0.309492
H	3.922072	-2.264409	-0.309492
H	-3.922072	-2.264409	-0.309492
H	-3.922072	2.264409	0.309492
H	3.922072	2.264409	0.309492
H	0.000000	-4.528819	0.309492
H	2.559149	-1.477525	-1.039705
H	0.000000	2.955051	-1.039705
H	-2.559149	-1.477525	-1.039705
H	2.559149	1.477525	1.039705
H	-2.559149	1.477525	1.039705
H	0.000000	-2.955051	1.039705

$[Fe(Tb^{3,5\text{-}NO2})_2]$ $^5A_{1g}$ D_{3d} OPBE

Fe	0.000000	0.000000	0.000000
N	0.000000	1.802512	1.457748
N	0.000000	1.481176	2.758865
N	1.561021	-0.901256	1.457748
N	1.282736	-0.740588	2.758865
N	-1.561021	-0.901256	1.457748
N	-1.282736	-0.740588	2.758865
C	0.000000	3.145572	1.412391
C	0.000000	3.718077	2.671786
C	0.000000	2.628145	3.508633
C	2.724145	-1.572786	1.412391
C	3.219949	-1.859038	2.671786
C	2.276041	-1.314073	3.508633
C	-2.724145	-1.572786	1.412391
C	-3.219949	-1.859038	2.671786
C	-2.276041	-1.314073	3.508633
H	0.000000	4.762815	2.939170
N	0.000000	2.780904	4.968687

H	4.124718	-2.381407	2.939170
N	3.402770	-1.964590	0.192404
N	2.408334	-1.390452	4.968687
N	0.000000	3.929181	0.192404
H	0.000000	0.000000	4.396370
H	-4.124718	-2.381407	2.939170
N	-2.408334	-1.390452	4.968687
N	-3.402770	-1.964590	0.192404
B	0.000000	0.000000	3.231210
N	-1.561021	0.901256	-1.457748
N	-1.282736	0.740588	-2.758865
N	1.561021	0.901256	-1.457748
N	1.282736	0.740588	-2.758865
N	0.000000	-1.802512	-1.457748
N	0.000000	-1.481176	-2.758865
C	-2.724145	1.572786	-1.412391
C	-3.219949	1.859038	-2.671786
C	-2.276041	1.314073	-3.508633
C	2.724145	1.572786	-1.412391
C	3.219949	1.859038	-2.671786
C	2.276041	1.314073	-3.508633
C	0.000000	-3.145572	-1.412391
C	0.000000	-3.718077	-2.671786
C	0.000000	-2.628145	-3.508633
H	-4.124718	2.381407	-2.939170
N	-2.408334	1.390452	-4.968687
H	4.124718	2.381407	-2.939170
N	3.402770	1.964590	-0.192404
N	2.408334	1.390452	-4.968687
N	-3.402770	1.964590	-0.192404
H	0.000000	0.000000	-4.396370
H	0.000000	-4.762815	-2.939170
N	0.000000	-2.780904	-4.968687
N	0.000000	-3.929181	-0.192404
B	0.000000	0.000000	-3.231210
O	0.000000	3.946635	5.344018
O	0.000000	1.798997	5.685785
O	3.417886	-1.973317	5.344018
O	1.557977	-0.899499	5.685785
O	-3.417886	-1.973317	5.344018
O	-1.557977	-0.899499	5.685785
O	-3.417886	1.973317	-5.344018
O	-1.557977	0.899499	-5.685785
O	3.417886	1.973317	-5.344018
O	1.557977	0.899499	-5.685785
O	0.000000	-3.946635	-5.344018
O	0.000000	-1.798997	-5.685785
O	0.000000	5.143365	0.343200
O	4.454285	-2.571683	0.343200
O	-4.454285	-2.571683	0.343200
O	-4.454285	2.571683	-0.343200
O	4.454285	2.571683	-0.343200
O	0.000000	-5.143365	-0.343200
O	2.891501	-1.669409	-0.877490
O	0.000000	3.338818	-0.877490
O	-2.891501	-1.669409	-0.877490
O	2.891501	1.669409	0.877490
O	-2.891501	1.669409	0.877490
O	0.000000	-3.338818	0.877490

$[Fe(Tb^{3,5\text{-}NO2})_2]$ ^3E_g D_{3d} OPBE

Fe	0.000000	0.000000	0.000000
N	0.000000	1.741899	1.263986
N	0.000000	1.469155	2.575665
N	1.508528	-0.870949	1.263986
N	1.272326	-0.734577	2.575665
N	-1.508528	-0.870949	1.263986
N	-1.272326	-0.734577	2.575665
C	0.000000	3.090200	1.167718
C	0.000000	3.696801	2.411562
C	0.000000	2.638388	3.285004
C	2.676192	-1.545100	1.167718
C	3.201523	-1.848400	2.411562
C	2.284911	-1.319194	3.285004
C	-2.676192	-1.545100	1.167718
C	-3.201523	-1.848400	2.411562
C	-2.284911	-1.319194	3.285004
H	0.000000	4.749889	2.643306
N	0.000000	2.834229	4.736589
H	4.113524	-2.374944	2.643306
N	3.357851	-1.938656	-0.054702
N	2.454514	-1.417114	4.736589
N	0.000000	3.877313	-0.054702
H	0.000000	0.000000	4.237188
H	-4.113524	-2.374944	2.643306
N	-2.454514	-1.417114	4.736589
N	-3.357851	-1.938656	-0.054702
B	0.000000	0.000000	3.071705
N	-1.508528	0.870949	-1.263986
N	-1.272326	0.734577	-2.575665
N	1.508528	0.870949	-1.263986
N	1.272326	0.734577	-2.575665
N	0.000000	-1.741899	-1.263986
N	0.000000	-1.469155	-2.575665
C	-2.676192	1.545100	-1.167718
C	-3.201523	1.848400	-2.411562
C	-2.284911	1.319194	-3.285004
C	2.676192	1.545100	-1.167718
C	3.201523	1.848400	-2.411562
C	2.284911	1.319194	-3.285004
C	0.000000	-3.090200	-1.167718
C	0.000000	-3.696801	-2.411562
C	0.000000	-2.638388	-3.285004
H	-4.113524	2.374944	-2.643306
N	-2.454514	1.417114	-4.736589
H	4.113524	2.374944	-2.643306
N	3.357851	1.938656	0.054702
N	2.454514	1.417114	-4.736589
N	-3.357851	1.938656	0.054702
H	0.000000	0.000000	-4.237188
H	0.000000	-4.749889	-2.643306
N	0.000000	-2.834229	-4.736589
N	0.000000	-3.877313	0.054702
B	0.000000	0.000000	-3.071705
O	0.000000	4.010706	5.077574
O	0.000000	1.872539	5.480915
O	3.473374	-2.005353	5.077574
O	1.621666	-0.936269	5.480915
O	-3.473374	-2.005353	5.077574

O	-1.621666	-0.936269	5.480915
O	-3.473374	2.005353	-5.077574
O	-1.621666	0.936269	-5.480915
O	3.473374	2.005353	-5.077574
O	1.621666	0.936269	-5.480915
O	0.000000	-4.010706	-5.077574
O	0.000000	-1.872539	-5.480915
O	0.000000	5.090401	0.109815
O	4.408417	-2.545200	0.109815
O	-4.408417	-2.545200	0.109815
O	-4.408417	2.545200	-0.109815
O	4.408417	2.545200	-0.109815
O	0.000000	-5.090401	-0.109815
O	2.862440	-1.652631	-1.133033
O	0.000000	3.305261	-1.133033
O	-2.862440	-1.652631	-1.133033
O	2.862440	1.652631	1.133033
O	-2.862440	1.652631	1.133033
O	0.000000	-3.305261	1.133033

$[Fe(Tb^{3,5\text{-}NO2})_2]$ $^1A_{1g}$ D_{3d} OPBE

Fe	0.000000	0.000000	0.000000
N	0.000000	1.666512	1.128802
N	0.000000	1.450516	2.450809
N	1.443242	-0.833256	1.128802
N	1.256184	-0.725258	2.450809
N	-1.443242	-0.833256	1.128802
N	-1.256184	-0.725258	2.450809
C	0.000000	3.018125	0.977768
C	0.000000	3.663744	2.203595
C	0.000000	2.640977	3.115161
C	2.613773	-1.509062	0.977768
C	3.172896	-1.831872	2.203595
C	2.287153	-1.320489	3.115161
C	-2.613773	-1.509062	0.977768
C	-3.172896	-1.831872	2.203595
C	-2.287153	-1.320489	3.115161
H	0.000000	4.724690	2.394566
N	0.000000	2.875283	4.558202
H	4.091702	-2.362345	2.394566
N	3.293282	-1.901377	-0.252503
N	2.490068	-1.437641	4.558202
N	0.000000	3.802755	-0.252503
H	0.000000	0.000000	4.140815
H	-4.091702	-2.362345	2.394566
N	-2.490068	-1.437641	4.558202
N	-3.293282	-1.901377	-0.252503
B	0.000000	0.000000	2.975318
N	-1.443242	0.833256	-1.128802
N	-1.256184	0.725258	-2.450809
N	1.443242	0.833256	-1.128802
N	1.256184	0.725258	-2.450809
N	0.000000	-1.666512	-1.128802
N	0.000000	-1.450516	-2.450809
C	-2.613773	1.509062	-0.977768
C	-3.172896	1.831872	-2.203595
C	-2.287153	1.320489	-3.115161
C	2.613773	1.509062	-0.977768
C	3.172896	1.831872	-2.203595
C	2.287153	1.320489	-3.115161
C	0.000000	-3.018125	-0.977768
C	0.000000	-3.663744	-2.203595
C	0.000000	-2.640977	-3.115161
H	-4.091702	2.362345	-2.394566
N	-2.490068	1.437641	-4.558202
H	4.091702	2.362345	-2.394566
N	3.293282	1.901377	0.252503
N	2.490068	1.437641	-4.558202
N	-3.293282	1.901377	0.252503
H	0.000000	0.000000	-4.140815
H	0.000000	-4.724690	-2.394566
N	0.000000	-2.875283	-4.558202
N	0.000000	-3.802755	0.252503
B	0.000000	0.000000	-2.975318
O	0.000000	4.060558	4.866986
O	0.000000	1.932199	5.327328
O	3.516546	-2.030279	4.866986
O	1.673333	-0.966099	5.327328
O	-3.516546	-2.030279	4.866986
O	-1.673333	-0.966099	5.327328
O	-3.516546	2.030279	-4.866986
O	-1.673333	0.966099	-5.327328
O	3.516546	2.030279	-4.866986
O	1.673333	0.966099	-5.327328
O	0.000000	-4.060558	-4.866986
O	0.000000	-1.932199	-5.327328
O	0.000000	5.015011	-0.082191
O	4.343127	-2.507505	-0.082191
O	-4.343127	-2.507505	-0.082191
O	-4.343127	2.507505	0.082191
O	4.343127	2.507505	0.082191
O	0.000000	-5.015011	0.082191
O	2.807845	-1.621110	-1.335667
O	0.000000	3.242220	-1.335667
O	-2.807845	-1.621110	-1.335667
O	2.807845	1.621110	1.335667
O	-2.807845	1.621110	1.335667
O	0.000000	-3.242220	1.335667

$[Co(Tb^{3CH3})_2]^+$ $^5A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.49336201	0.86219325	1.26730119
N	1.25304674	0.72344668	2.58797573
N	0.00000000	-1.72438598	1.26730119
N	0.00000000	-1.44689337	2.58797573
N	-1.49336201	0.86219325	1.26730119
N	-1.25304674	0.72344668	2.58797573
C	2.66769205	1.54019261	1.14641912
C	3.16006820	1.82446610	2.42506799
C	2.23547119	1.29065008	3.30628728
C	0.00000000	-3.08038574	1.14641912
C	0.00000000	-3.64893272	2.42506799
C	0.00000000	-2.58130016	3.30628728
C	-2.66769205	1.54019261	1.14641912
C	-3.16006820	1.82446610	2.42506799
C	-2.23547119	1.29065008	3.30628728
H	4.07374934	2.35198014	2.67253349
H	2.20916843	1.27546375	4.38863520

H	0.00000000	-4.70396028	2.67253349
C	0.00000000	-3.82667119	-0.14067807
H	0.00000000	-2.55092803	4.38863520
C	3.31399421	1.91333559	-0.14067807
H	0.00000000	0.00000000	4.30189723
H	-4.07374934	2.35198014	2.67253349
H	-2.20916843	1.27546375	4.38863520
C	-3.31399421	1.91333559	-0.14067807
B	0.00000000	0.00000000	3.10048019
N	0.00000000	1.72438598	-1.26730119
N	0.00000000	1.44689337	-2.58797573
N	1.49336201	-0.86219325	-1.26730119
N	1.25304674	-0.72344668	-2.58797573
N	-1.49336201	-0.86219325	-1.26730119
N	-1.25304674	-0.72344668	-2.58797573
C	0.00000000	3.08038574	-1.14641912
C	0.00000000	3.64893272	-2.42506799
C	0.00000000	2.58130016	-3.30628728
C	2.66769205	-1.54019261	-1.14641912
C	3.16006820	-1.82446610	-2.42506799
C	2.23547119	-1.29065008	-3.30628728
C	-2.66769205	-1.54019261	-1.14641912
C	-3.16006820	-1.82446610	-2.42506799
C	-2.23547119	-1.29065008	-3.30628728
H	0.00000000	4.70396028	-2.67253349
H	0.00000000	2.55092803	-4.38863520
H	4.07374934	-2.35198014	-2.67253349
C	3.31399421	-1.91333559	0.14067807
H	2.20916843	-1.27546375	-4.38863520
C	0.00000000	3.82667119	0.14067807
H	0.00000000	0.00000000	-4.30189723
H	-4.07374934	-2.35198014	-2.67253349
H	-2.20916843	-1.27546375	-4.38863520
C	-3.31399421	-1.91333559	0.14067807
B	0.00000000	0.00000000	-3.10048019
H	-0.87832946	-3.60026694	-0.75035958
H	0.00000000	-4.89947646	0.06691711
H	0.87832946	-3.60026694	-0.75035958
H	4.24307071	2.44973823	0.06691711
H	2.67875767	2.56078925	-0.75035958
H	3.55708713	1.03947769	-0.75035958
H	-4.24307071	2.44973823	0.06691711
H	-3.55708713	1.03947769	-0.75035958
H	-2.67875767	2.56078925	-0.75035958
H	3.55708713	-1.03947769	0.75035958
H	4.24307071	-2.44973823	-0.06691711
H	2.67875767	-2.56078925	0.75035958
H	-2.67875767	-2.56078925	0.75035958
H	-4.24307071	-2.44973823	-0.06691711
H	-3.55708713	-1.03947769	0.75035958
H	-0.87832946	3.60026694	0.75035958
H	0.00000000	4.89947646	-0.06691711
H	0.87832946	3.60026694	0.75035958

$[Co(Tb^{3CH3})_2]^+$ ^3E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.45781770	0.84167176	1.19664756
N	1.24454075	0.71853592	2.52170051
N	0.00000000	-1.68334299	1.19664756
N	0.00000000	-1.43707184	2.52170051
N	-1.45781770	0.84167176	1.19664756
N	-1.24454075	0.71853592	2.52170051
C	2.62666335	1.51650452	1.03561310
C	3.14410133	1.81524783	2.30389275
C	2.24158107	1.29417758	3.21178045
C	0.00000000	-3.03300956	1.03561310
C	0.00000000	-3.63049566	2.30389275
C	0.00000000	-2.58835462	3.21178045
C	-2.62666335	1.51650452	1.03561310
C	-3.14410133	1.81524783	2.30389275
C	-2.24158107	1.29417758	3.21178045
H	4.06361824	2.34613114	2.52069084
H	2.23643217	1.29120466	4.29436386
H	0.00000000	-4.69226229	2.52069084
C	0.00000000	-3.76546549	-0.25926034
H	0.00000000	-2.58240931	4.29436386
C	3.26098865	1.88273274	-0.25926034
H	0.00000000	0.00000000	4.25057391
H	-4.06361824	2.34613114	2.52069084
H	-2.23643217	1.29120466	4.29436386
C	-3.26098865	1.88273274	-0.25926034
B	0.00000000	0.00000000	3.05023904
N	0.00000000	1.68334299	-1.19664756
N	0.00000000	1.43707184	-2.52170051
N	1.45781770	-0.84167176	-1.19664756
N	1.24454075	-0.71853592	-2.52170051
N	-1.45781770	-0.84167176	-1.19664756
N	-1.24454075	-0.71853592	-2.52170051
C	0.00000000	3.03300956	-1.03561310
C	0.00000000	3.63049566	-2.30389275
C	0.00000000	2.58835462	-3.21178045
C	2.62666335	-1.51650452	-1.03561310
C	3.14410133	-1.81524783	-2.30389275
C	2.24158107	-1.29417758	-3.21178045
C	-2.62666335	-1.51650452	-1.03561310
C	-3.14410133	-1.81524783	-2.30389275
C	-2.24158107	-1.29417758	-3.21178045
H	0.00000000	4.69226229	-2.52069084
H	0.00000000	2.58240931	-4.29436386
H	4.06361824	-2.34613114	-2.52069084
C	3.26098865	-1.88273274	0.25926034
H	2.23643217	-1.29120466	-4.29436386
C	0.00000000	3.76546549	0.25926034
H	0.00000000	0.00000000	-4.25057391
H	-4.06361824	-2.34613114	-2.52069084
H	-2.23643217	-1.29120466	-4.29436386
C	-3.26098865	-1.88273274	0.25926034
B	0.00000000	0.00000000	-3.05023904
H	-0.87987254	-3.53773194	-0.86596999
H	0.00000000	-4.83938997	-0.05681617
H	0.87987254	-3.53773194	-0.86596999
H	4.19103459	2.41969525	-0.05681617
H	2.62382908	2.53085793	-0.86596999
H	3.50370214	1.00687402	-0.86596999
H	-4.19103459	2.41969525	-0.05681617
H	-3.50370214	1.00687402	-0.86596999
H	-2.62382908	2.53085793	-0.86596999
H	3.50370214	-1.00687402	0.86596999
H	4.19103459	-2.41969525	0.05681617

H	2.62382908	-2.53085793	0.86596999
H	-2.62382908	-2.53085793	0.86596999
H	-4.19103459	-2.41969525	0.05681617
H	-3.50370214	-1.00687402	0.86596999
H	-0.87987254	3.53773194	0.86596999
H	0.00000000	4.83938997	0.05681617
H	0.87987254	3.53773194	0.86596999

$[Co(Tb^{3CH3})_2]^+$ $^1A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.41460985	0.81672529	1.11080390
N	1.23458904	0.71279011	2.44208633
N	0.00000000	-1.63345110	1.11080390
N	0.00000000	-1.42558022	2.44208633
N	-1.41460985	0.81672529	1.11080390
N	-1.23458904	0.71279011	2.44208633
C	2.57669420	1.48765483	0.90533760
C	3.12401270	1.80364985	2.15937073
C	2.24805343	1.29791410	3.09780203
C	0.00000000	-2.97531019	0.90533760
C	0.00000000	-3.60729917	2.15937073
C	0.00000000	-2.59582819	3.09780203
C	-2.57669420	1.48765483	0.90533760
C	-3.12401270	1.80364985	2.15937073
C	-2.24805343	1.29791410	3.09780203
H	4.04914365	2.33777438	2.34062664
H	2.26835426	1.30963484	4.17992452
H	0.00000000	-4.67554822	2.34062664
C	0.00000000	-3.69053399	-0.39959709
H	0.00000000	-2.61926969	4.17992452
C	3.19609617	1.84526700	-0.39959709
H	0.00000000	0.00000000	4.18898985
H	-4.04914365	2.33777438	2.34062664
H	-2.26835426	1.30963484	4.17992452
C	-3.19609617	1.84526700	-0.39959709
B	0.00000000	0.00000000	2.98986839
N	0.00000000	1.63345110	-1.11080390
N	0.00000000	1.42558022	-2.44208633
N	1.41460985	-0.81672529	-1.11080390
N	1.23458904	-0.71279011	-2.44208633
N	-1.41460985	-0.81672529	-1.11080390
N	-1.23458904	-0.71279011	-2.44208633
C	0.00000000	2.97531019	-0.90533760
C	0.00000000	3.60729917	-2.15937073
C	0.00000000	2.59582819	-3.09780203
C	2.57669420	-1.48765483	-0.90533760
C	3.12401270	-1.80364985	-2.15937073
C	2.24805343	-1.29791410	-3.09780203
C	-2.57669420	-1.48765483	-0.90533760
C	-3.12401270	-1.80364985	-2.15937073
C	-2.24805343	-1.29791410	-3.09780203
H	0.00000000	4.67554822	-2.34062664
H	0.00000000	2.61926969	-4.17992452
H	4.04914365	-2.33777438	-2.34062664
C	3.19609617	-1.84526700	0.39959709
H	2.26835426	-1.30963484	-4.17992452
C	0.00000000	3.69053399	0.39959709
H	0.00000000	0.00000000	-4.18898985
H	-4.04914365	-2.33777438	-2.34062664
H	-2.26835426	-1.30963484	-4.17992452
C	-3.19609617	-1.84526700	0.39959709
B	0.00000000	0.00000000	-2.98986839
H	-0.88172677	-3.46052445	-1.00279988
H	0.00000000	-4.76603277	-0.20490378
H	0.88172677	-3.46052445	-1.00279988
H	4.12750528	2.38301639	-0.20490378
H	2.55603830	2.49385997	-1.00279988
H	3.43776560	0.96666396	-1.00279988
H	-4.12750528	2.38301639	-0.20490378
H	-3.43776560	0.96666396	-1.00279988
H	-2.55603830	2.49385997	-1.00279988
H	3.43776560	-0.96666396	1.00279988
H	4.12750528	-2.38301639	0.20490378
H	2.55603830	-2.49385997	1.00279988
H	-2.55603830	-2.49385997	1.00279988
H	-4.12750528	-2.38301639	0.20490378
H	-3.43776560	-0.96666396	1.00279988
H	-0.88172677	3.46052445	1.00279988
H	0.00000000	4.76603277	0.20490378
H	0.88172677	3.46052445	1.00279988

$[Co(Tb^{3CF3})_2]^+$ $^5A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.56304301	0.90242342	1.19561037
N	1.26873685	0.73250567	2.50070699
N	0.00000000	-1.80484685	1.19561037
N	0.00000000	-1.46501134	2.50070699
N	-1.56304301	0.90242342	1.19561037
N	-1.26873685	0.73250567	2.50070699
C	2.74391792	1.58420163	1.16202985
C	3.17943026	1.83564497	2.46202519
C	2.21321611	1.27780113	3.28098996
C	0.00000000	-3.16840327	1.16202985
C	0.00000000	-3.67128940	2.46202519
C	0.00000000	-2.55560225	3.28098996
C	-2.74391792	1.58420163	1.16202985
C	-3.17943026	1.83564497	2.46202519
C	-2.21321611	1.27780113	3.28098996
H	4.07754830	2.35417358	2.76884269
H	2.13963242	1.23531719	4.35983684
H	0.00000000	-4.70834716	2.76884269
C	0.00000000	-4.10124803	-0.04922513
H	0.00000000	-2.47063438	4.35983684
C	3.55178530	2.05062428	-0.04922513
H	0.00000000	0.00000000	4.18054683
H	-4.07754830	2.35417358	2.76884269
H	-2.13963242	1.23531719	4.35983684
C	-3.55178530	2.05062428	-0.04922513
B	0.00000000	0.00000000	2.98097609
N	0.00000000	1.80484685	-1.19561037
N	0.00000000	1.46501134	-2.50070699
N	1.56304301	-0.90242342	-1.19561037
N	1.26873685	-0.73250567	-2.50070699
N	-1.56304301	-0.90242342	-1.19561037
N	-1.26873685	-0.73250567	-2.50070699
C	0.00000000	3.16840327	-1.16202985
C	0.00000000	3.67128940	-2.46202519
C	0.00000000	2.55560225	-3.28098996

C	2.74391792	-1.58420163	-1.16202985
C	3.17943026	-1.83564497	-2.46202519
C	2.21321611	-1.27780113	-3.28098996
C	-2.74391792	-1.58420163	-1.16202985
C	-3.17943026	-1.83564497	-2.46202519
C	-2.21321611	-1.27780113	-3.28098996
H	0.00000000	4.70834716	-2.76884269
H	0.00000000	2.47063438	-4.35983684
H	4.07754830	-2.35417358	-2.76884269
C	3.55178530	-2.05062428	0.04922513
H	2.13963242	-1.23531719	-4.35983684
C	0.00000000	4.10124803	0.04922513
H	0.00000000	0.00000000	-4.18054683
H	-4.07754830	-2.35417358	-2.76884269
H	-2.13963242	-1.23531719	-4.35983684
C	-3.55178530	-2.05062428	0.04922513
B	0.00000000	0.00000000	-2.98097609
F	-1.07673229	-3.96944586	-0.84329316
F	0.00000000	-5.37563332	0.40679178
F	1.07673229	-3.96944586	-0.84329316
F	4.65543526	2.68781666	0.40679178
F	2.89927536	2.91720018	-0.84329316
F	3.97600712	1.05224567	-0.84329316
F	-4.65543526	2.68781666	0.40679178
F	-3.97600712	1.05224567	-0.84329316
F	-2.89927536	2.91720018	-0.84329316
F	3.97600712	-1.05224567	0.84329316
F	4.65543526	-2.68781666	-0.40679178
F	2.89927536	-2.91720018	0.84329316
F	-2.89927536	-2.91720018	0.84329316
F	-4.65543526	-2.68781666	-0.40679178
F	-3.97600712	-1.05224567	0.84329316
F	-1.07673229	3.96944586	0.84329316
F	0.00000000	5.37563332	-0.40679178
F	1.07673229	3.96944586	0.84329316

$[Co(Tb^{3CF3})_2]^+$ ^3E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.52331609	0.87948677	1.14539357
N	1.25827978	0.72646829	2.45510991
N	0.00000000	-1.75897353	1.14539357
N	0.00000000	-1.45293657	2.45510991
N	-1.52331609	0.87948677	1.14539357
N	-1.25827978	0.72646829	2.45510991
C	2.70327499	1.56073633	1.07194906
C	3.16392590	1.82669340	2.36254252
C	2.21928418	1.28130428	3.20836250
C	0.00000000	-3.12147318	1.07194906
C	0.00000000	-3.65338733	2.36254252
C	0.00000000	-2.56260856	3.20836250
C	-2.70327499	1.56073633	1.07194906
C	-3.16392590	1.82669340	2.36254252
C	-2.21928418	1.28130428	3.20836250
H	4.06904654	2.34926546	2.63987214
H	2.16606324	1.25057707	4.28862652
H	0.00000000	-4.69853039	2.63987214
C	0.00000000	-4.04199447	-0.14796643
H	0.00000000	-2.50115415	4.28862652
C	3.50046993	2.02099723	-0.14796643
H	0.00000000	0.00000000	4.15150294
H	-4.06904654	2.34926546	2.63987214
H	-2.16606324	1.25057707	4.28862652
C	-3.50046993	2.02099723	-0.14796643
B	0.00000000	0.00000000	2.95290377
N	0.00000000	1.75897353	-1.14539357
N	0.00000000	1.45293657	-2.45510991
N	1.52331609	-0.87948677	-1.14539357
N	1.25827978	-0.72646829	-2.45510991
N	-1.52331609	-0.87948677	-1.14539357
N	-1.25827978	-0.72646829	-2.45510991
C	0.00000000	3.12147318	-1.07194906
C	0.00000000	3.65338733	-2.36254252
C	0.00000000	2.56260856	-3.20836250
C	2.70327499	-1.56073633	-1.07194906
C	3.16392590	-1.82669340	-2.36254252
C	2.21928418	-1.28130428	-3.20836250
C	-2.70327499	-1.56073633	-1.07194906
C	-3.16392590	-1.82669340	-2.36254252
C	-2.21928418	-1.28130428	-3.20836250
H	0.00000000	4.69853039	-2.63987214
H	0.00000000	2.50115415	-4.28862652
H	4.06904654	-2.34926546	-2.63987214
C	3.50046993	-2.02099723	0.14796643
H	2.16606324	-1.25057707	-4.28862652
C	0.00000000	4.04199447	0.14796643
H	0.00000000	0.00000000	-4.15150294
H	-4.06904654	-2.34926546	-2.63987214
H	-2.16606324	-1.25057707	-4.28862652
C	-3.50046993	-2.02099723	0.14796643
B	0.00000000	0.00000000	-2.95290377
F	-1.07854843	-3.90459571	-0.93866889
F	0.00000000	-5.32042479	0.29562222
F	1.07854843	-3.90459571	-0.93866889
F	4.60762303	2.66021213	0.29562222
F	2.84220518	2.88634809	-0.93866889
F	3.92075308	1.01824762	-0.93866889
F	-4.60762303	2.66021213	0.29562222
F	-3.92075308	1.01824762	-0.93866889
F	-2.84220518	2.88634809	-0.93866889
F	3.92075308	-1.01824762	0.93866889
F	4.60762303	-2.66021213	-0.29562222
F	2.84220518	-2.88634809	0.93866889
F	-2.84220518	-2.88634809	0.93866889
F	-4.60762303	-2.66021213	-0.29562222
F	-3.92075308	-1.01824762	0.93866889
F	-1.07854843	3.90459571	0.93866889
F	0.00000000	5.32042479	-0.29562222
F	1.07854843	3.90459571	0.93866889

$[Co(Tb^{3CF3})_2]^+$ $^1A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.47804444	0.85334911	1.08195051
N	1.24615527	0.71946833	2.39802809
N	0.00000000	-1.70669876	1.08195051
N	0.00000000	-1.43893666	2.39802809
N	-1.47804444	0.85334911	1.08195051
N	-1.24615527	0.71946833	2.39802809
C	2.65856639	1.53492412	0.96785143

C	3.14403307	1.81520814	2.24823759
C	2.22337261	1.28366441	3.12134512
C	0.00000000	-3.06984771	0.96785143
C	0.00000000	-3.63041628	2.24823759
C	0.00000000	-2.56732935	3.12134512
C	-2.65856639	1.53492412	0.96785143
C	-3.14403307	1.81520814	2.24823759
C	-2.22337261	1.28366441	3.12134512
H	4.05497995	2.34114365	2.49664132
H	2.19202362	1.26556549	4.20250874
H	0.00000000	-4.68228783	2.49664132
C	0.00000000	-3.99290322	-0.25411197
H	0.00000000	-2.53113098	4.20250874
C	3.45795583	1.99645188	-0.25411197
H	0.00000000	0.00000000	4.11316987
H	-4.05497995	2.34114365	2.49664132
H	-2.19202362	1.26556549	4.20250874
C	-3.45795583	1.99645188	-0.25411197
B	0.00000000	0.00000000	2.91584125
N	0.00000000	1.70669876	-1.08195051
N	0.00000000	1.43893666	-2.39802809
N	1.47804444	-0.85334911	-1.08195051
N	1.24615527	-0.71946833	-2.39802809
N	-1.47804444	-0.85334911	-1.08195051
N	-1.24615527	-0.71946833	-2.39802809
C	0.00000000	3.06984771	-0.96785143
C	0.00000000	3.63041628	-2.24823759
C	0.00000000	2.56732935	-3.12134512
C	2.65856639	-1.53492412	-0.96785143
C	3.14403307	-1.81520814	-2.24823759
C	2.22337261	-1.28366441	-3.12134512
C	-2.65856639	-1.53492412	-0.96785143
C	-3.14403307	-1.81520814	-2.24823759
C	-2.22337261	-1.28366441	-3.12134512
H	0.00000000	4.68228783	-2.49664132
H	0.00000000	2.53113098	-4.20250874
H	4.05497995	-2.34114365	-2.49664132
C	3.45795583	-1.99645188	0.25411197
H	2.19202362	-1.26556549	-4.20250874
C	0.00000000	3.99290322	0.25411197
H	0.00000000	0.00000000	-4.11316987
H	-4.05497995	-2.34114365	-2.49664132
H	-2.19202362	-1.26556549	-4.20250874
C	-3.45795583	-1.99645188	0.25411197
B	0.00000000	0.00000000	-2.91584125
F	-1.07878603	-3.86323786	-1.04493033
F	0.00000000	-5.26957826	0.19478856
F	1.07878603	-3.86323786	-1.04493033
F	4.56358861	2.63478940	0.19478856
F	2.80626875	2.86587528	-1.04493033
F	3.88505478	0.99736259	-1.04493033
F	-4.56358861	2.63478940	0.19478856
F	-3.88505478	0.99736259	-1.04493033
F	-2.80626875	2.86587528	-1.04493033
F	3.88505478	-0.99736259	1.04493033
F	4.56358861	-2.63478940	-0.19478856
F	2.80626875	-2.86587528	1.04493033
F	-2.80626875	-2.86587528	1.04493033
F	-4.56358861	-2.63478940	-0.19478856
F	-3.88505478	-0.99736259	1.04493033
F	-1.07878603	3.86323786	1.04493033
F	0.00000000	5.26957826	-0.19478856
F	1.07878603	3.86323786	1.04493033

$[Co(Tb^{3NH2})_2]^+$ $^5A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.69165001	1.30065418
N	0.00000000	1.44521482	2.63837563
N	1.46501187	-0.84582474	1.30065418
N	1.25159257	-0.72260741	2.63837563
N	-1.46501187	-0.84582474	1.30065418
N	-1.25159257	-0.72260741	2.63837563
C	0.00000000	3.04509809	1.16550866
C	0.00000000	3.65674285	2.43639079
C	0.00000000	2.60231908	3.32513551
C	2.63713206	-1.52254878	1.16550866
C	3.16683214	-1.82837142	2.43639079
C	2.25367435	-1.30115954	3.32513551
C	-2.63713206	-1.52254878	1.16550866
C	-3.16683214	-1.82837142	2.43639079
C	-2.25367435	-1.30115954	3.32513551
H	0.00000000	4.71583396	2.66411746
H	0.00000000	2.59955413	4.40802796
H	4.08403231	-2.35791698	2.66411746
N	3.15577445	-1.82198743	-0.04441543
H	2.25127983	-1.29977733	4.40802796
N	0.00000000	3.64397433	-0.04441543
H	0.00000000	0.00000000	4.36067930
H	-4.08403231	-2.35791698	2.66411746
H	-2.25127983	-1.29977733	4.40802796
N	-3.15577445	-1.82198743	-0.04441543
B	0.00000000	0.00000000	3.15729954
N	-1.46501187	0.84582474	-1.30065418
N	-1.25159257	0.72260741	-2.63837563
N	1.46501187	0.84582474	-1.30065418
N	1.25159257	0.72260741	-2.63837563
N	0.00000000	-1.69165001	-1.30065418
N	0.00000000	-1.44521482	-2.63837563
C	-2.63713206	1.52254878	-1.16550866
C	-3.16683214	1.82837142	-2.43639079
C	-2.25367435	1.30115954	-3.32513551
C	2.63713206	1.52254878	-1.16550866
C	3.16683214	1.82837142	-2.43639079
C	2.25367435	1.30115954	-3.32513551
C	0.00000000	-3.04509809	-1.16550866
C	0.00000000	-3.65674285	-2.43639079
C	0.00000000	-2.60231908	-3.32513551
H	-4.08403231	2.35791698	-2.66411746
H	-2.25127983	1.29977733	-4.40802796
H	4.08403231	2.35791698	-2.66411746
N	3.15577445	1.82198743	0.04441543
H	2.25127983	1.29977733	-4.40802796
N	-3.15577445	1.82198743	0.04441543
H	0.00000000	0.00000000	-4.36067930
H	0.00000000	-4.71583396	-2.66411746
H	0.00000000	-2.59955413	-4.40802796
N	0.00000000	-3.64397433	0.04441543
B	0.00000000	0.00000000	-3.15729954
H	0.00000000	4.64449134	-0.11171090

H	4.02224769	-2.32224567	-0.11171090
H	-4.02224769	-2.32224567	-0.11171090
H	-4.02224769	2.32224567	0.11171090
H	4.02224769	2.32224567	0.11171090
H	0.00000000	-4.64449134	0.11171090
H	2.68186342	-1.54837475	-0.88713655
H	0.00000000	3.09674949	-0.88713655
H	-2.68186342	-1.54837475	-0.88713655
H	2.68186342	1.54837475	0.88713655
H	-2.68186342	1.54837475	0.88713655
H	0.00000000	-3.09674949	0.88713655

$[Co(Tb^{3NH2})_2]^+$ ^3E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.65150504	1.22554805
N	0.00000000	1.43536630	2.56963762
N	1.43024545	-0.82575252	1.22554805
N	1.24306382	-0.71768288	2.56963762
N	-1.43024545	-0.82575252	1.22554805
N	-1.24306382	-0.71768288	2.56963762
C	0.00000000	2.99863315	1.05112699
C	0.00000000	3.63791631	2.30965496
C	0.00000000	2.60830619	3.22615344
C	2.59689237	-1.49931684	1.05112699
C	3.15052766	-1.81895789	2.30965496
C	2.25885976	-1.30415310	3.22615344
C	-2.59689237	-1.49931684	1.05112699
C	-3.15052766	-1.81895789	2.30965496
C	-2.25885976	-1.30415310	3.22615344
H	0.00000000	4.70295590	2.50795937
H	0.00000000	2.63145822	4.30866541
H	4.07287937	-2.35147795	2.50795937
N	3.10232384	-1.79112740	-0.16571186
H	2.27890976	-1.31572938	4.30866541
N	0.00000000	3.58225533	-0.16571186
H	0.00000000	0.00000000	4.30631745
H	-4.07287937	-2.35147795	2.50795937
H	-2.27890976	-1.31572938	4.30866541
N	-3.10232384	-1.79112740	-0.16571186
B	0.00000000	0.00000000	3.10379019
N	-1.43024545	0.82575252	-1.22554805
N	-1.24306382	0.71768288	-2.56963762
N	1.43024545	0.82575252	-1.22554805
N	1.24306382	0.71768288	-2.56963762
N	0.00000000	-1.65150504	-1.22554805
N	0.00000000	-1.43536630	-2.56963762
C	-2.59689237	1.49931684	-1.05112699
C	-3.15052766	1.81895789	-2.30965496
C	-2.25885976	1.30415310	-3.22615344
C	2.59689237	1.49931684	-1.05112699
C	3.15052766	1.81895789	-2.30965496
C	2.25885976	1.30415310	-3.22615344
C	0.00000000	-2.99863315	-1.05112699
C	0.00000000	-3.63791631	-2.30965496
C	0.00000000	-2.60830619	-3.22615344
H	-4.07287937	2.35147795	-2.50795937
H	-2.27890976	1.31572938	-4.30866541
H	4.07287937	2.35147795	-2.50795937
N	3.10232384	1.79112740	0.16571186
H	2.27890976	1.31572938	-4.30866541
N	-3.10232384	1.79112740	0.16571186
H	0.00000000	0.00000000	-4.30631745
H	0.00000000	-4.70295590	-2.50795937
H	0.00000000	-2.63145822	-4.30866541
N	0.00000000	-3.58225533	0.16571186
B	0.00000000	0.00000000	-3.10379019
H	0.00000000	4.58203625	-0.24073490
H	3.96815995	-2.29101839	-0.24073490
H	-3.96815995	-2.29101839	-0.24073490
H	-3.96815995	2.29101839	0.24073490
H	3.96815995	2.29101839	0.24073490
H	0.00000000	-4.58203625	0.24073490
H	2.62256487	-1.51413857	-1.00303484
H	0.00000000	3.02827713	-1.00303484
H	-2.62256487	-1.51413857	-1.00303484
H	2.62256487	1.51413857	1.00303484
H	-2.62256487	1.51413857	1.00303484
H	0.00000000	-3.02827713	1.00303484

$[Co(Tb^{3NH2})_2]^+$ $^1A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.61059170	1.13695690
N	0.00000000	1.42392337	2.49009487
N	1.39481333	-0.80529612	1.13695690
N	1.23315338	-0.71196142	2.49009487
N	-1.39481333	-0.80529612	1.13695690
N	-1.23315338	-0.71196142	2.49009487
C	0.00000000	2.95001234	0.92100178
C	0.00000000	3.61517703	2.16653527
C	0.00000000	2.61251262	3.11134526
C	2.55478573	-1.47500644	0.92100178
C	3.13083486	-1.80758852	2.16653527
C	2.26250209	-1.30625605	3.11134526
C	-2.55478573	-1.47500644	0.92100178
C	-3.13083486	-1.80758852	2.16653527
C	-2.26250209	-1.30625605	3.11134526
H	0.00000000	4.68542320	2.33367802
H	0.00000000	2.66356447	4.19277612
H	4.05769569	-2.34271160	2.33367802
N	3.05472647	-1.76364723	-0.29830462
H	2.30671432	-1.33178197	4.19277612
N	0.00000000	3.52729392	-0.29830462
H	0.00000000	0.00000000	4.24145619
H	-4.05769569	-2.34271160	2.33367802
H	-2.30671432	-1.33178197	4.19277612
N	-3.05472647	-1.76364723	-0.29830462
B	0.00000000	0.00000000	3.04007620
N	-1.39481333	0.80529612	-1.13695690
N	-1.23315338	0.71196142	-2.49009487
N	1.39481333	0.80529612	-1.13695690
N	1.23315338	0.71196142	-2.49009487
N	0.00000000	-1.61059170	-1.13695690
N	0.00000000	-1.42392337	-2.49009487
C	-2.55478573	1.47500644	-0.92100178
C	-3.13083486	1.80758852	-2.16653527
C	-2.26250209	1.30625605	-3.11134526
C	2.55478573	1.47500644	-0.92100178
C	3.13083486	1.80758852	-2.16653527

C	2.26250209	1.30625605	-3.11134526
C	0.00000000	-2.95001234	-0.92100178
C	0.00000000	-3.61517703	-2.16653527
C	0.00000000	-2.61251262	-3.11134526
H	-4.05769569	2.34271160	-2.33367802
H	-2.30671432	1.33178197	-4.19277612
H	4.05769569	2.34271160	-2.33367802
N	3.05472647	1.76364723	0.29830462
H	2.30671432	1.33178197	-4.19277612
N	-3.05472647	1.76364723	0.29830462
H	0.00000000	0.00000000	-4.24145619
H	0.00000000	-4.68542320	-2.33367802
H	0.00000000	-2.66356447	-4.19277612
N	0.00000000	-3.52729392	0.29830462
B	0.00000000	0.00000000	-3.04007620
H	0.00000000	4.52698118	-0.36997427
H	3.92048056	-2.26349059	-0.36997427
H	-3.92048056	-2.26349059	-0.36997427
H	-3.92048056	2.26349059	0.36997427
H	3.92048056	2.26349059	0.36997427
H	0.00000000	-4.52698118	0.36997427
H	2.57924748	-1.48912912	-1.13740882
H	0.00000000	2.97825824	-1.13740882
H	-2.57924748	-1.48912912	-1.13740882
H	2.57924748	1.48912912	1.13740882
H	-2.57924748	1.48912912	1.13740882
H	0.00000000	-2.97825824	1.13740882

$[Co(Tb^{3NO2})_2]^+$ $^5A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.77193890	1.31647975
N	0.00000000	1.44899473	2.61837379
N	1.53454417	-0.88596919	1.31647975
N	1.25486606	-0.72449763	2.61837379
N	-1.53454417	-0.88596919	1.31647975
N	-1.25486606	-0.72449763	2.61837379
C	0.00000000	3.12668611	1.30848071
C	0.00000000	3.65810865	2.59213718
C	0.00000000	2.54205902	3.40440838
C	2.70778993	-1.56334305	1.30848071
C	3.16801485	-1.82905406	2.59213718
C	2.20148795	-1.27102977	3.40440838
C	-2.70778993	-1.56334305	1.30848071
C	-3.16801485	-1.82905406	2.59213718
C	-2.20148795	-1.27102977	3.40440838
H	0.00000000	4.70244895	2.87059342
H	0.00000000	2.45024201	4.48271286
H	4.07244015	-2.35122448	2.87059342
N	3.42656662	-1.97832914	0.11784089
H	2.12197166	-1.22512100	4.48271286
N	0.00000000	3.95665882	0.11784089
H	0.00000000	0.00000000	4.31024500
H	-4.07244015	-2.35122448	2.87059342
H	-2.12197166	-1.22512100	4.48271286
N	-3.42656662	-1.97832914	0.11784089
B	0.00000000	0.00000000	3.11112724
N	-1.53454417	0.88596919	-1.31647975
N	-1.25486606	0.72449763	-2.61837379
N	1.53454417	0.88596919	-1.31647975
N	1.25486606	0.72449763	-2.61837379
N	0.00000000	-1.77193890	-1.31647975
N	0.00000000	-1.44899473	-2.61837379
C	-2.70778993	1.56334305	-1.30848071
C	-3.16801485	1.82905406	-2.59213718
C	-2.20148795	1.27102977	-3.40440838
C	2.70778993	1.56334305	-1.30848071
C	3.16801485	1.82905406	-2.59213718
C	2.20148795	1.27102977	-3.40440838
C	0.00000000	-3.12668611	-1.30848071
C	0.00000000	-3.65810865	-2.59213718
C	0.00000000	-2.54205902	-3.40440838
H	-4.07244015	2.35122448	-2.87059342
H	-2.12197166	1.22512100	-4.48271286
H	4.07244015	2.35122448	-2.87059342
N	3.42656662	1.97832914	-0.11784089
H	2.12197166	1.22512100	-4.48271286
N	-3.42656662	1.97832914	-0.11784089
H	0.00000000	0.00000000	-4.31024500
H	0.00000000	-4.70244895	-2.87059342
H	0.00000000	-2.45024201	-4.48271286
N	0.00000000	-3.95665882	-0.11784089
B	0.00000000	0.00000000	-3.11112724
O	0.00000000	5.16316283	0.32007868
O	4.47143027	-2.58158168	0.32007868
O	-4.47143027	-2.58158168	0.32007868
O	-4.47143027	2.58158168	-0.32007868
O	4.47143027	2.58158168	-0.32007868
O	0.00000000	-5.16316283	-0.32007868
O	2.95761398	-1.70757931	-0.97772799
O	0.00000000	3.41515862	-0.97772799
O	-2.95761398	-1.70757931	-0.97772799
O	2.95761398	1.70757931	0.97772799
O	-2.95761398	1.70757931	0.97772799
O	0.00000000	-3.41515862	0.97772799

$[Co(Tb^{3NO2})_2]^+$ ^3E_g D_{3d} OPBE

[Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.78513447	1.36674048
N	0.00000000	1.45309797	2.66251564
N	1.54597175	-0.89256750	1.36674048
N	1.25841948	-0.72654872	2.66251564
N	-1.54597175	-0.89256750	1.36674048
N	-1.25841948	-0.72654872	2.66251564
C	0.00000000	3.13526195	1.37365788
C	0.00000000	3.66102918	2.66568594
C	0.00000000	2.53998094	3.46384769
C	2.71521640	-1.56763098	1.37365788
C	3.17054432	-1.83051459	2.66568594
C	2.19968822	-1.26999047	3.46384769
C	-2.71521640	-1.56763098	1.37365788
C	-3.17054432	-1.83051459	2.66568594
C	-2.19968822	-1.26999047	3.46384769
H	0.00000000	4.70226533	2.95543429
H	0.00000000	2.43622357	4.54081546
H	4.07228087	-2.35113240	2.95543429
N	3.43127101	-1.98104541	0.19512617
H	2.10983128	-1.21811152	4.54081546
N	0.00000000	3.96209029	0.19512617

H	0.00000000	0.00000000	4.34831189
H	-4.07228087	-2.35113240	2.95543429
H	-2.10983128	-1.21811152	4.54081546
N	-3.43127101	-1.98104541	0.19512617
B	0.00000000	0.00000000	3.14871628
N	-1.54597175	0.89256750	-1.36674048
N	-1.25841948	0.72654872	-2.66251564
N	1.54597175	0.89256750	-1.36674048
N	1.25841948	0.72654872	-2.66251564
N	0.00000000	-1.78513447	-1.36674048
N	0.00000000	-1.45309797	-2.66251564
C	-2.71521640	1.56763098	-1.37365788
C	-3.17054432	1.83051459	-2.66568594
C	-2.19968822	1.26999047	-3.46384769
C	2.71521640	1.56763098	-1.37365788
C	3.17054432	1.83051459	-2.66568594
C	2.19968822	1.26999047	-3.46384769
C	0.00000000	-3.13526195	-1.37365788
C	0.00000000	-3.66102918	-2.66568594
C	0.00000000	-2.53998094	-3.46384769
H	-4.07228087	2.35113240	-2.95543429
H	-2.10983128	1.21811152	-4.54081546
H	4.07228087	2.35113240	-2.95543429
N	3.43127101	1.98104541	-0.19512617
H	2.10983128	1.21811152	-4.54081546
N	-3.43127101	1.98104541	-0.19512617
H	0.00000000	0.00000000	-4.34831189
H	0.00000000	-4.70226533	-2.95543429
H	0.00000000	-2.43622357	-4.54081546
N	0.00000000	-3.96209029	-0.19512617
B	0.00000000	0.00000000	-3.14871628
O	0.00000000	5.17415914	0.38556595
O	4.48095335	-2.58707930	0.38556595
O	-4.48095335	-2.58707930	0.38556595
O	-4.48095335	2.58707930	-0.38556595
O	4.48095335	2.58707930	-0.38556595
O	0.00000000	-5.17415914	-0.38556595
O	2.97905095	-1.71995571	-0.91316519
O	0.00000000	3.43991141	-0.91316519
O	-2.97905095	-1.71995571	-0.91316519
O	2.97905095	1.71995571	0.91316519
O	-2.97905095	1.71995571	0.91316519
O	0.00000000	-3.43991141	0.91316519

$Co(Tb^{3NO2})_2]^+$ $^1A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.67113910	1.12531553
N	0.00000000	1.42749055	2.43812173
N	1.44724897	-0.83556929	1.12531553
N	1.23624272	-0.71374528	2.43812173
N	-1.44724897	-0.83556929	1.12531553
N	-1.23624272	-0.71374528	2.43812173
C	0.00000000	3.02650650	1.02101734
C	0.00000000	3.62104243	2.28166677
C	0.00000000	2.56381932	3.15785518
C	2.62103132	-1.51325325	1.02101734
C	3.13591496	-1.81052122	2.28166677
C	2.22033301	-1.28190966	3.15785518
C	-2.62103132	-1.51325325	1.02101734
C	-3.13591496	-1.81052122	2.28166677
C	-2.22033301	-1.28190966	3.15785518
H	0.00000000	4.68090138	2.49151095
H	0.00000000	2.53071505	4.23904896
H	4.05377925	-2.34045043	2.49151095
N	3.32720460	-1.92096263	-0.18772140
H	2.19166378	-1.26535752	4.23904896
N	0.00000000	3.84192525	-0.18772140
H	0.00000000	0.00000000	4.16729412
H	-4.05377925	-2.34045043	2.49151095
H	-2.19166378	-1.26535752	4.23904896
N	-3.32720460	-1.92096263	-0.18772140
B	0.00000000	0.00000000	2.97087939
N	-1.44724897	0.83556929	-1.12531553
N	-1.23624272	0.71374528	-2.43812173
N	1.44724897	0.83556929	-1.12531553
N	1.23624272	0.71374528	-2.43812173
N	0.00000000	-1.67113910	-1.12531553
N	0.00000000	-1.42749055	-2.43812173
C	-2.62103132	1.51325325	-1.02101734
C	-3.13591496	1.81052122	-2.28166677
C	-2.22033301	1.28190966	-3.15785518
C	2.62103132	1.51325325	-1.02101734
C	3.13591496	1.81052122	-2.28166677
C	2.22033301	1.28190966	-3.15785518
C	0.00000000	-3.02650650	-1.02101734
C	0.00000000	-3.62104243	-2.28166677
C	0.00000000	-2.56381932	-3.15785518
H	-4.05377925	2.34045043	-2.49151095
H	-2.19166378	1.26535752	-4.23904896
H	4.05377925	2.34045043	-2.49151095
N	3.32720460	1.92096263	0.18772140
H	2.19166378	1.26535752	-4.23904896
N	-3.32720460	1.92096263	0.18772140
H	0.00000000	0.00000000	-4.16729412
H	0.00000000	-4.68090138	-2.49151095
H	0.00000000	-2.53071505	-4.23904896
N	0.00000000	-3.84192525	0.18772140
B	0.00000000	0.00000000	-2.97087939
O	0.00000000	5.04839911	0.01235047
O	4.37204179	-2.52419929	0.01235047
O	-4.37204179	-2.52419929	0.01235047
O	-4.37204179	2.52419929	-0.01235047
O	4.37204179	2.52419929	-0.01235047
O	0.00000000	-5.04839911	-0.01235047
O	2.86105236	-1.65182943	-1.28261294
O	0.00000000	3.30365885	-1.28261294
O	-2.86105236	-1.65182943	-1.28261294
O	2.86105236	1.65182943	1.28261294
O	-2.86105236	1.65182943	1.28261294
O	0.00000000	-3.30365885	1.28261294

$[Co(Tb^{5CH3})_2]^+$ $^5A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.42870237	0.82486192	1.27917328
N	1.25660176	0.72549936	2.61556386
N	0.00000000	-1.64972330	1.27917328
N	0.00000000	-1.45099872	2.61556386
N	-1.42870237	0.82486192	1.27917328

N	-1.25660176	0.72549936	2.61556386
C	2.57579195	1.48713412	1.07312965
C	3.15544848	1.82179904	2.28969809
C	2.28662569	1.32018399	3.26418223
C	0.00000000	-2.97426824	1.07312965
C	0.00000000	-3.64359809	2.28969809
C	0.00000000	-2.64036798	3.26418223
C	-2.57579195	1.48713412	1.07312965
C	-3.15544848	1.82179904	2.28969809
C	-2.28662569	1.32018399	3.26418223
H	4.08254532	2.35705865	2.45907450
C	2.41512845	1.39437517	4.74446192
H	0.00000000	-4.71411731	2.45907450
H	0.00000000	-3.36888312	0.06539149
C	0.00000000	-2.78874981	4.74446192
H	2.91753832	1.68444156	0.06539149
H	0.00000000	0.00000000	4.34780018
H	-4.08254532	2.35705865	2.45907450
C	-2.41512845	1.39437517	4.74446192
H	-2.91753832	1.68444156	0.06539149
B	0.00000000	0.00000000	3.15180033
N	0.00000000	1.64972330	-1.27917328
N	0.00000000	1.45099872	-2.61556386
N	1.42870237	-0.82486192	-1.27917328
N	1.25660176	-0.72549936	-2.61556386
N	-1.42870237	-0.82486192	-1.27917328
N	-1.25660176	-0.72549936	-2.61556386
C	0.00000000	2.97426824	-1.07312965
C	0.00000000	3.64359809	-2.28969809
C	0.00000000	2.64036798	-3.26418223
C	2.57579195	-1.48713412	-1.07312965
C	3.15544848	-1.82179904	-2.28969809
C	2.28662569	-1.32018399	-3.26418223
C	-2.57579195	-1.48713412	-1.07312965
C	-3.15544848	-1.82179904	-2.28969809
C	-2.28662569	-1.32018399	-3.26418223
H	0.00000000	4.71411731	-2.45907450
C	0.00000000	2.78874981	-4.74446192
H	4.08254532	-2.35705865	-2.45907450
H	2.91753832	-1.68444156	-0.06539149
C	2.41512845	-1.39437517	-4.74446192
H	0.00000000	3.36888312	-0.06539149
H	0.00000000	0.00000000	-4.34780018
H	-4.08254532	-2.35705865	-2.45907450
C	-2.41512845	-1.39437517	-4.74446192
H	-2.91753832	-1.68444156	-0.06539149
B	0.00000000	0.00000000	-3.15180033
H	-3.33370765	-1.92471714	-5.00567439
H	-1.57537231	-1.93010205	-5.20014121
H	-2.45920362	-0.39926159	-5.20014121
H	3.33370765	-1.92471714	-5.00567439
H	2.45920362	-0.39926159	-5.20014121
H	1.57537231	-1.93010205	-5.20014121
H	0.88383131	2.32936310	-5.20014121
H	0.00000000	3.84943375	-5.00567439
H	-0.88383131	2.32936310	-5.20014121
H	-2.45920362	0.39926159	5.20014121
H	-3.33370765	1.92471714	5.00567439
H	-1.57537231	1.93010205	5.20014121
H	-0.88383131	-2.32936310	5.20014121
H	0.88383131	-2.32936310	5.20014121
H	0.00000000	-3.84943375	5.00567439
H	2.45920362	0.39926159	5.20014121
H	1.57537231	1.93010205	5.20014121
H	3.33370765	1.92471714	5.00567439

$[Co(Tb^{5CH3})_2]^+$ ^3E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.39233466	0.80386469	1.20974576
N	1.24792590	0.72049070	2.54849646
N	0.00000000	-1.60772938	1.20974576
N	0.00000000	-1.44098087	2.54849646
N	-1.39233466	0.80386469	1.20974576
N	-1.24792590	0.72049070	2.54849646
C	2.53187924	1.46178124	0.96465573
C	3.13689023	1.81108426	2.16686388
C	2.29267789	1.32367815	3.16612569
C	0.00000000	-2.92356248	0.96465573
C	0.00000000	-3.62216905	2.16686388
C	0.00000000	-2.64735683	3.16612569
C	-2.53187924	1.46178124	0.96465573
C	-3.13689023	1.81108426	2.16686388
C	-2.29267789	1.32367815	3.16612569
H	4.06788499	2.34859446	2.30482198
C	2.44952021	1.41423096	4.64323878
H	0.00000000	-4.69718893	2.30482198
H	0.00000000	-3.29320813	-0.05158843
C	0.00000000	-2.82846245	4.64323878
H	2.85200184	1.64660380	-0.05158843
H	0.00000000	0.00000000	4.29730344
H	-4.06788499	2.34859446	2.30482198
C	-2.44952021	1.41423096	4.64323878
H	-2.85200184	1.64660380	-0.05158843
B	0.00000000	0.00000000	3.10209048
N	0.00000000	1.60772938	-1.20974576
N	0.00000000	1.44098087	-2.54849646
N	1.39233466	-0.80386469	-1.20974576
N	1.24792590	-0.72049070	-2.54849646
N	-1.39233466	-0.80386469	-1.20974576
N	-1.24792590	-0.72049070	-2.54849646
C	0.00000000	2.92356248	-0.96465573
C	0.00000000	3.62216905	-2.16686388
C	0.00000000	2.64735683	-3.16612569
C	2.53187924	-1.46178124	-0.96465573
C	3.13689023	-1.81108426	-2.16686388
C	2.29267789	-1.32367815	-3.16612569
C	-2.53187924	-1.46178124	-0.96465573
C	-3.13689023	-1.81108426	-2.16686388
C	-2.29267789	-1.32367815	-3.16612569
H	0.00000000	4.69718893	-2.30482198
C	0.00000000	2.82846245	-4.64323878
H	4.06788499	-2.34859446	-2.30482198
H	2.85200184	-1.64660380	0.05158843
C	2.44952021	-1.41423096	-4.64323878
H	0.00000000	3.29320813	0.05158843
H	0.00000000	0.00000000	-4.29730344
H	-4.06788499	-2.34859446	-2.30482198
C	-2.44952021	-1.41423096	-4.64323878
H	-2.85200184	-1.64660380	0.05158843

B	0.00000000	0.00000000	-3.10209048
H	-3.37328112	-1.94756489	-4.87901635
H	-1.61950781	-1.95601903	-5.10953654
H	-2.50371590	-0.42452557	-5.10953654
H	3.37328112	-1.94756489	-4.87901635
H	2.50371590	-0.42452557	-5.10953654
H	1.61950781	-1.95601903	-5.10953654
H	0.88420809	2.38054460	-5.10953654
H	0.00000000	3.89512926	-4.87901635
H	-0.88420809	2.38054460	-5.10953654
H	-2.50371590	0.42452557	5.10953654
H	-3.37328112	1.94756489	4.87901635
H	-1.61950781	1.95601903	5.10953654
H	-0.88420809	-2.38054460	5.10953654
H	0.88420809	-2.38054460	5.10953654
H	0.00000000	-3.89512926	4.87901635
H	2.50371590	0.42452557	5.10953654
H	1.61950781	1.95601903	5.10953654
H	3.37328112	1.94756489	4.87901635

$[Co(Tb^{5CH3})_2]^+$ $^1A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.35437255	0.78194723	1.13192654
N	1.23853988	0.71507139	2.47355914
N	0.00000000	-1.56389499	1.13192654
N	0.00000000	-1.43014226	2.47355914
N	-1.35437255	0.78194723	1.13192654
N	-1.23853988	0.71507139	2.47355914
C	2.48571011	1.43512552	0.84856112
C	3.11600890	1.79902855	2.03539615
C	2.29780668	1.32663942	3.05833069
C	0.00000000	-2.87025105	0.84856112
C	0.00000000	-3.59805709	2.03539615
C	0.00000000	-2.65327832	3.05833069
C	-2.48571011	1.43512552	0.84856112
C	-3.11600890	1.79902855	2.03539615
C	-2.29780668	1.32663942	3.05833069
H	4.05001891	2.33827974	2.14095960
C	2.48173811	1.43283207	4.53191576
H	0.00000000	-4.67655948	2.14095960
H	0.00000000	-3.21513544	-0.17551381
C	0.00000000	-2.86566414	4.53191576
H	2.78438886	1.60756745	-0.17551381
H	0.00000000	0.00000000	4.23974748
H	-4.05001891	2.33827974	2.14095960
C	-2.48173811	1.43283207	4.53191576
H	-2.78438886	1.60756745	-0.17551381
B	0.00000000	0.00000000	3.04544047
N	0.00000000	1.56389499	-1.13192654
N	0.00000000	1.43014226	-2.47355914
N	1.35437255	-0.78194723	-1.13192654
N	1.23853988	-0.71507139	-2.47355914
N	-1.35437255	-0.78194723	-1.13192654
N	-1.23853988	-0.71507139	-2.47355914
C	0.00000000	2.87025105	-0.84856112
C	0.00000000	3.59805709	-2.03539615
C	0.00000000	2.65327832	-3.05833069
C	2.48571011	-1.43512552	-0.84856112
C	3.11600890	-1.79902855	-2.03539615
C	2.29780668	-1.32663942	-3.05833069
C	-2.48571011	-1.43512552	-0.84856112
C	-3.11600890	-1.79902855	-2.03539615
C	-2.29780668	-1.32663942	-3.05833069
H	0.00000000	4.67655948	-2.14095960
C	0.00000000	2.86566414	-4.53191576
H	4.05001891	-2.33827974	-2.14095960
H	2.78438886	-1.60756745	0.17551381
C	2.48173811	-1.43283207	-4.53191576
H	0.00000000	3.21513544	0.17551381
H	0.00000000	0.00000000	-4.23974748
H	-4.05001891	-2.33827974	-2.14095960
C	-2.48173811	-1.43283207	-4.53191576
H	-2.78438886	-1.60756745	0.17551381
B	0.00000000	0.00000000	-3.04544047
H	-3.40995628	-1.96873939	-4.74322417
H	-1.66124825	-1.98069880	-5.00792922
H	-2.54595959	-0.44833378	-5.00792922
H	3.40995628	-1.96873939	-4.74322417
H	2.54595959	-0.44833378	-5.00792922
H	1.66124825	-1.98069880	-5.00792922
H	0.88471133	2.42903258	-5.00792922
H	0.00000000	3.93747879	-4.74322417
H	-0.88471133	2.42903258	-5.00792922
H	-2.54595959	0.44833378	5.00792922
H	-3.40995628	1.96873939	4.74322417
H	-1.66124825	1.98069880	5.00792922
H	-0.88471133	-2.42903258	5.00792922
H	0.88471133	-2.42903258	5.00792922
H	0.00000000	-3.93747879	4.74322417
H	2.54595959	0.44833378	5.00792922
H	1.66124825	1.98069880	5.00792922
H	3.40995628	1.96873939	4.74322417

$[Co(Tb^{5CF3})_2]^+$ $^5A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.42365931	0.82195038	1.28691726
N	1.26091508	0.72798967	2.62281253
N	0.00000000	-1.64390024	1.28691726
N	0.00000000	-1.45597934	2.62281253
N	-1.42365931	0.82195038	1.28691726
N	-1.26091508	0.72798967	2.62281253
C	2.56786858	1.48255938	1.05576100
C	3.16791960	1.82899903	2.25715899
C	2.30863312	1.33289007	3.23486581
C	0.00000000	-2.96511877	1.05576100
C	0.00000000	-3.65799806	2.25715899
C	0.00000000	-2.66578013	3.23486581
C	-2.56786858	1.48255938	1.05576100
C	-3.16791960	1.82899903	2.25715899
C	-2.30863312	1.33289007	3.23486581
H	4.09559536	2.36459308	2.41248838
C	2.51032532	1.44933711	4.72914118
H	0.00000000	-4.72918616	2.41248838
H	0.00000000	-3.34514265	0.04244901
C	0.00000000	-2.89867368	4.72914118
H	2.89697873	1.67257159	0.04244901
H	0.00000000	0.00000000	4.35906583
H	-4.09559536	2.36459308	2.41248838

C	-2.51032532	1.44933711	4.72914118
H	-2.89697873	1.67257159	0.04244901
B	0.00000000	0.00000000	3.17408769
N	0.00000000	1.64390024	-1.28691726
N	0.00000000	1.45597934	-2.62281253
N	1.42365931	-0.82195038	-1.28691726
N	1.26091508	-0.72798967	-2.62281253
N	-1.42365931	-0.82195038	-1.28691726
N	-1.26091508	-0.72798967	-2.62281253
C	0.00000000	2.96511877	-1.05576100
C	0.00000000	3.65799806	-2.25715899
C	0.00000000	2.66578013	-3.23486581
C	2.56786858	-1.48255938	-1.05576100
C	3.16791960	-1.82899903	-2.25715899
C	2.30863312	-1.33289007	-3.23486581
C	-2.56786858	-1.48255938	-1.05576100
C	-3.16791960	-1.82899903	-2.25715899
C	-2.30863312	-1.33289007	-3.23486581
H	0.00000000	4.72918616	-2.41248838
C	0.00000000	2.89867368	-4.72914118
H	4.09559536	-2.36459308	-2.41248838
H	2.89697873	-1.67257159	-0.04244901
C	2.51032532	-1.44933711	-4.72914118
H	0.00000000	3.34514265	-0.04244901
H	0.00000000	0.00000000	-4.35906583
H	-4.09559536	-2.36459308	-2.41248838
C	-2.51032532	-1.44933711	-4.72914118
H	-2.89697873	-1.67257159	-0.04244901
B	0.00000000	0.00000000	-3.17408769
F	-3.65889607	-2.11246446	-4.96934796
F	-1.51016391	-2.13007495	-5.32242031
F	-2.59978115	-0.24280293	-5.32242031
F	3.65889607	-2.11246446	-4.96934796
F	2.59978115	-0.24280293	-5.32242031
F	1.51016391	-2.13007495	-5.32242031
F	1.08961723	2.37287788	-5.32242031
F	0.00000000	4.22492893	-4.96934796
F	-1.08961723	2.37287788	-5.32242031
F	-2.59978115	0.24280293	5.32242031
F	-3.65889607	2.11246446	4.96934796
F	-1.51016391	2.13007495	5.32242031
F	-1.08961723	-2.37287788	5.32242031
F	1.08961723	-2.37287788	5.32242031
F	0.00000000	-4.22492893	4.96934796
F	2.59978115	0.24280293	5.32242031
F	1.51016391	2.13007495	5.32242031
F	3.65889607	2.11246446	4.96934796

$[Co(Tb^{5CF3})_2]^+$ ^3E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.39079105	0.80297356	1.21889999
N	1.25091151	0.72221423	2.55584832
N	0.00000000	-1.60594711	1.21889999
N	0.00000000	-1.44442846	2.55584832
N	-1.39079105	0.80297356	1.21889999
N	-1.25091151	0.72221423	2.55584832
C	2.52864649	1.45991483	0.95605183
C	3.14846281	1.81776618	2.14650379
C	2.30893528	1.33306417	3.14321231
C	0.00000000	-2.91982966	0.95605183
C	0.00000000	-3.63553184	2.14650379
C	0.00000000	-2.66612886	3.14321231
C	-2.52864649	1.45991483	0.95605183
C	-3.14846281	1.81776618	2.14650379
C	-2.30893528	1.33306417	3.14321231
H	4.07915277	2.35510017	2.27656762
C	2.52437815	1.45745045	4.63409618
H	0.00000000	-4.71019981	2.27656762
H	0.00000000	-3.28102330	-0.06323298
C	0.00000000	-2.91490091	4.63409618
H	2.84144952	1.64051191	-0.06323298
H	0.00000000	0.00000000	4.30684715
H	-4.07915277	2.35510017	2.27656762
C	-2.52437815	1.45745045	4.63409618
H	-2.84144952	1.64051191	-0.06323298
B	0.00000000	0.00000000	3.12261938
N	0.00000000	1.60594711	-1.21889999
N	0.00000000	1.44442846	-2.55584832
N	1.39079105	-0.80297356	-1.21889999
N	1.25091151	-0.72221423	-2.55584832
N	-1.39079105	-0.80297356	-1.21889999
N	-1.25091151	-0.72221423	-2.55584832
C	0.00000000	2.91982966	-0.95605183
C	0.00000000	3.63553184	-2.14650379
C	0.00000000	2.66612886	-3.14321231
C	2.52864649	-1.45991483	-0.95605183
C	3.14846281	-1.81776618	-2.14650379
C	2.30893528	-1.33306417	-3.14321231
C	-2.52864649	-1.45991483	-0.95605183
C	-3.14846281	-1.81776618	-2.14650379
C	-2.30893528	-1.33306417	-3.14321231
H	0.00000000	4.71019981	-2.27656762
C	0.00000000	2.91490091	-4.63409618
H	4.07915277	-2.35510017	-2.27656762
H	2.84144952	-1.64051191	0.06323298
C	2.52437815	-1.45745045	-4.63409618
H	0.00000000	3.28102330	0.06323298
H	0.00000000	0.00000000	-4.30684715
H	-4.07915277	-2.35510017	-2.27656762
C	-2.52437815	-1.45745045	-4.63409618
H	-2.84144952	-1.64051191	0.06323298
B	0.00000000	0.00000000	-3.12261938
F	-3.67462428	-2.12154514	-4.86082958
F	-1.52828189	-2.14050715	-5.23273641
F	-2.61787424	-0.25327746	-5.23273641
F	3.67462428	-2.12154514	-4.86082958
F	2.61787424	-0.25327746	-5.23273641
F	1.52828189	-2.14050715	-5.23273641
F	1.08959236	2.39378461	-5.23273641
F	0.00000000	4.24309082	-4.86082958
F	-1.08959236	2.39378461	-5.23273641
F	-2.61787424	0.25327746	5.23273641
F	-3.67462428	2.12154514	4.86082958
F	-1.52828189	2.14050715	5.23273641
F	-1.08959236	-2.39378461	5.23273641
F	1.08959236	-2.39378461	5.23273641
F	0.00000000	-4.24309082	4.86082958
F	2.61787424	0.25327746	5.23273641
F	1.52828189	2.14050715	5.23273641

F	3.67462428	2.12154514	4.86082958

$[Co(Tb^{5CF3})_2]^+$ $^1A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.35398466	0.78172339	1.13701246
N	1.24234149	0.71726642	2.47646274
N	0.00000000	-1.56344677	1.13701246
N	0.00000000	-1.43453232	2.47646274
N	-1.35398466	0.78172339	1.13701246
N	-1.24234149	0.71726642	2.47646274
C	2.48349233	1.43384491	0.83617414
C	3.12818209	1.80605655	2.01084497
C	2.31436516	1.33619954	3.03093783
C	0.00000000	-2.86769036	0.83617414
C	0.00000000	-3.61211363	2.01084497
C	0.00000000	-2.67239855	3.03093783
C	-2.48349233	1.43384491	0.83617414
C	-3.12818209	1.80605655	2.01084497
C	-2.31436516	1.33619954	3.03093783
H	4.06167986	2.34501193	2.10955081
C	2.55815765	1.47695328	4.51534934
H	0.00000000	-4.69002440	2.10955081
H	0.00000000	-3.20425132	-0.19078692
C	0.00000000	-2.95390656	4.51534934
H	2.77496316	1.60212592	-0.19078692
H	0.00000000	0.00000000	4.24497998
H	-4.06167986	2.34501193	2.10955081
C	-2.55815765	1.47695328	4.51534934
H	-2.77496316	1.60212592	-0.19078692
B	0.00000000	0.00000000	3.06106284
N	0.00000000	1.56344677	-1.13701246
N	0.00000000	1.43453232	-2.47646274
N	1.35398466	-0.78172339	-1.13701246
N	1.24234149	-0.71726642	-2.47646274
N	-1.35398466	-0.78172339	-1.13701246
N	-1.24234149	-0.71726642	-2.47646274
C	0.00000000	2.86769036	-0.83617414
C	0.00000000	3.61211363	-2.01084497
C	0.00000000	2.67239855	-3.03093783
C	2.48349233	-1.43384491	-0.83617414
C	3.12818209	-1.80605655	-2.01084497
C	2.31436516	-1.33619954	-3.03093783
C	-2.48349233	-1.43384491	-0.83617414
C	-3.12818209	-1.80605655	-2.01084497
C	-2.31436516	-1.33619954	-3.03093783
H	0.00000000	4.69002440	-2.10955081
C	0.00000000	2.95390656	-4.51534934
H	4.06167986	-2.34501193	-2.10955081
H	2.77496316	-1.60212592	0.19078692
C	2.55815765	-1.47695328	-4.51534934
H	0.00000000	3.20425132	0.19078692
H	0.00000000	0.00000000	-4.24497998
H	-4.06167986	-2.34501193	-2.10955081
C	-2.55815765	-1.47695328	-4.51534934
H	-2.77496316	-1.60212592	0.19078692
B	0.00000000	0.00000000	-3.06106284
F	-3.71211490	-2.14319061	-4.71366962
F	-1.57317040	-2.16598810	-5.12536159
F	-2.66238599	-0.27941141	-5.12536159
F	3.71211490	-2.14319061	-4.71366962
F	2.66238599	-0.27941141	-5.12536159
F	1.57317040	-2.16598810	-5.12536159
F	1.08921558	2.44539950	-5.12536159
F	0.00000000	4.28638069	-4.71366962
F	-1.08921558	2.44539950	-5.12536159
F	-2.66238599	0.27941141	5.12536159
F	-3.71211490	2.14319061	4.71366962
F	-1.57317040	2.16598810	5.12536159
F	-1.08921558	-2.44539950	5.12536159
F	1.08921558	-2.44539950	5.12536159
F	0.00000000	-4.28638069	4.71366962
F	2.66238599	0.27941141	5.12536159
F	1.57317040	2.16598810	5.12536159
F	3.71211490	2.14319061	4.71366962

$[Co(Tb^{5NH2})_2]^+$ $^5A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.65390010	-1.28912552
N	0.00000000	1.44883333	-2.63595994
N	-1.43231983	-0.82695005	-1.28912552
N	-1.25472635	-0.72441667	-2.63595994
N	1.43231983	-0.82695005	-1.28912552
N	1.25472635	-0.72441667	-2.63595994
C	0.00000000	2.97736763	-1.10006901
C	0.00000000	3.65626606	-2.31147797
C	0.00000000	2.64134643	-3.28007395
C	-2.57847594	-1.48868355	-1.10006901
C	-3.16641938	-1.82813276	-2.31147797
C	-2.28747343	-1.32067348	-3.28007395
C	2.57847594	-1.48868355	-1.10006901
C	3.16641938	-1.82813276	-2.31147797
C	2.28747343	-1.32067348	-3.28007395
H	0.00000000	4.72627410	-2.48213076
N	0.00000000	2.76448809	-4.63246208
H	-4.09307330	-2.36313678	-2.48213076
H	-2.92700001	-1.68990426	-0.09538526
N	-2.39411694	-1.38224431	-4.63246208
H	0.00000000	3.37980852	-0.09538526
H	0.00000000	0.00000000	-4.36624783
H	4.09307330	-2.36313678	-2.48213076
N	2.39411694	-1.38224431	-4.63246208
H	2.92700001	-1.68990426	-0.09538526
B	0.00000000	0.00000000	-3.15555325
N	1.43231983	0.82695005	1.28912552
N	1.25472635	0.72441667	2.63595994
N	-1.43231983	0.82695005	1.28912552
N	-1.25472635	0.72441667	2.63595994
N	0.00000000	-1.65390010	1.28912552
N	0.00000000	-1.44883333	2.63595994
C	2.57847594	1.48868355	1.10006901
C	3.16641938	1.82813276	2.31147797
C	2.28747343	1.32067348	3.28007395
C	-2.57847594	1.48868355	1.10006901
C	-3.16641938	1.82813276	2.31147797
C	-2.28747343	1.32067348	3.28007395
C	0.00000000	-2.97736763	1.10006901
C	0.00000000	-3.65626606	2.31147797
C	0.00000000	-2.64134643	3.28007395

H	4.09307330	2.36313678	2.48213076
N	2.39411694	1.38224431	4.63246208
H	-4.09307330	2.36313678	2.48213076
H	-2.92700001	1.68990426	0.09538526
N	-2.39411694	1.38224431	4.63246208
H	2.92700001	1.68990426	0.09538526
H	0.00000000	0.00000000	4.36624783
H	0.00000000	-4.72627410	2.48213076
N	0.00000000	-2.76448809	4.63246208
H	0.00000000	-3.37980852	0.09538526
B	0.00000000	0.00000000	3.15555325
H	0.00000000	3.67698123	-5.04850917
H	0.00000000	1.96192042	-5.23233212
H	-3.18435955	-1.83849088	-5.04850917
H	-1.69907278	-0.98096021	-5.23233212
H	3.18435955	-1.83849088	-5.04850917
H	1.69907278	-0.98096021	-5.23233212
H	3.18435955	1.83849088	5.04850917
H	1.69907278	0.98096021	5.23233212
H	-3.18435955	1.83849088	5.04850917
H	-1.69907278	0.98096021	5.23233212
H	0.00000000	-3.67698123	5.04850917
H	0.00000000	-1.96192042	5.23233212

$[Co(Tb^{5NH2})_2]^+$ ^3E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.60888034	-1.20914408
N	0.00000000	1.43896100	-2.55979281
N	-1.39333110	-0.80443991	-1.20914408
N	-1.24617697	-0.71948050	-2.55979281
N	1.39333110	-0.80443991	-1.20914408
N	1.24617697	-0.71948050	-2.55979281
C	0.00000000	2.92326931	-0.97730042
C	0.00000000	3.63423376	-2.17228531
C	0.00000000	2.64959313	-3.16886841
C	-2.53162523	-1.46163466	-0.97730042
C	-3.14733884	-1.81711688	-2.17228531
C	-2.29461468	-1.32479630	-3.16886841
C	2.53162523	-1.46163466	-0.97730042
C	3.14733884	-1.81711688	-2.17228531
C	2.29461468	-1.32479630	-3.16886841
H	0.00000000	4.70900493	-2.30893210
N	0.00000000	2.80492676	-4.51893822
H	-4.07811769	-2.35450220	-2.30893210
H	-2.85567539	-1.64872474	0.03731917
N	-2.42913789	-1.40246364	-4.51893822
H	0.00000000	3.29745002	0.03731917
H	0.00000000	0.00000000	-4.30707046
H	4.07811769	-2.35450220	-2.30893210
N	2.42913789	-1.40246364	-4.51893822
H	2.85567539	-1.64872474	0.03731917
B	0.00000000	0.00000000	-3.09808302
N	1.39333110	0.80443991	1.20914408
N	1.24617697	0.71948050	2.55979281
N	-1.39333110	0.80443991	1.20914408
N	-1.24617697	0.71948050	2.55979281
N	0.00000000	-1.60888034	1.20914408
N	0.00000000	-1.43896100	2.55979281
C	2.53162523	1.46163466	0.97730042
C	3.14733884	1.81711688	2.17228531
C	2.29461468	1.32479630	3.16886841
C	-2.53162523	1.46163466	0.97730042
C	-3.14733884	1.81711688	2.17228531
C	-2.29461468	1.32479630	3.16886841
C	0.00000000	-2.92326931	0.97730042
C	0.00000000	-3.63423376	2.17228531
C	0.00000000	-2.64959313	3.16886841
H	4.07811769	2.35450220	2.30893210
N	2.42913789	1.40246364	4.51893822
H	-4.07811769	2.35450220	2.30893210
H	-2.85567539	1.64872474	-0.03731917
N	-2.42913789	1.40246364	4.51893822
H	2.85567539	1.64872474	-0.03731917
H	0.00000000	0.00000000	4.30707046
H	0.00000000	-4.70900493	2.30893210
N	0.00000000	-2.80492676	4.51893822
H	0.00000000	-3.29745002	-0.03731917
B	0.00000000	0.00000000	3.09808302
H	0.00000000	3.72720015	-4.91242595
H	0.00000000	2.01790102	-5.13889212
H	-3.22784998	-1.86359981	-4.91242595
H	-1.74755336	-1.00895051	-5.13889212
H	3.22784998	-1.86359981	-4.91242595
H	1.74755336	-1.00895051	-5.13889212
H	3.22784998	1.86359981	4.91242595
H	1.74755336	1.00895051	5.13889212
H	-3.22784998	1.86359981	4.91242595
H	-1.74755336	1.00895051	5.13889212
H	0.00000000	-3.72720015	4.91242595
H	0.00000000	-2.01790102	5.13889212

$[Co(Tb^{5NH2})_2]^+$ $^1A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.56470463	-1.12769630
N	0.00000000	1.42847482	-2.48243715
N	-1.35507371	-0.78235205	-1.12769630
N	-1.23709523	-0.71423741	-2.48243715
N	1.35507371	-0.78235205	-1.12769630
N	1.23709523	-0.71423741	-2.48243715
C	0.00000000	2.86937949	-0.85410690
C	0.00000000	3.60947515	-2.03235391
C	0.00000000	2.65604803	-3.05541546
C	-2.48495550	-1.43469001	-0.85410690
C	-3.12589710	-1.80473731	-2.03235391
C	-2.30020491	-1.32802375	-3.05541546
C	2.48495550	-1.43469001	-0.85410690
C	3.12589710	-1.80473731	-2.03235391
C	2.30020491	-1.32802375	-3.05541546
H	0.00000000	4.68777434	-2.13443749
N	0.00000000	2.84250840	-4.40250017
H	-4.05973143	-2.34388690	-2.13443749
H	-2.78657595	-1.60883007	0.16879167
N	-2.46168440	-1.42125420	-4.40250017
H	0.00000000	3.21766067	0.16879167
H	0.00000000	0.00000000	-4.24696651
H	4.05973143	-2.34388690	-2.13443749
N	2.46168440	-1.42125420	-4.40250017
H	2.78657595	-1.60883007	0.16879167

B	0.00000000	0.00000000	-3.04025188
N	1.35507371	0.78235205	1.12769630
N	1.23709523	0.71423741	2.48243715
N	-1.35507371	0.78235205	1.12769630
N	-1.23709523	0.71423741	2.48243715
N	0.00000000	-1.56470463	1.12769630
N	0.00000000	-1.42847482	2.48243715
C	2.48495550	1.43469001	0.85410690
C	3.12589710	1.80473731	2.03235391
C	2.30020491	1.32802375	3.05541546
C	-2.48495550	1.43469001	0.85410690
C	-3.12589710	1.80473731	2.03235391
C	-2.30020491	1.32802375	3.05541546
C	0.00000000	-2.86937949	0.85410690
C	0.00000000	-3.60947515	2.03235391
C	0.00000000	-2.65604803	3.05541546
H	4.05973143	2.34388690	2.13443749
N	2.46168440	1.42125420	4.40250017
H	-4.05973143	2.34388690	2.13443749
H	-2.78657595	1.60883007	-0.16879167
N	-2.46168440	1.42125420	4.40250017
H	2.78657595	1.60883007	-0.16879167
H	0.00000000	0.00000000	4.24696651
H	0.00000000	-4.68777434	2.13443749
N	0.00000000	-2.84250840	4.40250017
H	0.00000000	-3.21766067	-0.16879167
B	0.00000000	0.00000000	3.04025188
H	0.00000000	3.77377145	-4.77341003
H	0.00000000	2.07115001	-5.04151292
H	-3.26818175	-1.88688573	-4.77341003
H	-1.79366851	-1.03557500	-5.04151292
H	3.26818175	-1.88688573	-4.77341003
H	1.79366851	-1.03557500	-5.04151292
H	3.26818175	1.88688573	4.77341003
H	1.79366851	1.03557500	5.04151292
H	-3.26818175	1.88688573	4.77341003
H	-1.79366851	1.03557500	5.04151292
H	0.00000000	-3.77377145	4.77341003
H	0.00000000	-2.07115001	5.04151292

$[Co(Tb^{5NO2})_2]^+$ $^5A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.42295974	-0.82154609	-1.25786120
N	-1.26551469	-0.73064508	-2.59229064
N	1.42295974	-0.82154609	-1.25786120
N	1.26551469	-0.73064508	-2.59229064
N	0.00000000	1.64309218	-1.25786120
N	0.00000000	1.46129016	-2.59229064
C	-2.56539203	-1.48113008	-1.00265700
C	-3.18130672	-1.83672819	-2.18798758
C	-2.32925092	-1.34479338	-3.17059671
C	2.56539203	-1.48113008	-1.00265700
C	3.18130672	-1.83672819	-2.18798758
C	2.32925092	-1.34479338	-3.17059671
C	0.00000000	2.96225962	-1.00265700
C	0.00000000	3.67345638	-2.18798758
C	0.00000000	2.68958729	-3.17059671
H	-4.10780295	-2.37164119	-2.34661852
N	-2.58999190	-1.49533266	-4.60607678
H	-2.87911265	-1.66225634	0.01692097
H	0.00000000	0.00000000	-4.31555371
H	0.00000000	4.74328238	-2.34661852
N	0.00000000	2.99066480	-4.60607678
H	0.00000000	3.32451320	0.01692097
B	0.00000000	0.00000000	-3.14819822
N	-1.42295974	0.82154609	1.25786120
N	-1.26551469	0.73064508	2.59229064
N	0.00000000	-1.64309218	1.25786120
N	0.00000000	-1.46129016	2.59229064
N	1.42295974	0.82154609	1.25786120
N	1.26551469	0.73064508	2.59229064
C	-2.56539203	1.48113008	1.00265700
C	-3.18130672	1.83672819	2.18798758
C	-2.32925092	1.34479338	3.17059671
C	0.00000000	-2.96225962	1.00265700
C	0.00000000	-3.67345638	2.18798758
C	0.00000000	-2.68958729	3.17059671
C	2.56539203	1.48113008	1.00265700
C	3.18130672	1.83672819	2.18798758
C	2.32925092	1.34479338	3.17059671
H	-4.10780295	2.37164119	2.34661852
N	-2.58999190	1.49533266	4.60607678
H	0.00000000	-4.74328238	2.34661852
H	0.00000000	-3.32451320	-0.01692097
N	0.00000000	-2.99066480	4.60607678
H	-2.87911265	1.66225634	-0.01692097
H	0.00000000	0.00000000	4.31555371
H	4.10780295	2.37164119	2.34661852
N	2.58999190	1.49533266	4.60607678
H	2.87911265	1.66225634	-0.01692097
B	0.00000000	0.00000000	3.14819822
O	-3.62662155	-2.09383107	-4.85792493
O	-1.79764369	-1.03787005	-5.40713365
O	3.62662155	-2.09383107	-4.85792493
O	1.79764369	-1.03787005	-5.40713365
O	0.00000000	4.18766162	-4.85792493
O	0.00000000	2.07574009	-5.40713365
O	-3.62662155	2.09383107	4.85792493
O	-1.79764369	1.03787005	5.40713365
O	0.00000000	-4.18766162	4.85792493
O	0.00000000	-2.07574009	5.40713365
O	3.62662155	2.09383107	4.85792493
O	1.79764369	1.03787005	5.40713365

$[Co(Tb^{5NO2})_2]^+$ ^3E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.39006291	-0.80255339	-1.19314123
N	-1.25675099	-0.72558562	-2.52839884
N	1.39006291	-0.80255339	-1.19314123
N	1.25675099	-0.72558562	-2.52839884
N	0.00000000	1.60510678	-1.19314123
N	0.00000000	1.45117071	-2.52839884
C	-2.52526928	-1.45796481	-0.90406970
C	-3.16249394	-1.82586683	-2.07658836
C	-2.33176557	-1.34624544	-3.07959939

C	2.52526928	-1.45796481	-0.90406970
C	3.16249394	-1.82586683	-2.07658836
C	2.33176557	-1.34624544	-3.07959939
C	0.00000000	2.91593015	-0.90406970
C	0.00000000	3.65173366	-2.07658836
C	0.00000000	2.69249088	-3.07959939
H	-4.09231446	-2.36269863	-2.20823867
N	-2.61099706	-1.50745982	-4.50852877
H	4.09231446	-2.36269863	-2.20823867
H	2.82128680	-1.62887054	0.12168960
N	2.61099706	-1.50745982	-4.50852877
H	-2.82128680	-1.62887054	0.12168960
H	0.00000000	0.00000000	-4.26790764
H	0.00000000	4.72539778	-2.20823867
N	0.00000000	3.01491964	-4.50852877
H	0.00000000	3.25774109	0.12168960
B	0.00000000	0.00000000	-3.10066329
N	-1.39006291	0.80255339	1.19314123
N	-1.25675099	0.72558562	2.52839884
N	0.00000000	-1.60510678	1.19314123
N	0.00000000	-1.45117071	2.52839884
N	1.39006291	0.80255339	1.19314123
N	1.25675099	0.72558562	2.52839884
C	-2.52526928	1.45796481	0.90406970
C	-3.16249394	1.82586683	2.07658836
C	-2.33176557	1.34624544	3.07959939
C	0.00000000	-2.91593015	0.90406970
C	0.00000000	-3.65173366	2.07658836
C	0.00000000	-2.69249088	3.07959939
C	2.52526928	1.45796481	0.90406970
C	3.16249394	1.82586683	2.07658836
C	2.33176557	1.34624544	3.07959939
H	-4.09231446	2.36269863	2.20823867
N	-2.61099706	1.50745982	4.50852877
H	0.00000000	-4.72539778	2.20823867
H	0.00000000	-3.25774109	-0.12168960
N	0.00000000	-3.01491964	4.50852877
H	-2.82128680	1.62887054	-0.12168960
H	0.00000000	0.00000000	4.26790764
H	4.09231446	2.36269863	2.20823867
N	2.61099706	1.50745982	4.50852877
H	2.82128680	1.62887054	-0.12168960
B	0.00000000	0.00000000	3.10066329
O	-3.65046310	-2.10759603	-4.74311252
O	-1.82760782	-1.05516991	-5.32163766
O	3.65046310	-2.10759603	-4.74311252
O	1.82760782	-1.05516991	-5.32163766
O	0.00000000	4.21519154	-4.74311252
O	0.00000000	2.11033982	-5.32163766
O	-3.65046310	2.10759603	4.74311252
O	-1.82760782	1.05516991	5.32163766
O	0.00000000	-4.21519154	4.74311252
O	0.00000000	-2.11033982	5.32163766
O	3.65046310	2.10759603	4.74311252
O	1.82760782	1.05516991	5.32163766

$[Co(Tb^{5NO2})_2]^+$ $^1A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.35318931	-0.78126406	-1.11661532
N	-1.24696068	-0.71993295	-2.45376633
N	1.35318931	-0.78126406	-1.11661532
N	1.24696068	-0.71993295	-2.45376633
N	0.00000000	1.56252865	-1.11661532
N	0.00000000	1.43986642	-2.45376633
C	-2.48022942	-1.43196104	-0.79193651
C	-3.14033994	-1.81307608	-1.94945035
C	-2.33373993	-1.34738529	-2.97400842
C	2.48022942	-1.43196104	-0.79193651
C	3.14033994	-1.81307608	-1.94945035
C	2.33373993	-1.34738529	-2.97400842
C	0.00000000	2.86392209	-0.79193651
C	0.00000000	3.62615217	-1.94945035
C	0.00000000	2.69477111	-2.97400842
H	-4.07295398	-2.35152081	-2.05125824
N	-2.63292352	-1.52011880	-4.39625535
H	4.07295398	-2.35152081	-2.05125824
H	2.75685101	-1.59166832	0.24037665
N	2.63292352	-1.52011880	-4.39625535
H	-2.75685101	-1.59166832	0.24037665
H	0.00000000	0.00000000	-4.21149470
H	0.00000000	4.70304216	-2.05125824
N	0.00000000	3.04023812	-4.39625535
H	0.00000000	3.18333718	0.24037665
B	0.00000000	0.00000000	-3.04458690
N	-1.35318931	0.78126406	1.11661532
N	-1.24696068	0.71993295	2.45376633
N	0.00000000	-1.56252865	1.11661532
N	0.00000000	-1.43986642	2.45376633
N	1.35318931	0.78126406	1.11661532
N	1.24696068	0.71993295	2.45376633
C	-2.48022942	1.43196104	0.79193651
C	-3.14033994	1.81307608	1.94945035
C	-2.33373993	1.34738529	2.97400842
C	0.00000000	-2.86392209	0.79193651
C	0.00000000	-3.62615217	1.94945035
C	0.00000000	-2.69477111	2.97400842
C	2.48022942	1.43196104	0.79193651
C	3.14033994	1.81307608	1.94945035
C	2.33373993	1.34738529	2.97400842
H	-4.07295398	2.35152081	2.05125824
N	-2.63292352	1.52011880	4.39625535
H	0.00000000	-4.70304216	2.05125824
H	0.00000000	-3.18333718	-0.24037665
N	0.00000000	-3.04023812	4.39625535
H	-2.75685101	1.59166832	-0.24037665
H	0.00000000	0.00000000	4.21149470
H	4.07295398	2.35152081	2.05125824
N	2.63292352	1.52011880	4.39625535
H	2.75685101	1.59166832	-0.24037665
B	0.00000000	0.00000000	3.04458690
O	-3.67447452	-2.12145889	-4.61373291
O	-1.85806673	-1.07275500	-5.22088443
O	3.67447452	-2.12145889	-4.61373291
O	1.85806673	-1.07275500	-5.22088443
O	0.00000000	4.24291778	-4.61373291
O	0.00000000	2.14551052	-5.22088443
O	-3.67447452	2.12145889	4.61373291
O	-1.85806673	1.07275500	5.22088443
O	0.00000000	-4.24291778	4.61373291

O	0.00000000	-2.14551052	5.22088443
O	3.67447452	2.12145889	4.61373291
O	1.85806673	1.07275500	5.22088443

$[Co(Tb^{3,5\text{-}CH3})_2]^+$ $^5A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.48935508	0.85987969	1.27981888
N	-1.26131620	0.72822145	2.60820935
N	1.48935508	0.85987969	1.27981888
N	1.26131620	0.72822145	2.60820935
N	0.00000000	-1.71975885	1.27981888
N	0.00000000	-1.45644290	2.60820935
C	-2.65957394	1.53550568	1.14092044
C	-3.16303053	1.82617640	2.40899793
C	-2.25670442	1.30290900	3.32416712
C	2.65957394	1.53550568	1.14092044
C	3.16303053	1.82617640	2.40899793
C	2.25670442	1.30290900	3.32416712
C	0.00000000	-3.07101137	1.14092044
C	0.00000000	-3.65235332	2.40899793
C	0.00000000	-2.60581800	3.32416712
H	-4.08055509	2.35590981	2.63840579
C	-2.32578057	1.34278991	4.81012435
H	4.08055509	2.35590981	2.63840579
C	3.30147018	1.90610439	-0.14964709
C	2.32578057	1.34278991	4.81012435
C	-3.30147018	1.90610439	-0.14964709
H	0.00000000	0.00000000	4.30661273
H	0.00000000	-4.71181909	2.63840579
C	0.00000000	-2.68557983	4.81012435
C	0.00000000	-3.81220930	-0.14964709
B	0.00000000	0.00000000	3.11139553
N	-1.48935508	-0.85987969	-1.27981888
N	-1.26131620	-0.72822145	-2.60820935
N	0.00000000	1.71975885	-1.27981888
N	0.00000000	1.45644290	-2.60820935
N	1.48935508	-0.85987969	-1.27981888
N	1.26131620	-0.72822145	-2.60820935
C	-2.65957394	-1.53550568	-1.14092044
C	-3.16303053	-1.82617640	-2.40899793
C	-2.25670442	-1.30290900	-3.32416712
C	0.00000000	3.07101137	-1.14092044
C	0.00000000	3.65235332	-2.40899793
C	0.00000000	2.60581800	-3.32416712
C	2.65957394	-1.53550568	-1.14092044
C	3.16303053	-1.82617640	-2.40899793
C	2.25670442	-1.30290900	-3.32416712
H	-4.08055509	-2.35590981	-2.63840579
C	-2.32578057	-1.34278991	-4.81012435
H	0.00000000	4.71181909	-2.63840579
C	0.00000000	3.81220930	0.14964709
C	0.00000000	2.68557983	-4.81012435
C	-3.30147018	-1.90610439	0.14964709
H	0.00000000	0.00000000	-4.30661273
H	4.08055509	-2.35590981	-2.63840579
C	2.32578057	-1.34278991	-4.81012435
C	3.30147018	-1.90610439	0.14964709
B	0.00000000	0.00000000	-3.11139553
H	3.54297027	1.03155167	-0.75894654
H	4.23100864	2.44277373	0.05582926
H	2.66483502	2.55252615	-0.75894654
H	-4.23100864	2.44277373	0.05582926
H	-3.54297027	1.03155167	-0.75894654
H	-2.66483502	2.55252615	-0.75894654
H	0.00000000	-4.88554798	0.05582926
H	0.87813525	-3.58407782	-0.75894654
H	-0.87813525	-3.58407782	-0.75894654
H	-0.87813525	3.58407782	0.75894654
H	0.00000000	4.88554798	-0.05582926
H	0.87813525	3.58407782	0.75894654
H	3.54297027	-1.03155167	0.75894654
H	4.23100864	-2.44277373	-0.05582926
H	2.66483502	-2.55252615	0.75894654
H	-2.66483502	-2.55252615	0.75894654
H	-4.23100864	-2.44277373	-0.05582926
H	-3.54297027	-1.03155167	0.75894654
H	3.23442977	-1.86739878	-5.11504316
H	2.35503561	-0.33939259	-5.24729037
H	1.47144031	-1.86982452	-5.24729037
H	0.00000000	3.73479808	-5.11504316
H	-0.88359530	2.20921711	-5.24729037
H	0.88359530	2.20921711	-5.24729037
H	-2.35503561	-0.33939259	-5.24729037
H	-3.23442977	-1.86739878	-5.11504316
H	-1.47144031	-1.86982452	-5.24729037
H	0.88359530	-2.20921711	5.24729037
H	0.00000000	-3.73479808	5.11504316
H	-0.88359530	-2.20921711	5.24729037
H	2.35503561	0.33939259	5.24729037
H	1.47144031	1.86982452	5.24729037
H	3.23442977	1.86739878	5.11504316
H	-1.47144031	1.86982452	5.24729037
H	-2.35503561	0.33939259	5.24729037
H	-3.23442977	1.86739878	5.11504316

$[Co(Tb^{3,5\text{-}CH3})_2]^+$ ^3E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	-1.67720000	-1.19840000
N	0.00000000	-1.44530000	-2.53080000
N	1.45250000	0.83860000	-1.19840000
N	1.25170000	0.72270000	-2.53080000
N	-1.45250000	0.83860000	-1.19840000
N	-1.25170000	0.72270000	-2.53080000
C	0.00000000	-3.02130000	-1.02020000
C	0.00000000	-3.63100000	-2.27800000
C	0.00000000	-2.61050000	-3.21860000
C	2.61650000	1.51060000	-1.02020000
C	3.14460000	1.81550000	-2.27800000
C	2.26070000	1.30520000	-3.21860000
C	-2.61650000	1.51060000	-1.02020000
C	-3.14460000	1.81550000	-2.27800000
C	-2.26070000	1.30520000	-3.21860000
H	0.00000000	-4.69670000	-2.47680000
C	0.00000000	-2.71600000	-4.70220000
H	4.06750000	2.34840000	-2.47680000
C	3.24230000	1.87190000	0.27980000
C	2.35210000	1.35800000	-4.70220000
C	0.00000000	-3.74390000	0.27980000

H	0.00000000	0.00000000	-4.24530000
H	-4.06750000	2.34840000	-2.47680000
C	-2.35210000	1.35800000	-4.70220000
C	-3.24230000	1.87190000	0.27980000
B	0.00000000	0.00000000	-3.05060000
N	-1.45250000	-0.83860000	1.19840000
N	-1.25170000	-0.72270000	2.53080000
N	1.45250000	-0.83860000	1.19840000
N	1.25170000	-0.72270000	2.53080000
N	0.00000000	1.67720000	1.19840000
N	0.00000000	1.44530000	2.53080000
C	-2.61650000	-1.51060000	1.02020000
C	-3.14460000	-1.81550000	2.27800000
C	-2.26070000	-1.30520000	3.21860000
C	2.61650000	-1.51060000	1.02020000
C	3.14460000	-1.81550000	2.27800000
C	2.26070000	-1.30520000	3.21860000
C	0.00000000	3.02130000	1.02020000
C	0.00000000	3.63100000	2.27800000
C	0.00000000	2.61050000	3.21860000
H	-4.06750000	-2.34840000	2.47680000
C	-2.35210000	-1.35800000	4.70220000
H	4.06750000	-2.34840000	2.47680000
C	3.24230000	-1.87190000	-0.27980000
C	2.35210000	-1.35800000	4.70220000
C	-3.24230000	-1.87190000	-0.27980000
H	0.00000000	0.00000000	4.24530000
H	0.00000000	4.69670000	2.47680000
C	0.00000000	2.71600000	4.70220000
C	0.00000000	3.74390000	-0.27980000
B	0.00000000	0.00000000	3.05060000
H	2.60110000	2.51750000	0.88490000
H	4.17360000	2.40960000	0.08430000
H	3.48080000	0.99380000	0.88490000
H	0.00000000	-4.81920000	0.08430000
H	-0.87970000	-3.51140000	0.88490000
H	0.87970000	-3.51140000	0.88490000
H	-4.17360000	2.40960000	0.08430000
H	-2.60110000	2.51750000	0.88490000
H	-3.48080000	0.99380000	0.88490000
H	2.60110000	-2.51750000	-0.88490000
H	4.17360000	-2.40960000	-0.08430000
H	3.48080000	-0.99380000	-0.88490000
H	0.87970000	3.51140000	-0.88490000
H	0.00000000	4.81920000	-0.08430000
H	-0.87970000	3.51140000	-0.88490000
H	-3.48080000	-0.99380000	-0.88490000
H	-4.17360000	-2.40960000	-0.08430000
H	-2.60110000	-2.51750000	-0.88490000
H	0.00000000	3.77050000	4.98850000
H	0.88390000	2.24780000	5.14790000
H	-0.88390000	2.24780000	5.14790000
H	3.26540000	-1.88530000	4.98850000
H	1.50460000	-1.88940000	5.14790000
H	2.38860000	-0.35840000	5.14790000
H	-1.50460000	-1.88940000	5.14790000
H	-3.26540000	-1.88530000	4.98850000
H	-2.38860000	-0.35840000	5.14790000
H	-1.50460000	1.88940000	-5.14790000
H	-3.26540000	1.88530000	-4.98850000
H	-2.38860000	0.35840000	-5.14790000
H	1.50460000	1.88940000	-5.14790000
H	2.38860000	0.35840000	-5.14790000
H	3.26540000	1.88530000	-4.98850000
H	0.88390000	-2.24780000	-5.14790000
H	-0.88390000	-2.24780000	-5.14790000
H	0.00000000	-3.77050000	-4.98850000

$[Co(Tb^{3,5\text{-}CH3})_2]^{+}$ $^1A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.41312392	0.81586749	1.11449174
N	-1.24138738	0.71671555	2.45226664
N	1.41312392	0.81586749	1.11449174
N	1.24138738	0.71671555	2.45226664
N	0.00000000	-1.63173445	1.11449174
N	0.00000000	-1.43343057	2.45226664
C	-2.57077271	1.48423635	0.89720150
C	-3.12410584	1.80370330	2.14401666
C	-2.26401448	1.30712919	3.10983552
C	2.57077271	1.48423635	0.89720150
C	3.12410584	1.80370330	2.14401666
C	2.26401448	1.30712919	3.10983552
C	0.00000000	-2.96847269	0.89720150
C	0.00000000	-3.60740659	2.14401666
C	0.00000000	-2.61425838	3.10983552
H	-4.05157205	2.33917617	2.31145628
C	-2.37933649	1.37371027	4.59307119
H	4.05157205	2.33917617	2.31145628
C	3.18825747	1.84074147	-0.40935406
C	2.37933649	1.37371027	4.59307119
C	-3.18825747	1.84074147	-0.40935406
H	0.00000000	0.00000000	4.18450190
H	0.00000000	-4.67835234	2.31145628
C	0.00000000	-2.74742107	4.59307119
C	0.00000000	-3.68148241	-0.40935406
B	0.00000000	0.00000000	2.99055579
N	-1.41312392	-0.81586749	-1.11449174
N	-1.24138738	-0.71671555	-2.45226664
N	0.00000000	1.63173445	-1.11449174
N	0.00000000	1.43343057	-2.45226664
N	1.41312392	-0.81586749	-1.11449174
N	1.24138738	-0.71671555	-2.45226664
C	-2.57077271	-1.48423635	-0.89720150
C	-3.12410584	-1.80370330	-2.14401666
C	-2.26401448	-1.30712919	-3.10983552
C	0.00000000	2.96847269	-0.89720150
C	0.00000000	3.60740659	-2.14401666
C	0.00000000	2.61425838	-3.10983552
C	2.57077271	-1.48423635	-0.89720150
C	3.12410584	-1.80370330	-2.14401666
C	2.26401448	-1.30712919	-3.10983552
H	-4.05157205	-2.33917617	-2.31145628
C	-2.37933649	-1.37371027	-4.59307119
H	0.00000000	4.67835234	-2.31145628
C	0.00000000	3.68148241	0.40935406
C	0.00000000	2.74742107	-4.59307119
C	-3.18825747	-1.84074147	0.40935406
H	0.00000000	0.00000000	-4.18450190
H	4.05157205	-2.33917617	-2.31145628

C	2.37933649	-1.37371027	-4.59307119
C	3.18825747	-1.84074147	0.40935406
B	0.00000000	0.00000000	-2.99055579
H	3.42830920	0.96141187	-1.01224887
H	4.11984173	2.37859141	-0.21544129
H	2.54676182	2.48829726	-1.01224887
H	-4.11984173	2.37859141	-0.21544129
H	-3.42830920	0.96141187	-1.01224887
H	-2.54676182	2.48829726	-1.01224887
H	0.00000000	-4.75718334	-0.21544129
H	0.88154738	-3.44970913	-1.01224887
H	-0.88154738	-3.44970913	-1.01224887
H	-0.88154738	3.44970913	1.01224887
H	0.00000000	4.75718334	0.21544129
H	0.88154738	3.44970913	1.01224887
H	3.42830920	-0.96141187	1.01224887
H	4.11984173	-2.37859141	0.21544129
H	2.54676182	-2.48829726	1.01224887
H	-2.54676182	-2.48829726	1.01224887
H	-4.11984173	-2.37859141	0.21544129
H	-3.42830920	-0.96141187	1.01224887
H	3.29717061	-1.90362255	-4.85901768
H	2.42337779	-0.37778758	-5.04687772
H	1.53886226	-1.90981286	-5.04687772
H	0.00000000	3.80724456	-4.85901768
H	-0.88451501	2.28760044	-5.04687772
H	0.88451501	2.28760044	-5.04687772
H	-2.42337779	-0.37778758	-5.04687772
H	-3.29717061	-1.90362255	-4.85901768
H	-1.53886226	-1.90981286	-5.04687772
H	0.88451501	-2.28760044	5.04687772
H	0.00000000	-3.80724456	4.85901768
H	-0.88451501	-2.28760044	5.04687772
H	2.42337779	0.37778758	5.04687772
H	1.53886226	1.90981286	5.04687772
H	3.29717061	1.90362255	4.85901768
H	-1.53886226	1.90981286	5.04687772
H	-2.42337779	0.37778758	5.04687772
H	-3.29717061	1.90362255	4.85901768

$[Co(Tb^{3,5\text{-}CF3})_2]^+$ $^5A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.53905858	0.88857591	1.21421572
N	1.28482860	0.74179643	2.53561735
N	0.00000000	-1.77715183	1.21421572
N	0.00000000	-1.48359234	2.53561735
N	-1.53905858	0.88857591	1.21421572
N	-1.28482860	0.74179643	2.53561735
C	2.71533864	1.56770136	1.10783733
C	3.20303898	1.84927551	2.37529675
C	2.27938813	1.31600508	3.25697537
C	0.00000000	-3.13540271	1.10783733
C	0.00000000	-3.69855050	2.37529675
C	0.00000000	-2.63201069	3.25697537
C	-2.71533864	1.56770136	1.10783733
C	-3.20303898	1.84927551	2.37529675
C	-2.27938813	1.31600508	3.25697537
H	4.11196493	2.37404419	2.63083168
C	2.41314827	1.39323215	4.76494320
H	0.00000000	-4.74808784	2.63083168
C	0.00000000	-4.03286351	-0.13482272
C	0.00000000	-2.78646377	4.76494320
C	3.49256243	2.01643202	-0.13482272
H	0.00000000	0.00000000	4.21507459
H	-4.11196493	2.37404419	2.63083168
C	-2.41314827	1.39323215	4.76494320
C	-3.49256243	2.01643202	-0.13482272
B	0.00000000	0.00000000	3.02925823
N	0.00000000	1.77715183	-1.21421572
N	0.00000000	1.48359234	-2.53561735
N	1.53905858	-0.88857591	-1.21421572
N	1.28482860	-0.74179643	-2.53561735
N	-1.53905858	-0.88857591	-1.21421572
N	-1.28482860	-0.74179643	-2.53561735
C	0.00000000	3.13540271	-1.10783733
C	0.00000000	3.69855050	-2.37529675
C	0.00000000	2.63201069	-3.25697537
C	2.71533864	-1.56770136	-1.10783733
C	3.20303898	-1.84927551	-2.37529675
C	2.27938813	-1.31600508	-3.25697537
C	-2.71533864	-1.56770136	-1.10783733
C	-3.20303898	-1.84927551	-2.37529675
C	-2.27938813	-1.31600508	-3.25697537
H	0.00000000	4.74808784	-2.63083168
C	0.00000000	2.78646377	-4.76494320
H	4.11196493	-2.37404419	-2.63083168
C	3.49256243	-2.01643202	0.13482272
C	2.41314827	-1.39323215	-4.76494320
C	0.00000000	4.03286351	0.13482272
H	0.00000000	0.00000000	-4.21507459
H	-4.11196493	-2.37404419	-2.63083168
C	-2.41314827	-1.39323215	-4.76494320
C	-3.49256243	-2.01643202	0.13482272
B	0.00000000	0.00000000	-3.02925823
F	-1.07823622	-3.87584498	-0.92007678
F	0.00000000	-5.31634642	0.28362736
F	1.07823622	-3.87584498	-0.92007678
F	4.60409130	2.65817321	0.28362736
F	2.81746191	2.87170258	-0.92007678
F	3.89569813	1.00414240	-0.92007678
F	-4.60409130	2.65817321	0.28362736
F	-3.89569813	1.00414240	-0.92007678
F	-2.81746191	2.87170258	-0.92007678
F	3.89569813	-1.00414240	0.92007678
F	4.60409130	-2.65817321	-0.28362736
F	2.81746191	-2.87170258	0.92007678
F	-2.81746191	-2.87170258	0.92007678
F	-4.60409130	-2.65817321	-0.28362736
F	-3.89569813	-1.00414240	0.92007678
F	-1.07823622	3.87584498	0.92007678
F	0.00000000	5.31634642	-0.28362736
F	1.07823622	3.87584498	0.92007678
F	-3.55124395	-2.05031154	-5.06204500
F	-1.39401427	-2.06249108	-5.33065696
F	-2.48317694	-0.17600594	-5.33065696
F	3.55124395	-2.05031154	-5.06204500
F	2.48317694	-0.17600594	-5.33065696
F	1.39401427	-2.06249108	-5.33065696
F	1.08916267	2.23849702	-5.33065696

F	0.00000000	4.10062307	-5.06204500
F	-1.08916267	2.23849702	-5.33065696
F	-2.48317694	0.17600594	5.33065696
F	-3.55124395	2.05031154	5.06204500
F	-1.39401427	2.06249108	5.33065696
F	-1.08916267	-2.23849702	5.33065696
F	1.08916267	-2.23849702	5.33065696
F	0.00000000	-4.10062307	5.06204500
F	2.48317694	0.17600594	5.33065696
F	1.39401427	2.06249108	5.33065696
F	3.55124395	2.05031154	5.06204500

$[Co(Tb^{3,5\text{-}CF3})_2]^+$ ^3E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.50890000	0.87120000	1.15380000
N	1.27530000	0.73630000	2.47760000
N	0.00000000	-1.74240000	1.15380000
N	0.00000000	-1.47260000	2.47760000
N	-1.50890000	0.87120000	1.15380000
N	-1.27530000	0.73630000	2.47760000
C	2.68390000	1.54960000	1.01800000
C	3.18670000	1.83990000	2.28010000
C	2.28000000	1.31640000	3.17890000
C	0.00000000	-3.09910000	1.01800000
C	0.00000000	-3.67970000	2.28010000
C	0.00000000	-2.63270000	3.17890000
C	-2.68390000	1.54960000	1.01800000
C	-3.18670000	1.83990000	2.28010000
C	-2.28000000	1.31640000	3.17890000
H	4.09960000	2.36690000	2.51540000
C	2.43310000	1.40470000	4.68390000
H	0.00000000	-4.73380000	2.51540000
C	0.00000000	-4.00160000	-0.22370000
C	0.00000000	-2.80940000	4.68390000
C	3.46550000	2.00080000	-0.22370000
H	0.00000000	0.00000000	4.16940000
H	-4.09960000	2.36690000	2.51540000
C	-2.43310000	1.40470000	4.68390000
C	-3.46550000	2.00080000	-0.22370000
B	0.00000000	0.00000000	2.98400000
N	0.00000000	1.74240000	-1.15380000
N	0.00000000	1.47260000	-2.47760000
N	1.50890000	-0.87120000	-1.15380000
N	1.27530000	-0.73630000	-2.47760000
N	-1.50890000	-0.87120000	-1.15380000
N	-1.27530000	-0.73630000	-2.47760000
C	0.00000000	3.09910000	-1.01800000
C	0.00000000	3.67970000	-2.28010000
C	0.00000000	2.63270000	-3.17890000
C	2.68390000	-1.54960000	-1.01800000
C	3.18670000	-1.83990000	-2.28010000
C	2.28000000	-1.31640000	-3.17890000
C	-2.68390000	-1.54960000	-1.01800000
C	-3.18670000	-1.83990000	-2.28010000
C	-2.28000000	-1.31640000	-3.17890000
H	0.00000000	4.73380000	-2.51540000
C	0.00000000	2.80940000	-4.68390000
H	4.09960000	-2.36690000	-2.51540000
C	3.46550000	-2.00080000	0.22370000
C	2.43310000	-1.40470000	-4.68390000
C	0.00000000	4.00160000	0.22370000
H	0.00000000	0.00000000	-4.16940000
H	-4.09960000	-2.36690000	-2.51540000
C	-2.43310000	-1.40470000	-4.68390000
C	-3.46550000	-2.00080000	0.22370000
B	0.00000000	0.00000000	-2.98400000
F	-1.07880000	-3.85210000	-1.00890000
F	0.00000000	-5.28250000	0.20240000
F	1.07880000	-3.85210000	-1.00890000
F	4.57480000	2.64130000	0.20240000
F	2.79660000	2.86040000	-1.00890000
F	3.87550000	0.99180000	-1.00890000
F	-4.57480000	2.64130000	0.20240000
F	-3.87550000	0.99180000	-1.00890000
F	-2.79660000	2.86040000	-1.00890000
F	3.87550000	-0.99180000	1.00890000
F	4.57480000	-2.64130000	-0.20240000
F	2.79660000	-2.86040000	1.00890000
F	-2.79660000	-2.86040000	1.00890000
F	-4.57480000	-2.64130000	-0.20240000
F	-3.87550000	-0.99180000	1.00890000
F	-1.07880000	3.85210000	1.00890000
F	0.00000000	5.28250000	-0.20240000
F	1.07880000	3.85210000	1.00890000
F	-3.57510000	-2.06410000	-4.95970000
F	-1.42140000	-2.07800000	-5.25840000
F	-2.51030000	-0.19200000	-5.25840000
F	3.57510000	-2.06410000	-4.95970000
F	2.51030000	-0.19200000	-5.25840000
F	1.42140000	-2.07800000	-5.25840000
F	1.08890000	2.27000000	-5.25840000
F	0.00000000	4.12810000	-4.95970000
F	-1.08890000	2.27000000	-5.25840000
F	-2.51030000	0.19200000	5.25840000
F	-3.57510000	2.06410000	4.95970000
F	-1.42140000	2.07800000	5.25840000
F	-1.08890000	-2.27000000	5.25840000
F	1.08890000	-2.27000000	5.25840000
F	0.00000000	-4.12810000	4.95970000
F	2.51030000	0.19200000	5.25840000
F	1.42140000	2.07800000	5.25840000
F	3.57510000	2.06410000	4.95970000

$[Co(Tb^{3,5\text{-}CF3})_2]^+$ $^1A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.46798425	0.84754139	1.09000723
N	1.26190782	0.72856277	2.41845644
N	0.00000000	-1.69508226	1.09000723
N	0.00000000	-1.45712554	2.41845644
N	-1.46798425	0.84754139	1.09000723
N	-1.26190782	0.72856277	2.41845644
C	2.64219841	1.52547407	0.92212364
C	3.16395394	1.82670981	2.17622979
C	2.27779055	1.31508325	3.09491854
C	0.00000000	-3.05094761	0.92212364
C	0.00000000	-3.65341961	2.17622979
C	0.00000000	-2.63016597	3.09491854
C	-2.64219841	1.52547407	0.92212364

C	-3.16395394	1.82670981	2.17622979
C	-2.27779055	1.31508325	3.09491854
H	4.08073024	2.35601035	2.38805098
C	2.45176868	1.41552956	4.59652354
H	0.00000000	-4.71202124	2.38805098
C	0.00000000	-3.95738432	-0.31924734
C	0.00000000	-2.83105912	4.59652354
C	3.42719528	1.97869216	-0.31924734
H	0.00000000	0.00000000	4.12670305
H	-4.08073024	2.35601035	2.38805098
C	-2.45176868	1.41552956	4.59652354
C	-3.42719528	1.97869216	-0.31924734
B	0.00000000	0.00000000	2.94235515
N	0.00000000	1.69508226	-1.09000723
N	0.00000000	1.45712554	-2.41845644
N	1.46798425	-0.84754139	-1.09000723
N	1.26190782	-0.72856277	-2.41845644
N	-1.46798425	-0.84754139	-1.09000723
N	-1.26190782	-0.72856277	-2.41845644
C	0.00000000	3.05094761	-0.92212364
C	0.00000000	3.65341961	-2.17622979
C	0.00000000	2.63016597	-3.09491854
C	2.64219841	-1.52547407	-0.92212364
C	3.16395394	-1.82670981	-2.17622979
C	2.27779055	-1.31508325	-3.09491854
C	-2.64219841	-1.52547407	-0.92212364
C	-3.16395394	-1.82670981	-2.17622979
C	-2.27779055	-1.31508325	-3.09491854
H	0.00000000	4.71202124	-2.38805098
C	0.00000000	2.83105912	-4.59652354
H	4.08073024	-2.35601035	-2.38805098
C	3.42719528	-1.97869216	0.31924734
C	2.45176868	-1.41552956	-4.59652354
C	0.00000000	3.95738432	0.31924734
H	0.00000000	0.00000000	-4.12670305
H	-4.08073024	-2.35601035	-2.38805098
C	-2.45176868	-1.41552956	-4.59652354
C	-3.42719528	-1.97869216	0.31924734
B	0.00000000	0.00000000	-2.94235515
F	-1.07972267	-3.81381165	-1.10313295
F	0.00000000	-5.23672112	0.11114204
F	1.07972267	-3.81381165	-1.10313295
F	4.53513316	2.61836056	0.11114204
F	2.76299634	2.84197287	-1.10313295
F	3.84271902	0.97183878	-1.10313295
F	-4.53513316	2.61836056	0.11114204
F	-3.84271902	0.97183878	-1.10313295
F	-2.76299634	2.84197287	-1.10313295
F	3.84271902	-0.97183878	1.10313295
F	4.53513316	-2.61836056	-0.11114204
F	2.76299634	-2.84197287	1.10313295
F	-2.76299634	-2.84197287	1.10313295
F	-4.53513316	-2.61836056	-0.11114204
F	-3.84271902	-0.97183878	1.10313295
F	-1.07972267	3.81381165	1.10313295
F	0.00000000	5.23672112	-0.11114204
F	1.07972267	3.81381165	1.10313295
F	-3.59727867	-2.07688999	-4.85058524
F	-1.44784271	-2.09319077	-5.17997480
F	-2.53667782	-0.20727291	-5.17997480
F	3.59727867	-2.07688999	-4.85058524
F	2.53667782	-0.20727291	-5.17997480
F	1.44784271	-2.09319077	-5.17997480
F	1.08883511	2.30046368	-5.17997480
F	0.00000000	4.15377999	-4.85058524
F	-1.08883511	2.30046368	-5.17997480
F	-2.53667782	0.20727291	5.17997480
F	-3.59727867	2.07688999	4.85058524
F	-1.44784271	2.09319077	5.17997480
F	-1.08883511	-2.30046368	5.17997480
F	1.08883511	-2.30046368	5.17997480
F	0.00000000	-4.15377999	4.85058524
F	2.53667782	0.20727291	5.17997480
F	1.44784271	2.09319077	5.17997480
F	3.59727867	2.07688999	4.85058524

$[Co(Tb^{3,5\text{-}NH2})_2]^+$ $^5A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.68203169	1.30578190
N	0.00000000	1.45033302	2.66329776
N	1.45668209	-0.84101558	1.30578190
N	1.25602548	-0.72516651	2.66329776
N	-1.45668209	-0.84101558	1.30578190
N	-1.25602548	-0.72516651	2.66329776
C	0.00000000	3.02887457	1.15565379
C	0.00000000	3.66862129	2.40381676
C	0.00000000	2.62961775	3.32964093
C	2.62308188	-1.51443702	1.15565379
C	3.17711934	-1.83431038	2.40381676
C	2.27731588	-1.31480861	3.32964093
C	-2.62308188	-1.51443702	1.15565379
C	-3.17711934	-1.83431038	2.40381676
C	-2.27731588	-1.31480861	3.32964093
H	0.00000000	4.73238609	2.60824428
N	0.00000000	2.71362940	4.68757642
H	4.09836666	-2.36619331	2.60824428
N	3.12164358	-1.80228140	-0.06662289
N	2.35007193	-1.35681470	4.68757642
N	0.00000000	3.60456333	-0.06662289
H	0.00000000	0.00000000	4.37637363
H	-4.09836666	-2.36619331	2.60824428
N	-2.35007193	-1.35681470	4.68757642
N	-3.12164358	-1.80228140	-0.06662289
B	0.00000000	0.00000000	3.16405290
N	-1.45668209	0.84101558	-1.30578190
N	-1.25602548	0.72516651	-2.66329776
N	1.45668209	0.84101558	-1.30578190
N	1.25602548	0.72516651	-2.66329776
N	0.00000000	-1.68203169	-1.30578190
N	0.00000000	-1.45033302	-2.66329776
C	-2.62308188	1.51443702	-1.15565379
C	-3.17711934	1.83431038	-2.40381676
C	-2.27731588	1.31480861	-3.32964093
C	2.62308188	1.51443702	-1.15565379
C	3.17711934	1.83431038	-2.40381676
C	2.27731588	1.31480861	-3.32964093
C	0.00000000	-3.02887457	-1.15565379
C	0.00000000	-3.66862129	-2.40381676
C	0.00000000	-2.62961775	-3.32964093

H	-4.09836666	2.36619331	-2.60824428
N	-2.35007193	1.35681470	-4.68757642
H	4.09836666	2.36619331	-2.60824428
N	3.12164358	1.80228140	0.06662289
N	2.35007193	1.35681470	-4.68757642
N	-3.12164358	1.80228140	0.06662289
H	0.00000000	0.00000000	-4.37637363
H	0.00000000	-4.73238609	-2.60824428
N	0.00000000	-2.71362940	-4.68757642
N	0.00000000	-3.60456333	0.06662289
B	0.00000000	0.00000000	-3.16405290
H	0.00000000	3.61235017	5.13111216
H	0.00000000	1.89139696	5.25916458
H	3.12838688	-1.80617508	5.13111216
H	1.63799779	-0.94569848	5.25916458
H	-3.12838688	-1.80617508	5.13111216
H	-1.63799779	-0.94569848	5.25916458
H	-3.12838688	1.80617508	-5.13111216
H	-1.63799779	0.94569848	-5.25916458
H	3.12838688	1.80617508	-5.13111216
H	1.63799779	0.94569848	-5.25916458
H	0.00000000	-3.61235017	-5.13111216
H	0.00000000	-1.89139696	-5.25916458
H	0.00000000	4.60228681	-0.15624276
H	3.98569742	-2.30114367	-0.15624276
H	-3.98569742	-2.30114367	-0.15624276
H	-3.98569742	2.30114367	0.15624276
H	3.98569742	2.30114367	0.15624276
H	0.00000000	-4.60228681	0.15624276
H	2.62760052	-1.51704587	-0.89338984
H	0.00000000	3.03409120	-0.89338984
H	-2.62760052	-1.51704587	-0.89338984
H	2.62760052	1.51704587	0.89338984
H	-2.62760052	1.51704587	0.89338984
H	0.00000000	-3.03409120	0.89338984

$[Co(Tb^{3,5\text{-}NH2})_2]^+$ ^3E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.64561477	1.22912052
N	0.00000000	1.44089250	2.59244516
N	1.42514418	-0.82280765	1.22912052
N	1.24784917	-0.72044625	2.59244516
N	-1.42514418	-0.82280765	1.22912052
N	-1.24784917	-0.72044625	2.59244516
C	0.00000000	2.98604085	1.04526424
C	0.00000000	3.64912799	2.28379301
C	0.00000000	2.63319816	3.23241096
C	2.58598708	-1.49302016	1.04526424
C	3.16023753	-1.82456399	2.28379301
C	2.28041686	-1.31659934	3.23241096
C	-2.58598708	-1.49302016	1.04526424
C	-3.16023753	-1.82456399	2.28379301
C	-2.28041686	-1.31659934	3.23241096
H	0.00000000	4.71773635	2.46124466
N	0.00000000	2.74325115	4.58958232
H	4.08567964	-2.35886791	2.46124466
N	3.07708209	-1.77655439	-0.18044150
N	2.37572538	-1.37162531	4.58958232
N	0.00000000	3.55310825	-0.18044150
H	0.00000000	0.00000000	4.31815726
H	-4.08567964	-2.35886791	2.46124466
N	-2.37572538	-1.37162531	4.58958232
N	-3.07708209	-1.77655439	-0.18044150
B	0.00000000	0.00000000	3.10745422
N	-1.42514418	0.82280765	-1.22912052
N	-1.24784917	0.72044625	-2.59244516
N	1.42514418	0.82280765	-1.22912052
N	1.24784917	0.72044625	-2.59244516
N	0.00000000	-1.64561477	-1.22912052
N	0.00000000	-1.44089250	-2.59244516
C	-2.58598708	1.49302016	-1.04526424
C	-3.16023753	1.82456399	-2.28379301
C	-2.28041686	1.31659934	-3.23241096
C	2.58598708	1.49302016	-1.04526424
C	3.16023753	1.82456399	-2.28379301
C	2.28041686	1.31659934	-3.23241096
C	0.00000000	-2.98604085	-1.04526424
C	0.00000000	-3.64912799	-2.28379301
C	0.00000000	-2.63319816	-3.23241096
H	-4.08567964	2.35886791	-2.46124466
N	-2.37572538	1.37162531	-4.58958232
H	4.08567964	2.35886791	-2.46124466
N	3.07708209	1.77655439	0.18044150
N	2.37572538	1.37162531	-4.58958232
N	-3.07708209	1.77655439	0.18044150
H	0.00000000	0.00000000	-4.31815726
H	0.00000000	-4.71773635	-2.46124466
N	0.00000000	-2.74325115	-4.58958232
N	0.00000000	-3.55310825	0.18044150
B	0.00000000	0.00000000	-3.10745422
H	0.00000000	3.65069276	5.01470692
H	0.00000000	1.93317445	5.17807452
H	3.16159275	-1.82534665	5.01470692
H	1.67417817	-0.96658722	5.17807452
H	-3.16159275	-1.82534665	5.01470692
H	-1.67417817	-0.96658722	5.17807452
H	-3.16159275	1.82534665	-5.01470692
H	-1.67417817	0.96658722	-5.17807452
H	3.16159275	1.82534665	-5.01470692
H	1.67417817	0.96658722	-5.17807452
H	0.00000000	-3.65069276	-5.01470692
H	0.00000000	-1.93317445	-5.17807452
H	0.00000000	4.55064546	-0.27131553
H	3.94097453	-2.27532299	-0.27131553
H	-3.94097453	-2.27532299	-0.27131553
H	-3.94097453	2.27532299	0.27131553
H	3.94097453	2.27532299	0.27131553
H	0.00000000	-4.55064546	0.27131553
H	2.58208440	-1.49076692	-1.00546588
H	0.00000000	2.98153385	-1.00546588
H	-2.58208440	-1.49076692	-1.00546588
H	2.58208440	1.49076692	1.00546588
H	-2.58208440	1.49076692	1.00546588
H	0.00000000	-2.98153385	1.00546588

$[Co(Tb^{3,5\text{-}NH2})_2]^+$ $^1A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.60612650	1.13950277

N	0.00000000	1.43021687	2.51147787
N	1.39094610	-0.80306299	1.13950277
N	1.23860391	-0.71510844	2.51147787
N	-1.39094610	-0.80306299	1.13950277
N	-1.23860391	-0.71510844	2.51147787
C	0.00000000	2.93800425	0.91786376
C	0.00000000	3.62557166	2.14528086
C	0.00000000	2.63623828	3.11925593
C	2.54438634	-1.46900239	0.91786376
C	3.13983722	-1.81278610	2.14528086
C	2.28304951	-1.31811914	3.11925593
C	-2.54438634	-1.46900239	0.91786376
C	-3.13983722	-1.81278610	2.14528086
C	-2.28304951	-1.31811914	3.11925593
H	0.00000000	4.69862723	2.29240007
N	0.00000000	2.77848113	4.47445240
H	4.06913068	-2.34931362	2.29240007
N	3.03180621	-1.75041409	-0.30908926
N	2.40623563	-1.38924056	4.47445240
N	0.00000000	3.50082818	-0.30908926
H	0.00000000	0.00000000	4.25126449
H	-4.06913068	-2.34931362	2.29240007
N	-2.40623563	-1.38924056	4.47445240
N	-3.03180621	-1.75041409	-0.30908926
B	0.00000000	0.00000000	3.04253687
N	-1.39094610	0.80306299	-1.13950277
N	-1.23860391	0.71510844	-2.51147787
N	1.39094610	0.80306299	-1.13950277
N	1.23860391	0.71510844	-2.51147787
N	0.00000000	-1.60612650	-1.13950277
N	0.00000000	-1.43021687	-2.51147787
C	-2.54438634	1.46900239	-0.91786376
C	-3.13983722	1.81278610	-2.14528086
C	-2.28304951	1.31811914	-3.11925593
C	2.54438634	1.46900239	-0.91786376
C	3.13983722	1.81278610	-2.14528086
C	2.28304951	1.31811914	-3.11925593
C	0.00000000	-2.93800425	-0.91786376
C	0.00000000	-3.62557166	-2.14528086
C	0.00000000	-2.63623828	-3.11925593
H	-4.06913068	2.34931362	-2.29240007
N	-2.40623563	1.38924056	-4.47445240
H	4.06913068	2.34931362	-2.29240007
N	3.03180621	1.75041409	0.30908926
N	2.40623563	1.38924056	-4.47445240
N	-3.03180621	1.75041409	0.30908926
H	0.00000000	0.00000000	-4.25126449
H	0.00000000	-4.69862723	-2.29240007
N	0.00000000	-2.77848113	-4.47445240
N	0.00000000	-3.50082818	0.30908926
B	0.00000000	0.00000000	-3.04253687
H	0.00000000	3.69624170	4.87635035
H	0.00000000	1.98428292	5.08393653
H	3.20103921	-1.84812085	4.87635035
H	1.71843961	-0.99214119	5.08393653
H	-3.20103921	-1.84812085	4.87635035
H	-1.71843961	-0.99214119	5.08393653
H	-3.20103921	1.84812085	-4.87635035
H	-1.71843961	0.99214119	-5.08393653
H	3.20103921	1.84812085	-4.87635035
H	1.71843961	0.99214119	-5.08393653
H	0.00000000	-3.69624170	-4.87635035
H	0.00000000	-1.98428292	-5.08393653
H	0.00000000	4.49862681	-0.39555417
H	3.89592514	-2.24931340	-0.39555417
H	-3.89592514	-2.24931340	-0.39555417
H	-3.89592514	2.24931340	0.39555417
H	3.89592514	2.24931340	0.39555417
H	0.00000000	-4.49862681	0.39555417
H	2.54146581	-1.46731590	-1.13669601
H	0.00000000	2.93463181	-1.13669601
H	-2.54146581	-1.46731590	-1.13669601
H	2.54146581	1.46731590	1.13669601
H	-2.54146581	1.46731590	1.13669601
H	0.00000000	-2.93463181	1.13669601

$[Co(Tb^{3,5\text{-}NO2})_2]^+$ $^5A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.75629272	1.31083343
N	0.00000000	1.47120165	2.62252783
N	1.52099406	-0.87814636	1.31083343
N	1.27409794	-0.73560083	2.62252783
N	-1.52099406	-0.87814636	1.31083343
N	-1.27409794	-0.73560083	2.62252783
C	0.00000000	3.10502529	1.22293285
C	0.00000000	3.70456354	2.46659782
C	0.00000000	2.63541012	3.33432944
C	2.68903059	-1.55251238	1.22293285
C	3.20824608	-1.85228177	2.46659782
C	2.28233195	-1.31770480	3.33432944
C	-2.68903059	-1.55251238	1.22293285
C	-3.20824608	-1.85228177	2.46659782
C	-2.28233195	-1.31770480	3.33432944
H	0.00000000	4.75737543	2.70595686
N	0.00000000	2.82223139	4.79311130
H	4.12000789	-2.37868772	2.70595686
N	3.36298174	-1.94161853	-0.00895791
N	2.44412419	-1.41111569	4.79311130
N	0.00000000	3.88323653	-0.00895791
H	0.00000000	0.00000000	4.28342894
H	-4.12000789	-2.37868772	2.70595686
N	-2.44412419	-1.41111569	4.79311130
N	-3.36298174	-1.94161853	-0.00895791
B	0.00000000	0.00000000	3.11840131
N	-1.52099406	0.87814636	-1.31083343
N	-1.27409794	0.73560083	-2.62252783
N	1.52099406	0.87814636	-1.31083343
N	1.27409794	0.73560083	-2.62252783
N	0.00000000	-1.75629272	-1.31083343
N	0.00000000	-1.47120165	-2.62252783
C	-2.68903059	1.55251238	-1.22293285
C	-3.20824608	1.85228177	-2.46659782
C	-2.28233195	1.31770480	-3.33432944
C	2.68903059	1.55251238	-1.22293285
C	3.20824608	1.85228177	-2.46659782
C	2.28233195	1.31770480	-3.33432944
C	0.00000000	-3.10502529	-1.22293285
C	0.00000000	-3.70456354	-2.46659782
C	0.00000000	-2.63541012	-3.33432944

H	-4.12000789	2.37868772	-2.70595686
N	-2.44412419	1.41111569	-4.79311130
H	4.12000789	2.37868772	-2.70595686
N	3.36298174	1.94161853	0.00895791
N	2.44412419	1.41111569	-4.79311130
N	-3.36298174	1.94161853	0.00895791
H	0.00000000	0.00000000	-4.28342894
H	0.00000000	-4.75737543	-2.70595686
N	0.00000000	-2.82223139	-4.79311130
N	0.00000000	-3.88323653	0.00895791
B	0.00000000	0.00000000	-3.11840131
O	0.00000000	3.99569199	5.13568054
O	0.00000000	1.85810960	5.53148237
O	3.46037099	-1.99784626	5.13568054
O	1.60917033	-0.92905480	5.53148237
O	-3.46037099	-1.99784626	5.13568054
O	-1.60917033	-0.92905480	5.53148237
O	-3.46037099	1.99784626	-5.13568054
O	-1.60917033	0.92905480	-5.53148237
O	3.46037099	1.99784626	-5.13568054
O	1.60917033	0.92905480	-5.53148237
O	0.00000000	-3.99569199	-5.13568054
O	0.00000000	-1.85810960	-5.53148237
O	0.00000000	5.09307384	0.14022721
O	4.41073153	-2.54653692	0.14022721
O	-4.41073153	-2.54653692	0.14022721
O	-4.41073153	2.54653692	-0.14022721
O	4.41073153	2.54653692	-0.14022721
O	0.00000000	-5.09307384	-0.14022721
O	2.84521832	-1.64268736	-1.07459812
O	0.00000000	3.28537525	-1.07459812
O	-2.84521832	-1.64268736	-1.07459812
O	2.84521832	1.64268736	1.07459812
O	-2.84521832	1.64268736	1.07459812
O	0.00000000	-3.28537525	1.07459812

$[Co(Tb^{3,5\text{-}NO2})_2]^+$ ^3E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.76216077	1.33355736
N	0.00000000	1.47228647	2.64035105
N	1.52607575	-0.88108012	1.33355736
N	1.27503776	-0.73614323	2.64035105
N	-1.52607575	-0.88108012	1.33355736
N	-1.27503776	-0.73614323	2.64035105
C	0.00000000	3.10742776	1.24988121
C	0.00000000	3.70651091	2.49803994
C	0.00000000	2.63617531	3.35979186
C	2.69111185	-1.55371414	1.24988121
C	3.20993257	-1.85325545	2.49803994
C	2.28299501	-1.31808739	3.35979186
C	-2.69111185	-1.55371414	1.24988121
C	-3.20993257	-1.85325545	2.49803994
C	-2.28299501	-1.31808739	3.35979186
H	0.00000000	4.75912013	2.73779110
N	0.00000000	2.81595958	4.81011377
H	4.12151923	-2.37956033	2.73779110
N	3.36813804	-1.94459515	0.02355527
N	2.43869271	-1.40797979	4.81011377
N	0.00000000	3.88919083	0.02355527
H	0.00000000	0.00000000	4.29664514
H	-4.12151923	-2.37956033	2.73779110
N	-2.43869271	-1.40797979	4.81011377
N	-3.36813804	-1.94459515	0.02355527
B	0.00000000	0.00000000	3.13157570
N	-1.52607575	0.88108012	-1.33355736
N	-1.27503776	0.73614323	-2.64035105
N	1.52607575	0.88108012	-1.33355736
N	1.27503776	0.73614323	-2.64035105
N	0.00000000	-1.76216077	-1.33355736
N	0.00000000	-1.47228647	-2.64035105
C	-2.69111185	1.55371414	-1.24988121
C	-3.20993257	1.85325545	-2.49803994
C	-2.28299501	1.31808739	-3.35979186
C	2.69111185	1.55371414	-1.24988121
C	3.20993257	1.85325545	-2.49803994
C	2.28299501	1.31808739	-3.35979186
C	0.00000000	-3.10742776	-1.24988121
C	0.00000000	-3.70651091	-2.49803994
C	0.00000000	-2.63617531	-3.35979186
H	-4.12151923	2.37956033	-2.73779110
N	-2.43869271	1.40797979	-4.81011377
H	4.12151923	2.37956033	-2.73779110
N	3.36813804	1.94459515	-0.02355527
N	2.43869271	1.40797979	-4.81011377
N	-3.36813804	1.94459515	-0.02355527
H	0.00000000	0.00000000	-4.29664514
H	0.00000000	-4.75912013	-2.73779110
N	0.00000000	-2.81595958	-4.81011377
N	0.00000000	-3.88919083	-0.02355527
B	0.00000000	0.00000000	-3.13157570
O	0.00000000	3.98727013	5.16798046
O	0.00000000	1.85525098	5.55637116
O	3.45307734	-1.99363507	5.16798046
O	1.60669484	-0.92762549	5.55637116
O	-3.45307734	-1.99363507	5.16798046
O	-1.60669484	-0.92762549	5.55637116
O	-3.45307734	1.99363507	-5.16798046
O	-1.60669484	0.92762549	-5.55637116
O	3.45307734	1.99363507	-5.16798046
O	1.60669484	0.92762549	-5.55637116
O	0.00000000	-3.98727013	-5.16798046
O	0.00000000	-1.85525098	-5.55637116
O	0.00000000	5.09967162	0.17441523
O	4.41644505	-2.54983581	0.17441523
O	-4.41644505	-2.54983581	0.17441523
O	-4.41644505	2.54983581	-0.17441523
O	4.41644505	2.54983581	-0.17441523
O	0.00000000	-5.09967162	-0.17441523
O	2.85791963	-1.65002070	-1.04768575
O	0.00000000	3.30004140	-1.04768575
O	-2.85791963	-1.65002070	-1.04768575
O	2.85791963	1.65002070	1.04768575
O	-2.85791963	1.65002070	1.04768575
O	0.00000000	-3.30004140	1.04768575

$[Co(Tb^{3,5\text{-}NO2})_2]^+$ $^1A_{1g}$ D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.66338983	1.11664655

N	0.00000000	1.44691083	2.43702527
N	1.44053795	-0.83169518	1.11664655
N	1.25306156	-0.72345568	2.43702527
N	-1.44053795	-0.83169518	1.11664655
N	-1.25306156	-0.72345568	2.43702527
C	0.00000000	3.01148210	0.94816815
C	0.00000000	3.65901884	2.17206252
C	0.00000000	2.63928899	3.08946219
C	2.60801991	-1.50574105	0.94816815
C	3.16880332	-1.82950968	2.17206252
C	2.28569116	-1.31964423	3.08946219
C	-2.60801991	-1.50574105	0.94816815
C	-3.16880332	-1.82950968	2.17206252
C	-2.28569116	-1.31964423	3.08946219
H	0.00000000	4.72242539	2.35817892
N	0.00000000	2.87985720	4.54283692
H	4.08974001	-2.36121270	2.35817892
N	3.28260395	-1.89521233	-0.29371930
N	2.49402931	-1.43992886	4.54283692
N	0.00000000	3.79042466	-0.29371930
H	0.00000000	0.00000000	4.13744164
H	-4.08974001	-2.36121270	2.35817892
N	-2.49402931	-1.43992886	4.54283692
N	-3.28260395	-1.89521233	-0.29371930
B	0.00000000	0.00000000	2.97223885
N	-1.44053795	0.83169518	-1.11664655
N	-1.25306156	0.72345568	-2.43702527
N	1.44053795	0.83169518	-1.11664655
N	1.25306156	0.72345568	-2.43702527
N	0.00000000	-1.66338983	-1.11664655
N	0.00000000	-1.44691083	-2.43702527
C	-2.60801991	1.50574105	-0.94816815
C	-3.16880332	1.82950968	-2.17206252
C	-2.28569116	1.31964423	-3.08946219
C	2.60801991	1.50574105	-0.94816815
C	3.16880332	1.82950968	-2.17206252
C	2.28569116	1.31964423	-3.08946219
C	0.00000000	-3.01148210	-0.94816815
C	0.00000000	-3.65901884	-2.17206252
C	0.00000000	-2.63928899	-3.08946219
H	-4.08974001	2.36121270	-2.35817892
N	-2.49402931	1.43992886	-4.54283692
H	4.08974001	2.36121270	-2.35817892
N	3.28260395	1.89521233	0.29371930
N	2.49402931	1.43992886	-4.54283692
N	-3.28260395	1.89521233	0.29371930
H	0.00000000	0.00000000	-4.13744164
H	0.00000000	-4.72242539	-2.35817892
N	0.00000000	-2.87985720	-4.54283692
N	0.00000000	-3.79042466	0.29371930
B	0.00000000	0.00000000	-2.97223885
O	0.00000000	4.06542750	4.83153804
O	0.00000000	1.93811009	5.30881993
O	3.52076335	-2.03271375	4.83153804
O	1.67845286	-0.96905531	5.30881993
O	-3.52076335	-2.03271375	4.83153804
O	-1.67845286	-0.96905531	5.30881993
O	-3.52076335	2.03271375	-4.83153804
O	-1.67845286	0.96905531	-5.30881993
O	3.52076335	2.03271375	-4.83153804
O	1.67845286	0.96905531	-5.30881993
O	0.00000000	-4.06542750	-4.83153804
O	0.00000000	-1.93811009	-5.30881993
O	0.00000000	4.99774943	-0.13139048
O	4.32817829	-2.49887498	-0.13139048
O	-4.32817829	-2.49887498	-0.13139048
O	-4.32817829	2.49887498	0.13139048
O	4.32817829	2.49887498	0.13139048
O	0.00000000	-4.99774943	0.13139048
O	2.78023588	-1.60516975	-1.36660607
O	0.00000000	3.21034003	-1.36660607
O	-2.78023588	-1.60516975	-1.36660607
O	2.78023588	1.60516975	1.36660607
O	-2.78023588	1.60516975	1.36660607
O	0.00000000	-3.21034003	1.36660607

$[Co(Tb^{3CH3})_2]$ ^4E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.52156557	0.87847657	1.34106585
N	1.26009803	0.72751817	2.65557230
N	0.00000000	-1.75695260	1.34106585
N	0.00000000	-1.45503635	2.65557230
N	-1.52156557	0.87847657	1.34106585
N	-1.26009803	0.72751817	2.65557230
C	2.68829398	1.55208745	1.25285518
C	3.16752430	1.82877095	2.54507321
C	2.22903427	1.28693367	3.40278698
C	0.00000000	-3.10417491	1.25285518
C	0.00000000	-3.65754191	2.54507321
C	0.00000000	-2.57386734	3.40278698
C	-2.68829398	1.55208745	1.25285518
C	-3.16752430	1.82877095	2.54507321
C	-2.22903427	1.28693367	3.40278698
H	4.07789809	2.35437573	2.81084561
H	2.17973136	1.25846817	4.48398447
H	0.00000000	-4.70875145	2.81084561
C	0.00000000	-3.86352785	-0.03036631
H	0.00000000	-2.51693686	4.48398447
C	3.34591313	1.93176366	-0.03036631
H	0.00000000	0.00000000	4.35649192
H	-4.07789809	2.35437573	2.81084561
H	-2.17973136	1.25846817	4.48398447
C	-3.34591313	1.93176366	-0.03036631
B	0.00000000	0.00000000	3.14966457
N	0.00000000	1.75695260	-1.34106585
N	0.00000000	1.45503635	-2.65557230
N	1.52156557	-0.87847657	-1.34106585
N	1.26009803	-0.72751817	-2.65557230
N	-1.52156557	-0.87847657	-1.34106585
N	-1.26009803	-0.72751817	-2.65557230
C	0.00000000	3.10417491	-1.25285518
C	0.00000000	3.65754191	-2.54507321
C	0.00000000	2.57386734	-3.40278698
C	2.68829398	-1.55208745	-1.25285518
C	3.16752430	-1.82877095	-2.54507321
C	2.22903427	-1.28693367	-3.40278698
C	-2.68829398	-1.55208745	-1.25285518
C	-3.16752430	-1.82877095	-2.54507321
C	-2.22903427	-1.28693367	-3.40278698

H	0.00000000	4.70875145	-2.81084561
H	0.00000000	2.51693686	-4.48398447
H	4.07789809	-2.35437573	-2.81084561
C	3.34591313	-1.93176366	0.03036631
H	2.17973136	-1.25846817	-4.48398447
C	0.00000000	3.86352785	0.03036631
H	0.00000000	0.00000000	-4.35649192
H	-4.07789809	-2.35437573	-2.81084561
H	-2.17973136	-1.25846817	-4.48398447
C	-3.34591313	-1.93176366	0.03036631
B	0.00000000	0.00000000	-3.14966457
H	-0.87686363	-3.63759933	-0.64252014
H	0.00000000	-4.93653950	0.18214810
H	0.87686363	-3.63759933	-0.64252014
H	4.27516849	2.46827002	0.18214810
H	2.71182120	2.57818595	-0.64252014
H	3.58868483	1.05941338	-0.64252014
H	-4.27516849	2.46827002	0.18214810
H	-3.58868483	1.05941338	-0.64252014
H	-2.71182120	2.57818595	-0.64252014
H	3.58868483	-1.05941338	0.64252014
H	4.27516849	-2.46827002	-0.18214810
H	2.71182120	-2.57818595	0.64252014
H	-2.71182120	-2.57818595	0.64252014
H	-4.27516849	-2.46827002	-0.18214810
H	-3.58868483	-1.05941338	0.64252014
H	-0.87686363	3.63759933	0.64252014
H	0.00000000	4.93653950	-0.18214810
H	0.87686363	3.63759933	0.64252014

$[Co(Tb^{3CH3})_2]$ ^2E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.47605897	0.85220345	1.23002118
N	1.25024316	0.72182793	2.55212926
N	0.00000000	-1.70440636	1.23002118
N	0.00000000	-1.44365639	2.55212926
N	-1.47605897	0.85220345	1.23002118
N	-1.25024316	0.72182793	2.55212926
C	2.64106650	1.52482054	1.09834601
C	3.15093036	1.81919073	2.37625033
C	2.23723493	1.29166822	3.26681171
C	0.00000000	-3.04964055	1.09834601
C	0.00000000	-3.63838146	2.37625033
C	0.00000000	-2.58333643	3.26681171
C	-2.64106650	1.52482054	1.09834601
C	-3.15093036	1.81919073	2.37625033
C	-2.23723493	1.29166822	3.26681171
H	4.06834326	2.34885905	2.60746215
H	2.21379026	1.27813239	4.34906068
H	0.00000000	-4.69771811	2.60746215
C	0.00000000	-3.79294937	-0.19377624
H	0.00000000	-2.55626478	4.34906068
C	3.28479051	1.89647495	-0.19377624
H	0.00000000	0.00000000	4.27109647
H	-4.06834326	2.34885905	2.60746215
H	-2.21379026	1.27813239	4.34906068
C	-3.28479051	1.89647495	-0.19377624
B	0.00000000	0.00000000	3.06479565
N	0.00000000	1.70440636	-1.23002118
N	0.00000000	1.44365639	-2.55212926
N	1.47605897	-0.85220345	-1.23002118
N	1.25024316	-0.72182793	-2.55212926
N	-1.47605897	-0.85220345	-1.23002118
N	-1.25024316	-0.72182793	-2.55212926
C	0.00000000	3.04964055	-1.09834601
C	0.00000000	3.63838146	-2.37625033
C	0.00000000	2.58333643	-3.26681171
C	2.64106650	-1.52482054	-1.09834601
C	3.15093036	-1.81919073	-2.37625033
C	2.23723493	-1.29166822	-3.26681171
C	-2.64106650	-1.52482054	-1.09834601
C	-3.15093036	-1.81919073	-2.37625033
C	-2.23723493	-1.29166822	-3.26681171
H	0.00000000	4.69771811	-2.60746215
H	0.00000000	2.55626478	-4.34906068
H	4.06834326	-2.34885905	-2.60746215
C	3.28479051	-1.89647495	0.19377624
H	2.21379026	-1.27813239	-4.34906068
C	0.00000000	3.79294937	0.19377624
H	0.00000000	0.00000000	-4.27109647
H	-4.06834326	-2.34885905	-2.60746215
H	-2.21379026	-1.27813239	-4.34906068
C	-3.28479051	-1.89647495	0.19377624
B	0.00000000	0.00000000	-3.06479565
H	-0.87813313	-3.56483058	-0.80289471
H	0.00000000	-4.86735116	0.01275476
H	0.87813313	-3.56483058	-0.80289471
H	4.21524975	2.43367558	0.01275476
H	2.64816700	2.54290094	-0.80289471
H	3.52630066	1.02192964	-0.80289471
H	-4.21524975	2.43367558	0.01275476
H	-3.52630066	1.02192964	-0.80289471
H	-2.64816700	2.54290094	-0.80289471
H	3.52630066	-1.02192964	0.80289471
H	4.21524975	-2.43367558	-0.01275476
H	2.64816700	-2.54290094	0.80289471
H	-2.64816700	-2.54290094	0.80289471
H	-4.21524975	-2.43367558	-0.01275476
H	-3.52630066	-1.02192964	0.80289471
H	-0.87813313	3.56483058	0.80289471
H	0.00000000	4.86735116	-0.01275476
H	0.87813313	3.56483058	0.80289471

$[Co(Tb^{3CF3})_2]$ ^4E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.60872688	0.92879868	1.23822396
N	1.27848535	0.73813400	2.52812737
N	0.00000000	-1.85759735	1.23822396
N	0.00000000	-1.47626800	2.52812737
N	-1.60872688	0.92879868	1.23822396
N	-1.27848535	0.73813400	2.52812737
C	2.78295903	1.60674247	1.25582651
C	3.18676413	1.83987891	2.57688576
C	2.20026926	1.27032597	3.35211561
C	0.00000000	-3.21348440	1.25582651
C	0.00000000	-3.67975835	2.57688576
C	0.00000000	-2.54065247	3.35211561
C	-2.78295903	1.60674247	1.25582651

C	-3.18676413	1.83987891	2.57688576
C	-2.20026926	1.27032597	3.35211561
H	4.07583853	2.35318666	2.91599789
H	2.08954474	1.20639924	4.42625071
H	0.00000000	-4.70637333	2.91599789
C	0.00000000	-4.17553446	0.07389590
H	0.00000000	-2.41279848	4.42625071
C	3.61611897	2.08776723	0.07389590
H	0.00000000	0.00000000	4.18542055
H	-4.07583853	2.35318666	2.91599789
H	-2.08954474	1.20639924	4.42625071
C	-3.61611897	2.08776723	0.07389590
B	0.00000000	0.00000000	2.98126926
N	0.00000000	1.85759735	-1.23822396
N	0.00000000	1.47626800	-2.52812737
N	1.60872688	-0.92879868	-1.23822396
N	1.27848535	-0.73813400	-2.52812737
N	-1.60872688	-0.92879868	-1.23822396
N	-1.27848535	-0.73813400	-2.52812737
C	0.00000000	3.21348440	-1.25582651
C	0.00000000	3.67975835	-2.57688576
C	0.00000000	2.54065247	-3.35211561
C	2.78295903	-1.60674247	-1.25582651
C	3.18676413	-1.83987891	-2.57688576
C	2.20026926	-1.27032597	-3.35211561
C	-2.78295903	-1.60674247	-1.25582651
C	-3.18676413	-1.83987891	-2.57688576
C	-2.20026926	-1.27032597	-3.35211561
H	0.00000000	4.70637333	-2.91599789
H	0.00000000	2.41279848	-4.42625071
H	4.07583853	-2.35318666	-2.91599789
C	3.61611897	-2.08776723	-0.07389590
H	2.08954474	-1.20639924	-4.42625071
C	0.00000000	4.17553446	-0.07389590
H	0.00000000	0.00000000	-4.18542055
H	-4.07583853	-2.35318666	-2.91599789
H	-2.08954474	-1.20639924	-4.42625071
C	-3.61611897	-2.08776723	-0.07389590
B	0.00000000	0.00000000	-2.98126926
F	-1.07398586	-4.08027198	-0.73077632
F	0.00000000	-5.44676374	0.56760610
F	1.07398586	-4.08027198	-0.73077632
F	4.71703572	2.72338160	0.56760610
F	2.99662598	2.97023485	-0.73077632
F	4.07061184	1.11003712	-0.73077632
F	-4.71703572	2.72338160	0.56760610
F	-4.07061184	1.11003712	-0.73077632
F	-2.99662598	2.97023485	-0.73077632
F	4.07061184	-1.11003712	0.73077632
F	4.71703572	-2.72338160	-0.56760610
F	2.99662598	-2.97023485	0.73077632
F	-2.99662598	-2.97023485	0.73077632
F	-4.71703572	-2.72338160	-0.56760610
F	-4.07061184	-1.11003712	0.73077632
F	-1.07398586	4.08027198	0.73077632
F	0.00000000	5.44676374	-0.56760610
F	1.07398586	4.08027198	0.73077632

$[Co(Tb^{3CF3})_2]$ ^2E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.54874834	0.89417038	1.17124176
N	1.26477755	0.73021962	2.47294741
N	0.00000000	-1.78834022	1.17124176
N	0.00000000	-1.46043925	2.47294741
N	-1.54874834	0.89417038	1.17124176
N	-1.26477755	0.73021962	2.47294741
C	2.72472042	1.57311802	1.13473488
C	3.16978601	1.83007643	2.43881442
C	2.21171959	1.27693698	3.25710925
C	0.00000000	-3.14623656	1.13473488
C	0.00000000	-3.66015340	2.43881442
C	0.00000000	-2.55387343	3.25710925
C	-2.72472042	1.57311802	1.13473488
C	-3.16978601	1.83007643	2.43881442
C	-2.21171959	1.27693698	3.25710925
H	4.06980379	2.34970256	2.73633428
H	2.13355588	1.23180927	4.33496181
H	0.00000000	-4.69940512	2.73633428
C	0.00000000	-4.07741759	-0.06908885
H	0.00000000	-2.46361802	4.33496181
C	3.53114686	2.03870880	-0.06908885
H	0.00000000	0.00000000	4.15452242
H	-4.06980379	2.34970256	2.73633428
H	-2.13355588	1.23180927	4.33496181
C	-3.53114686	2.03870880	-0.06908885
B	0.00000000	0.00000000	2.95082463
N	0.00000000	1.78834022	-1.17124176
N	0.00000000	1.46043925	-2.47294741
N	1.54874834	-0.89417038	-1.17124176
N	1.26477755	-0.73021962	-2.47294741
N	-1.54874834	-0.89417038	-1.17124176
N	-1.26477755	-0.73021962	-2.47294741
C	0.00000000	3.14623656	-1.13473488
C	0.00000000	3.66015340	-2.43881442
C	0.00000000	2.55387343	-3.25710925
C	2.72472042	-1.57311802	-1.13473488
C	3.16978601	-1.83007643	-2.43881442
C	2.21171959	-1.27693698	-3.25710925
C	-2.72472042	-1.57311802	-1.13473488
C	-3.16978601	-1.83007643	-2.43881442
C	-2.21171959	-1.27693698	-3.25710925
H	0.00000000	4.69940512	-2.73633428
H	0.00000000	2.46361802	-4.33496181
H	4.06980379	-2.34970256	-2.73633428
C	3.53114686	-2.03870880	0.06908885
H	2.13355588	-1.23180927	-4.33496181
C	0.00000000	4.07741759	0.06908885
H	0.00000000	0.00000000	-4.15452242
H	-4.06980379	-2.34970256	-2.73633428
H	-2.13355588	-1.23180927	-4.33496181
C	-3.53114686	-2.03870880	0.06908885
B	0.00000000	0.00000000	-2.95082463
F	-1.07700641	-3.96288988	-0.86809570
F	0.00000000	-5.36164505	0.38954113
F	1.07700641	-3.96288988	-0.86809570
F	4.64332080	2.68082252	0.38954113
F	2.89346023	2.91415953	-0.86809570
F	3.97046664	1.04873035	-0.86809570
F	-4.64332080	2.68082252	0.38954113

F	-3.97046664	1.04873035	-0.86809570
F	-2.89346023	2.91415953	-0.86809570
F	3.97046664	-1.04873035	0.86809570
F	4.64332080	-2.68082252	-0.38954113
F	2.89346023	-2.91415953	0.86809570
F	-2.89346023	-2.91415953	0.86809570
F	-4.64332080	-2.68082252	-0.38954113
F	-3.97046664	-1.04873035	0.86809570
F	-1.07700641	3.96288988	0.86809570
F	0.00000000	5.36164505	-0.38954113
F	1.07700641	3.96288988	0.86809570

$[Co(Tb^{3NH2})_2]$ ^4E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.71882009	1.35929442
N	0.00000000	1.44954772	2.69612686
N	1.48854226	-0.85941031	1.35929442
N	1.25534496	-0.72477386	2.69612686
N	-1.48854226	-0.85941031	1.35929442
N	-1.25534496	-0.72477386	2.69612686
C	0.00000000	3.06356426	1.24648600
C	0.00000000	3.66097732	2.52609798
C	0.00000000	2.59111481	3.40227950
C	2.65312433	-1.53178239	1.24648600
C	3.17049934	-1.83048866	2.52609798
C	2.24397136	-1.29555767	3.40227950
C	-2.65312433	-1.53178239	1.24648600
C	-3.17049934	-1.83048866	2.52609798
C	-2.24397136	-1.29555767	3.40227950
H	0.00000000	4.71738657	2.76911416
H	0.00000000	2.56973023	4.48510527
H	4.08537642	-2.35869328	2.76911416
N	3.19023183	-1.84188132	0.03859237
H	2.22545174	-1.28486511	4.48510527
N	0.00000000	3.68376211	0.03859237
H	0.00000000	0.00000000	4.40915511
H	-4.08537642	-2.35869328	2.76911416
H	-2.22545174	-1.28486511	4.48510527
N	-3.19023183	-1.84188132	0.03859237
B	0.00000000	0.00000000	3.20036610
N	-1.48854226	0.85941031	-1.35929442
N	-1.25534496	0.72477386	-2.69612686
N	1.48854226	0.85941031	-1.35929442
N	1.25534496	0.72477386	-2.69612686
N	0.00000000	-1.71882009	-1.35929442
N	0.00000000	-1.44954772	-2.69612686
C	-2.65312433	1.53178239	-1.24648600
C	-3.17049934	1.83048866	-2.52609798
C	-2.24397136	1.29555767	-3.40227950
C	2.65312433	1.53178239	-1.24648600
C	3.17049934	1.83048866	-2.52609798
C	2.24397136	1.29555767	-3.40227950
C	0.00000000	-3.06356426	-1.24648600
C	0.00000000	-3.66097732	-2.52609798
C	0.00000000	-2.59111481	-3.40227950
H	-4.08537642	2.35869328	-2.76911416
H	-2.22545174	1.28486511	-4.48510527
H	4.08537642	2.35869328	-2.76911416
N	3.19023183	1.84188132	-0.03859237
H	2.22545174	1.28486511	-4.48510527
N	-3.19023183	1.84188132	-0.03859237
H	0.00000000	0.00000000	-4.40915511
H	0.00000000	-4.71738657	-2.76911416
H	0.00000000	-2.56973023	-4.48510527
N	0.00000000	-3.68376211	-0.03859237
B	0.00000000	0.00000000	-3.20036610
H	0.00000000	4.68278631	-0.01613514
H	4.05541176	-2.34139289	-0.01613514
H	-4.05541176	-2.34139289	-0.01613514
H	-4.05541176	2.34139289	0.01613514
H	4.05541176	2.34139289	0.01613514
H	0.00000000	-4.68278631	0.01613514
H	2.72133051	-1.57116059	-0.80739060
H	0.00000000	3.14232171	-0.80739060
H	-2.72133051	-1.57116059	-0.80739060
H	2.72133051	1.57116059	0.80739060
H	-2.72133051	1.57116059	0.80739060
H	0.00000000	-3.14232171	0.80739060

$[Co(Tb^{3NH2})_2]$ ^2E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.66959814	1.26325457
N	0.00000000	1.43907742	2.60758439
N	1.44591439	-0.83479933	1.26325457
N	1.24627751	-0.71953871	2.60758439
N	-1.44591439	-0.83479933	1.26325457
N	-1.24627751	-0.71953871	2.60758439
C	0.00000000	3.01017874	1.10869830
C	0.00000000	3.64187455	2.37269161
C	0.00000000	2.60016480	3.28090053
C	2.60689117	-1.50508911	1.10869830
C	3.15395620	-1.82093754	2.37269161
C	2.25180847	-1.30008213	3.28090053
C	-2.60689117	-1.50508911	1.10869830
C	-3.15395620	-1.82093754	2.37269161
C	-2.25180847	-1.30008213	3.28090053
H	0.00000000	4.70545044	2.58220346
H	0.00000000	2.60860782	4.36377657
H	4.07503947	-2.35272522	2.58220346
N	3.12110382	-1.80197024	-0.11089544
H	2.25912065	-1.30430391	4.36377657
N	0.00000000	3.60394048	-0.11089544
H	0.00000000	0.00000000	4.33757012
H	-4.07503947	-2.35272522	2.58220346
H	-2.25912065	-1.30430391	4.36377657
N	-3.12110382	-1.80197024	-0.11089544
B	0.00000000	0.00000000	3.12942830
N	-1.44591439	0.83479933	-1.26325457
N	-1.24627751	0.71953871	-2.60758439
N	1.44591439	0.83479933	-1.26325457
N	1.24627751	0.71953871	-2.60758439
N	0.00000000	-1.66959814	-1.26325457
N	0.00000000	-1.43907742	-2.60758439
C	-2.60689117	1.50508911	-1.10869830
C	-3.15395620	1.82093754	-2.37269161
C	-2.25180847	1.30008213	-3.28090053
C	2.60689117	1.50508911	-1.10869830
C	3.15395620	1.82093754	-2.37269161

C	2.25180847	1.30008213	-3.28090053
C	0.00000000	-3.01017874	-1.10869830
C	0.00000000	-3.64187455	-2.37269161
C	0.00000000	-2.60016480	-3.28090053
H	-4.07503947	2.35272522	-2.58220346
H	-2.25912065	1.30430391	-4.36377657
H	4.07503947	2.35272522	-2.58220346
N	3.12110382	1.80197024	0.11089544
H	2.25912065	1.30430391	-4.36377657
N	-3.12110382	1.80197024	0.11089544
H	0.00000000	0.00000000	-4.33757012
H	0.00000000	-4.70545044	-2.58220346
H	0.00000000	-2.60860782	-4.36377657
N	0.00000000	-3.60394048	0.11089544
B	0.00000000	0.00000000	-3.12942830
H	0.00000000	4.60160840	-0.18504111
H	3.98511003	-2.30080447	-0.18504111
H	-3.98511003	-2.30080447	-0.18504111
H	-3.98511003	2.30080447	0.18504111
H	3.98511003	2.30080447	0.18504111
H	0.00000000	-4.60160840	0.18504111
H	2.63567735	-1.52170898	-0.94370507
H	0.00000000	3.04341848	-0.94370507
H	-2.63567735	-1.52170898	-0.94370507
H	2.63567735	1.52170898	0.94370507
H	-2.63567735	1.52170898	0.94370507
H	0.00000000	-3.04341848	0.94370507

$[Co(Tb^{3NO2})_2]$ ^4E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.80599093	1.41033198
N	0.00000000	1.45544540	2.70076616
N	1.56403363	-0.90299547	1.41033198
N	1.26045258	-0.72772296	2.70076616
N	-1.56403363	-0.90299547	1.41033198
N	-1.26045258	-0.72772296	2.70076616
C	0.00000000	3.15207286	1.43583462
C	0.00000000	3.66185629	2.73575218
C	0.00000000	2.53237031	3.51780101
C	2.72977512	-1.57603643	1.43583462
C	3.17126082	-1.83092841	2.73575218
C	2.19309679	-1.26618516	3.51780101
C	-2.72977512	-1.57603643	1.43583462
C	-3.17126082	-1.83092841	2.73575218
C	-2.19309679	-1.26618516	3.51780101
H	0.00000000	4.70017772	3.03328791
H	0.00000000	2.40940540	4.59252031
H	4.07047320	-2.35008886	3.03328791
N	3.45739119	-1.99612590	0.25949476
H	2.08660622	-1.20470270	4.59252031
N	0.00000000	3.99225128	0.25949476
H	0.00000000	0.00000000	4.37836546
H	-4.07047320	-2.35008886	3.03328791
H	-2.08660622	-1.20470270	4.59252031
N	-3.45739119	-1.99612590	0.25949476
B	0.00000000	0.00000000	3.17533549
N	-1.56403363	0.90299547	-1.41033198
N	-1.26045258	0.72772296	-2.70076616
N	1.56403363	0.90299547	-1.41033198
N	1.26045258	0.72772296	-2.70076616
N	0.00000000	-1.80599093	-1.41033198
N	0.00000000	-1.45544540	-2.70076616
C	-2.72977512	1.57603643	-1.43583462
C	-3.17126082	1.83092841	-2.73575218
C	-2.19309679	1.26618516	-3.51780101
C	2.72977512	1.57603643	-1.43583462
C	3.17126082	1.83092841	-2.73575218
C	2.19309679	1.26618516	-3.51780101
C	0.00000000	-3.15207286	-1.43583462
C	0.00000000	-3.66185629	-2.73575218
C	0.00000000	-2.53237031	-3.51780101
H	-4.07047320	2.35008886	-3.03328791
H	-2.08660622	1.20470270	-4.59252031
H	4.07047320	2.35008886	-3.03328791
N	3.45739119	1.99612590	-0.25949476
H	2.08660622	1.20470270	-4.59252031
N	-3.45739119	1.99612590	-0.25949476
H	0.00000000	0.00000000	-4.37836546
H	0.00000000	-4.70017772	-3.03328791
H	0.00000000	-2.40940540	-4.59252031
N	0.00000000	-3.99225128	-0.25949476
B	0.00000000	0.00000000	-3.17533549
O	0.00000000	5.20289822	0.47289713
O	4.50584214	-2.60144911	0.47289713
O	-4.50584214	-2.60144911	0.47289713
O	-4.50584214	2.60144911	-0.47289713
O	4.50584214	2.60144911	-0.47289713
O	0.00000000	-5.20289822	-0.47289713
O	3.00281947	-1.73367833	-0.84327040
O	0.00000000	3.46735719	-0.84327040
O	-3.00281947	-1.73367833	-0.84327040
O	3.00281947	1.73367833	0.84327040
O	-3.00281947	1.73367833	0.84327040
O	0.00000000	-3.46735719	0.84327040

$[Co(Tb^{3NO2})_2]$ ^2E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	0.00000000	1.75754740	1.26053460
N	0.00000000	1.44530054	2.55879213
N	1.52208046	-0.87877344	1.26053460
N	1.25166718	-0.72265027	2.55879213
N	-1.52208046	-0.87877344	1.26053460
N	-1.25166718	-0.72265027	2.55879213
C	0.00000000	3.10849670	1.24574463
C	0.00000000	3.64719967	2.53540620
C	0.00000000	2.54185529	3.34758797
C	2.69203685	-1.55424808	1.24574463
C	3.15856745	-1.82359983	2.53540620
C	2.20131121	-1.27092764	3.34758797
C	-2.69203685	-1.55424808	1.24574463
C	-3.15856745	-1.82359983	2.53540620
C	-2.20131121	-1.27092764	3.34758797
H	0.00000000	4.69327990	2.80343713
H	0.00000000	2.44503596	4.42475261
H	4.06449985	-2.34664021	2.80343713
N	3.41991169	-1.97448679	0.06699754
H	2.11746360	-1.22251798	4.42475261
N	0.00000000	3.94897357	0.06699754

H	0.00000000	0.00000000	4.25302930
H	-4.06449985	-2.34664021	2.80343713
H	-2.11746360	-1.22251798	4.42475261
N	-3.41991169	-1.97448679	0.06699754
B	0.00000000	0.00000000	3.05059941
N	-1.52208046	0.87877344	-1.26053460
N	-1.25166718	0.72265027	-2.55879213
N	1.52208046	0.87877344	-1.26053460
N	1.25166718	0.72265027	-2.55879213
N	0.00000000	-1.75754740	-1.26053460
N	0.00000000	-1.44530054	-2.55879213
C	-2.69203685	1.55424808	-1.24574463
C	-3.15856745	1.82359983	-2.53540620
C	-2.20131121	1.27092764	-3.34758797
C	2.69203685	1.55424808	-1.24574463
C	3.15856745	1.82359983	-2.53540620
C	2.20131121	1.27092764	-3.34758797
C	0.00000000	-3.10849670	-1.24574463
C	0.00000000	-3.64719967	-2.53540620
C	0.00000000	-2.54185529	-3.34758797
H	-4.06449985	2.34664021	-2.80343713
H	-2.11746360	1.22251798	-4.42475261
H	4.06449985	2.34664021	-2.80343713
N	3.41991169	1.97448679	-0.06699754
H	2.11746360	1.22251798	-4.42475261
N	-3.41991169	1.97448679	-0.06699754
H	0.00000000	0.00000000	-4.25302930
H	0.00000000	-4.69327990	-2.80343713
H	0.00000000	-2.44503596	-4.42475261
N	0.00000000	-3.94897357	-0.06699754
B	0.00000000	0.00000000	-3.05059941
O	0.00000000	5.15889396	0.28792111
O	4.46773291	-2.57944698	0.28792111
O	-4.46773291	-2.57944698	0.28792111
O	-4.46773291	2.57944698	-0.28792111
O	4.46773291	2.57944698	-0.28792111
O	0.00000000	-5.15889396	-0.28792111
O	2.97616958	-1.71829197	-1.04076676
O	0.00000000	3.43658447	-1.04076676
O	-2.97616958	-1.71829197	-1.04076676
O	2.97616958	1.71829197	1.04076676
O	-2.97616958	1.71829197	1.04076676
O	0.00000000	-3.43658447	1.04076676

$[Co(Tb^{5CH3})_2]$ ^4E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.45217667	0.83841467	1.33571164
N	1.26181309	0.72850773	2.66712530
N	0.00000000	-1.67682882	1.33571164
N	0.00000000	-1.45701600	2.66712530
N	-1.45217667	0.83841467	1.33571164
N	-1.26181309	0.72850773	2.66712530
C	2.59754378	1.49969256	1.15986710
C	3.16343535	1.82641029	2.39415186
C	2.28139530	1.31716451	3.34273277
C	0.00000000	-2.99938511	1.15986710
C	0.00000000	-3.65282059	2.39415186
C	0.00000000	-2.63432848	3.34273277
C	-2.59754378	1.49969256	1.15986710
C	-3.16343535	1.82641029	2.39415186
C	-2.28139530	1.31716451	3.34273277
H	4.08813343	2.36028505	2.58400690
C	2.37928886	1.37368328	4.82891120
H	0.00000000	-4.72057010	2.58400690
H	0.00000000	-3.41234339	0.15915112
C	0.00000000	-2.74736603	4.82891120
H	2.95517606	1.70617170	0.15915112
H	0.00000000	0.00000000	4.38715827
H	-4.08813343	2.36028505	2.58400690
C	-2.37928886	1.37368328	4.82891120
H	-2.95517606	1.70617170	0.15915112
B	0.00000000	0.00000000	3.18716207
N	0.00000000	1.67682882	-1.33571164
N	0.00000000	1.45701600	-2.66712530
N	1.45217667	-0.83841467	-1.33571164
N	1.26181309	-0.72850773	-2.66712530
N	-1.45217667	-0.83841467	-1.33571164
N	-1.26181309	-0.72850773	-2.66712530
C	0.00000000	2.99938511	-1.15986710
C	0.00000000	3.65282059	-2.39415186
C	0.00000000	2.63432848	-3.34273277
C	2.59754378	-1.49969256	-1.15986710
C	3.16343535	-1.82641029	-2.39415186
C	2.28139530	-1.31716451	-3.34273277
C	-2.59754378	-1.49969256	-1.15986710
C	-3.16343535	-1.82641029	-2.39415186
C	-2.28139530	-1.31716451	-3.34273277
H	0.00000000	4.72057010	-2.58400690
C	0.00000000	2.74736603	-4.82891120
H	4.08813343	-2.36028505	-2.58400690
H	2.95517606	-1.70617170	-0.15915112
C	2.37928886	-1.37368328	-4.82891120
H	0.00000000	3.41234339	-0.15915112
H	0.00000000	0.00000000	-4.38715827
H	-4.08813343	-2.36028505	-2.58400690
C	-2.37928886	-1.37368328	-4.82891120
H	-2.95517606	-1.70617170	-0.15915112
B	0.00000000	0.00000000	-3.18716207
H	-3.29364735	-1.90158839	-5.11341171
H	-1.53211313	-1.90494337	-5.27765192
H	-2.41578569	-0.37437703	-5.27765192
H	3.29364735	-1.90158839	-5.11341171
H	2.41578569	-0.37437703	-5.27765192
H	1.53211313	-1.90494337	-5.27765192
H	0.88367309	2.27932040	-5.27765192
H	0.00000000	3.80317678	-5.11341171
H	-0.88367309	2.27932040	-5.27765192
H	-2.41578569	0.37437703	5.27765192
H	-3.29364735	1.90158839	5.11341171
H	-1.53211313	1.90494337	5.27765192
H	-0.88367309	-2.27932040	5.27765192
H	0.88367309	-2.27932040	5.27765192
H	0.00000000	-3.80317678	5.11341171
H	2.41578569	0.37437703	5.27765192
H	1.53211313	1.90494337	5.27765192
H	3.29364735	1.90158839	5.11341171

$[Co(Tb^{5CH3})_2]$ ^2E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.40297800	0.81000950	1.22375414
N	1.25206195	0.72287835	2.56127768
N	0.00000000	-1.62001900	1.22375414
N	0.00000000	-1.44575669	2.56127768
N	-1.40297800	0.81000950	1.22375414
N	-1.25206195	0.72287835	2.56127768
C	2.54136474	1.46725769	0.99789123
C	3.14289375	1.81455037	2.21063796
C	2.29209262	1.32334053	3.19516482
C	0.00000000	-2.93451539	0.99789123
C	0.00000000	-3.62910075	2.21063796
C	0.00000000	-2.64668054	3.19516482
C	-2.54136474	1.46725769	0.99789123
C	-3.14289375	1.81455037	2.21063796
C	-2.29209262	1.32334053	3.19516482
H	4.07310268	2.35160707	2.36044221
C	2.43293632	1.40465656	4.67672882
H	0.00000000	-4.70321361	2.36044221
H	0.00000000	-3.31061859	-0.01632988
C	0.00000000	-2.80931311	4.67672882
H	2.86708022	1.65530930	-0.01632988
H	0.00000000	0.00000000	4.30277778
H	-4.07310268	2.35160707	2.36044221
C	-2.43293632	1.40465656	4.67672882
H	-2.86708022	1.65530930	-0.01632988
B	0.00000000	0.00000000	3.10306416
N	0.00000000	1.62001900	-1.22375414
N	0.00000000	1.44575669	-2.56127768
N	1.40297800	-0.81000950	-1.22375414
N	1.25206195	-0.72287835	-2.56127768
N	-1.40297800	-0.81000950	-1.22375414
N	-1.25206195	-0.72287835	-2.56127768
C	0.00000000	2.93451539	-0.99789123
C	0.00000000	3.62910075	-2.21063796
C	0.00000000	2.64668054	-3.19516482
C	2.54136474	-1.46725769	-0.99789123
C	3.14289375	-1.81455037	-2.21063796
C	2.29209262	-1.32334053	-3.19516482
C	-2.54136474	-1.46725769	-0.99789123
C	-3.14289375	-1.81455037	-2.21063796
C	-2.29209262	-1.32334053	-3.19516482
H	0.00000000	4.70321361	-2.36044221
C	0.00000000	2.80931311	-4.67672882
H	4.07310268	-2.35160707	-2.36044221
H	2.86708022	-1.65530930	0.01632988
C	2.43293632	-1.40465656	-4.67672882
H	0.00000000	3.31061859	0.01632988
H	0.00000000	0.00000000	-4.30277778
H	-4.07310268	-2.35160707	-2.36044221
C	-2.43293632	-1.40465656	-4.67672882
H	-2.86708022	-1.65530930	0.01632988
B	0.00000000	0.00000000	-3.10306416
H	-3.35522612	-1.93714063	-4.92469334
H	-1.59960651	-1.94396437	-5.14162955
H	-2.48332564	-0.41331759	-5.14162955
H	3.35522612	-1.93714063	-4.92469334
H	2.48332564	-0.41331759	-5.14162955
H	1.59960651	-1.94396437	-5.14162955
H	0.88371913	2.35728197	-5.14162955
H	0.00000000	3.87428126	-4.92469334
H	-0.88371913	2.35728197	-5.14162955
H	-2.48332564	0.41331759	5.14162955
H	-3.35522612	1.93714063	4.92469334
H	-1.59960651	1.94396437	5.14162955
H	-0.88371913	-2.35728197	5.14162955
H	0.88371913	-2.35728197	5.14162955
H	0.00000000	-3.87428126	4.92469334
H	2.48332564	0.41331759	5.14162955
H	1.59960651	1.94396437	5.14162955
H	3.35522612	1.93714063	4.92469334

$[Co(Tb^{5CF3})_2]$ ^4E_g D_{3d} OPBE

Co	0.000000	0.000000	0.000000
N	1.438972	0.830791	1.343839
N	1.266273	0.731083	2.675048
N	0.000000	-1.661582	1.343839
N	0.000000	-1.462166	2.675048
N	-1.438972	0.830791	1.343839
N	-1.266273	0.731083	2.675048
C	2.580228	1.489696	1.130763
C	3.175185	1.833194	2.342190
C	2.310695	1.334080	3.305706
C	0.000000	-2.979391	1.130763
C	0.000000	-3.666387	2.342190
C	0.000000	-2.668161	3.305706
C	-2.580228	1.489696	1.130763
C	-3.175185	1.833194	2.342190
C	-2.310695	1.334080	3.305706
H	4.101347	2.367914	2.507088
C	2.503777	1.445556	4.792331
H	0.000000	-4.735827	2.507088
H	0.000000	-3.367649	0.120470
C	0.000000	-2.891112	4.792331
H	2.916469	1.683824	0.120470
H	0.000000	0.000000	4.401874
H	-4.101347	2.367914	2.507088
C	-2.503777	1.445556	4.792331
H	-2.916469	1.683824	0.120470
B	0.000000	0.000000	3.214013
N	0.000000	1.661582	-1.343839
N	0.000000	1.462166	-2.675048
N	1.438972	-0.830791	-1.343839
N	1.266273	-0.731083	-2.675048
N	-1.438972	-0.830791	-1.343839
N	-1.266273	-0.731083	-2.675048
C	0.000000	2.979391	-1.130763
C	0.000000	3.666387	-2.342190
C	0.000000	2.668161	-3.305706
C	2.580228	-1.489696	-1.130763
C	3.175185	-1.833194	-2.342190
C	2.310695	-1.334080	-3.305706
C	-2.580228	-1.489696	-1.130763
C	-3.175185	-1.833194	-2.342190
C	-2.310695	-1.334080	-3.305706
H	0.000000	4.735827	-2.507088
C	0.000000	2.891112	-4.792331
H	4.101347	-2.367914	-2.507088
H	2.916469	-1.683824	-0.120470

C	2.503777	-1.445556	-4.792331
H	0.000000	3.367649	-0.120470
H	0.000000	0.000000	-4.401874
H	-4.101347	-2.367914	-2.507088
C	-2.503777	-1.445556	-4.792331
H	-2.916469	-1.683824	-0.120470
B	0.000000	0.000000	-3.214013
F	-3.657355	-2.111575	-5.047566
F	-1.509097	-2.128134	-5.402596
F	-2.597567	-0.242850	-5.402596
F	3.657355	-2.111575	-5.047566
F	2.597567	-0.242850	-5.402596
F	1.509097	-2.128134	-5.402596
F	1.088469	2.370984	-5.402596
F	0.000000	4.223150	-5.047566
F	-1.088469	2.370984	-5.402596
F	-2.597567	0.242850	5.402596
F	-3.657355	2.111575	5.047566
F	-1.509097	2.128134	5.402596
F	-1.088469	-2.370984	5.402596
F	1.088469	-2.370984	5.402596
F	0.000000	-4.223150	5.047566
F	2.597567	0.242850	5.402596
F	1.509097	2.128134	5.402596
F	3.657355	2.111575	5.047566

$[Co(Tb^{5CF3})_2]$ ^2E_g D_{3d} OPBE

Co	0.000000	0.000000	0.000000
N	1.396453	0.806243	1.230909
N	1.254597	0.724342	2.566121
N	0.000000	-1.612485	1.230909
N	0.000000	-1.448684	2.566121
N	-1.396453	0.806243	1.230909
N	-1.254597	0.724342	2.566121
C	2.532661	1.462233	0.981050
C	3.153134	1.820463	2.176538
C	2.311807	1.334722	3.165933
C	0.000000	-2.924465	0.981050
C	0.000000	-3.640925	2.176538
C	0.000000	-2.669444	3.165933
C	-2.532661	1.462233	0.981050
C	-3.153134	1.820463	2.176538
C	-2.311807	1.334722	3.165933
H	4.083028	2.357337	2.311484
C	2.523569	1.456984	4.647694
H	0.000000	-4.714675	2.311484
H	0.000000	-3.287154	-0.037724
C	0.000000	-2.913967	4.647694
H	2.846759	1.643577	-0.037724
H	0.000000	0.000000	4.310705
H	-4.083028	2.357337	2.311484
C	-2.523569	1.456984	4.647694
H	-2.846759	1.643577	-0.037724
B	0.000000	0.000000	3.123425
N	0.000000	1.612485	-1.230909
N	0.000000	1.448684	-2.566121
N	1.396453	-0.806243	-1.230909
N	1.254597	-0.724342	-2.566121
N	-1.396453	-0.806243	-1.230909
N	-1.254597	-0.724342	-2.566121
C	0.000000	2.924465	-0.981050
C	0.000000	3.640925	-2.176538
C	0.000000	2.669444	-3.165933
C	2.532661	-1.462233	-0.981050
C	3.153134	-1.820463	-2.176538
C	2.311807	-1.334722	-3.165933
C	-2.532661	-1.462233	-0.981050
C	-3.153134	-1.820463	-2.176538
C	-2.311807	-1.334722	-3.165933
H	0.000000	4.714675	-2.311484
C	0.000000	2.913967	-4.647694
H	4.083028	-2.357337	-2.311484
H	2.846759	-1.643577	0.037724
C	2.523569	-1.456984	-4.647694
H	0.000000	3.287154	0.037724
H	0.000000	0.000000	-4.310705
H	-4.083028	-2.357337	-2.311484
C	-2.523569	-1.456984	-4.647694
H	-2.846759	-1.643577	0.037724
B	0.000000	0.000000	-3.123425
F	-3.679494	-2.124357	-4.885492
F	-1.534384	-2.142796	-5.265042
F	-2.622907	-0.257418	-5.265042
F	3.679494	-2.124357	-4.885492
F	2.622907	-0.257418	-5.265042
F	1.534384	-2.142796	-5.265042
F	1.088524	2.400213	-5.265042
F	0.000000	4.248714	-4.885492
F	-1.088524	2.400213	-5.265042
F	-2.622907	0.257418	5.265042
F	-3.679494	2.124357	4.885492
F	-1.534384	2.142796	5.265042
F	-1.088524	-2.400213	5.265042
F	1.088524	-2.400213	5.265042
F	0.000000	-4.248714	4.885492
F	2.622907	0.257418	5.265042
F	1.534384	2.142796	5.265042
F	3.679494	2.124357	4.885492

$[Co(Tb^{5NH2})_2]$ ^4E_g D_{3d} OPBE

Co	0.000000	0.000000	0.000000
N	0.000000	1.682150	-1.338372
N	0.000000	1.454345	-2.682597
N	-1.456785	-0.841075	-1.338372
N	-1.259500	-0.727172	-2.682597
N	1.456785	-0.841075	-1.338372
N	1.259500	-0.727172	-2.682597
C	0.000000	3.002987	-1.180679
C	0.000000	3.663278	-2.412466
C	0.000000	2.632055	-3.353207
C	-2.600663	-1.501494	-1.180679
C	-3.172492	-1.831639	-2.412466
C	-2.279426	-1.316027	-3.353207
C	2.600663	-1.501494	-1.180679
C	3.172492	-1.831639	-2.412466
C	2.279426	-1.316027	-3.353207
H	0.000000	4.730085	-2.605211
N	0.000000	2.714926	-4.719772

H	-4.096374	-2.365043	-2.605211
H	-2.966252	-1.712566	-0.183651
N	-2.351195	-1.357463	-4.719772
H	0.000000	3.425133	-0.183651
H	0.000000	0.000000	-4.401872
H	4.096374	-2.365043	-2.605211
N	2.351195	-1.357463	-4.719772
H	2.966252	-1.712566	-0.183651
B	0.000000	0.000000	-3.186390
N	1.456785	0.841075	1.338372
N	1.259500	0.727172	2.682597
N	-1.456785	0.841075	1.338372
N	-1.259500	0.727172	2.682597
N	0.000000	-1.682150	1.338372
N	0.000000	-1.454345	2.682597
C	2.600663	1.501494	1.180679
C	3.172492	1.831639	2.412466
C	2.279426	1.316027	3.353207
C	-2.600663	1.501494	1.180679
C	-3.172492	1.831639	2.412466
C	-2.279426	1.316027	3.353207
C	0.000000	-3.002987	1.180679
C	0.000000	-3.663278	2.412466
C	0.000000	-2.632055	3.353207
H	4.096374	2.365043	2.605211
N	2.351195	1.357463	4.719772
H	-4.096374	2.365043	2.605211
H	-2.966252	1.712566	0.183651
N	-2.351195	1.357463	4.719772
H	2.966252	1.712566	0.183651
H	0.000000	0.000000	4.401872
H	0.000000	-4.730085	2.605211
N	0.000000	-2.714926	4.719772
H	0.000000	-3.425133	0.183651
B	0.000000	0.000000	3.186390
H	0.000000	3.612211	-5.163482
H	0.000000	1.889462	-5.286017
H	-3.128266	-1.806105	-5.163482
H	-1.636322	-0.944731	-5.286017
H	3.128266	-1.806105	-5.163482
H	1.636322	-0.944731	-5.286017
H	3.128266	1.806105	5.163482
H	1.636322	0.944731	5.286017
H	-3.128266	1.806105	5.163482
H	-1.636322	0.944731	5.286017
H	0.000000	-3.612211	5.163482
H	0.000000	-1.889462	5.286017

$[Co(Tb^{5NH2})_2]$ ^2E_g D_{3d} OPBE

Co	0.000000	0.000000	0.000000
N	0.000000	1.626030	-1.225305
N	0.000000	1.443469	-2.575332
N	-1.408183	-0.813015	-1.225305
N	-1.250081	-0.721735	-2.575332
N	1.408183	-0.813015	-1.225305
N	1.250081	-0.721735	-2.575332
C	0.000000	2.938560	-1.017075
C	0.000000	3.639895	-2.228332
C	0.000000	2.643785	-3.204234
C	-2.544868	-1.469280	-1.017075
C	-3.152241	-1.819947	-2.228332
C	-2.289585	-1.321892	-3.204234
C	2.544868	-1.469280	-1.017075
C	3.152241	-1.819947	-2.228332
C	2.289585	-1.321892	-3.204234
H	0.000000	4.713087	-2.381150
N	0.000000	2.766970	-4.568844
H	-4.081653	-2.356544	-2.381150
H	-2.878666	-1.661998	-0.006223
N	-2.396267	-1.383485	-4.568844
H	0.000000	3.323997	-0.006223
H	0.000000	0.000000	-4.314764
H	4.081653	-2.356544	-2.381150
N	2.396267	-1.383485	-4.568844
H	2.878666	-1.661998	-0.006223
B	0.000000	0.000000	-3.100808
N	1.408183	0.813015	1.225305
N	1.250081	0.721735	2.575332
N	-1.408183	0.813015	1.225305
N	-1.250081	0.721735	2.575332
N	0.000000	-1.626030	1.225305
N	0.000000	-1.443469	2.575332
C	2.544868	1.469280	1.017075
C	3.152241	1.819947	2.228332
C	2.289585	1.321892	3.204234
C	-2.544868	1.469280	1.017075
C	-3.152241	1.819947	2.228332
C	-2.289585	1.321892	3.204234
C	0.000000	-2.938560	1.017075
C	0.000000	-3.639895	2.228332
C	0.000000	-2.643785	3.204234
H	4.081653	2.356544	2.381150
N	2.396267	1.383485	4.568844
H	-4.081653	2.356544	2.381150
H	-2.878666	1.661998	0.006223
N	-2.396267	1.383485	4.568844
H	2.878666	1.661998	0.006223
H	0.000000	0.000000	4.314764
H	0.000000	-4.713087	2.381150
N	0.000000	-2.766970	4.568844
H	0.000000	-3.323997	0.006223
B	0.000000	0.000000	3.100808
H	0.000000	3.676998	-4.985616
H	0.000000	1.959416	-5.160263
H	-3.184374	-1.838499	-4.985616
H	-1.696904	-0.979708	-5.160263
H	3.184374	-1.838499	-4.985616
H	1.696904	-0.979708	-5.160263
H	3.184374	1.838499	4.985616
H	1.696904	0.979708	5.160263
H	-3.184374	1.838499	4.985616
H	-1.696904	0.979708	5.160263
H	0.000000	-3.676998	4.985616
H	0.000000	-1.959416	5.160263

$[Co(Tb^{5NO2})_2]$ ^4E_g D_{3d} OPBE

Co	0.000000	0.000000	0.000000
N	-1.430967	-0.826169	-1.297009

N	-1.270057	-0.733268	-2.626865
N	1.430967	-0.826169	-1.297009
N	1.270057	-0.733268	-2.626865
N	0.000000	1.652338	-1.297009
N	0.000000	1.466536	-2.626865
C	-2.570459	-1.484055	-1.050329
C	-3.186483	-1.839717	-2.239846
C	-2.334211	-1.347657	-3.216891
C	2.570459	-1.484055	-1.050329
C	3.186483	-1.839717	-2.239846
C	2.334211	-1.347657	-3.216891
C	0.000000	2.968110	-1.050329
C	0.000000	3.679434	-2.239846
C	0.000000	2.695315	-3.216891
H	-4.111839	-2.373971	-2.402399
N	-2.590420	-1.495580	-4.641448
H	4.111839	-2.373971	-2.402399
H	2.883605	-1.664850	-0.030406
N	2.590420	-1.495580	-4.641448
H	-2.883605	-1.664850	-0.030406
H	0.000000	0.000000	-4.342817
H	0.000000	4.747943	-2.402399
N	0.000000	2.991159	-4.641448
H	0.000000	3.329700	-0.030406
B	0.000000	0.000000	-3.174647
N	-1.430967	0.826169	1.297009
N	-1.270057	0.733268	2.626865
N	0.000000	-1.652338	1.297009
N	0.000000	-1.466536	2.626865
N	1.430967	0.826169	1.297009
N	1.270057	0.733268	2.626865
C	-2.570459	1.484055	1.050329
C	-3.186483	1.839717	2.239846
C	-2.334211	1.347657	3.216891
C	0.000000	-2.968110	1.050329
C	0.000000	-3.679434	2.239846
C	0.000000	-2.695315	3.216891
C	2.570459	1.484055	1.050329
C	3.186483	1.839717	2.239846
C	2.334211	1.347657	3.216891
H	-4.111839	2.373971	2.402399
N	-2.590420	1.495580	4.641448
H	0.000000	-4.747943	2.402399
H	0.000000	-3.329700	0.030406
N	0.000000	-2.991159	4.641448
H	-2.883605	1.664850	0.030406
H	0.000000	0.000000	4.342817
H	4.111839	2.373971	2.402399
N	2.590420	1.495580	4.641448
H	2.883605	1.664850	0.030406
B	0.000000	0.000000	3.174647
O	-3.628513	-2.094923	-4.910459
O	-1.799702	-1.039058	-5.449412
O	3.628513	-2.094923	-4.910459
O	1.799702	-1.039058	-5.449412
O	0.000000	4.189846	-4.910459
O	0.000000	2.078117	-5.449412
O	-3.628513	2.094923	4.910459
O	-1.799702	1.039058	5.449412
O	0.000000	-4.189846	4.910459
O	0.000000	-2.078117	5.449412
O	3.628513	2.094923	4.910459
O	1.799702	1.039058	5.449412

$[Co(Tb^{5NO2})_2]$ ^2E_g D_{3d} OPBE

Co	0.000000	0.000000	0.000000
N	-1.388358	-0.801569	-1.194305
N	-1.259268	-0.727039	-2.527955
N	1.388358	-0.801569	-1.194305
N	1.259268	-0.727039	-2.527955
N	0.000000	1.603138	-1.194305
N	0.000000	1.454077	-2.527955
C	-2.521829	-1.455979	-0.908839
C	-3.163893	-1.826674	-2.080464
C	-2.336826	-1.349167	-3.084643
C	2.521829	-1.455979	-0.908839
C	3.163893	-1.826674	-2.080464
C	2.336826	-1.349167	-3.084643
C	0.000000	2.911957	-0.908839
C	0.000000	3.653348	-2.080464
C	0.000000	2.698334	-3.084643
H	-4.093166	-2.363190	-2.210908
N	-2.616589	-1.510688	-4.500015
H	4.093166	-2.363190	-2.210908
H	2.813432	-1.624336	0.118385
N	2.616589	-1.510688	-4.500015
H	-2.813432	-1.624336	0.118385
H	0.000000	0.000000	-4.263795
H	0.000000	4.726381	-2.210908
N	0.000000	3.021377	-4.500015
H	0.000000	3.248672	0.118385
B	0.000000	0.000000	-3.095652
N	-1.388358	0.801569	1.194305
N	-1.259268	0.727039	2.527955
N	0.000000	-1.603138	1.194305
N	0.000000	-1.454077	2.527955
N	1.388358	0.801569	1.194305
N	1.259268	0.727039	2.527955
C	-2.521829	1.455979	0.908839
C	-3.163893	1.826674	2.080464
C	-2.336826	1.349167	3.084643
C	0.000000	-2.911957	0.908839
C	0.000000	-3.653348	2.080464
C	0.000000	-2.698334	3.084643
C	2.521829	1.455979	0.908839
C	3.163893	1.826674	2.080464
C	2.336826	1.349167	3.084643
H	-4.093166	2.363190	2.210908
N	-2.616589	1.510688	4.500015
H	0.000000	-4.726381	2.210908
H	0.000000	-3.248672	-0.118385
N	0.000000	-3.021377	4.500015
H	-2.813432	1.624336	-0.118385
H	0.000000	0.000000	4.263795
H	4.093166	2.363190	2.210908
N	2.616589	1.510688	4.500015
H	2.813432	1.624336	-0.118385
B	0.000000	0.000000	3.095652
O	-3.658851	-2.112438	-4.747607

O	-1.837199	-1.060708	-5.323555
O	3.658851	-2.112438	-4.747607
O	1.837199	-1.060708	-5.323555
O	0.000000	4.224877	-4.747607
O	0.000000	2.121415	-5.323555
O	-3.658851	2.112438	4.747607
O	-1.837199	1.060708	5.323555
O	0.000000	-4.224877	4.747607
O	0.000000	-2.121415	5.323555
O	3.658851	2.112438	4.747607
O	1.837199	1.060708	5.323555

$[Co(Tb^{3,5\text{-}CH3})_2]$ ^4E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.51070000	0.87220000	-1.33860000
N	-1.26830000	0.73230000	-2.66300000
N	0.00000000	-1.74440000	-1.33860000
N	0.00000000	-1.46450000	-2.66300000
N	1.51070000	0.87220000	-1.33860000
N	1.26830000	0.73230000	-2.66300000
C	-2.67260000	1.54300000	-1.22080000
C	-3.17100000	1.83080000	-2.49900000
C	-2.25580000	1.30240000	-3.39640000
C	0.00000000	-3.08600000	-1.22080000
C	0.00000000	-3.66160000	-2.49900000
C	0.00000000	-2.60470000	-3.39640000
C	2.67260000	1.54300000	-1.22080000
C	3.17100000	1.83080000	-2.49900000
C	2.25580000	1.30240000	-3.39640000
H	-4.08680000	2.35950000	-2.74120000
C	-2.30670000	1.33180000	-4.88510000
H	0.00000000	-4.71900000	-2.74120000
C	0.00000000	-3.82750000	0.07240000
C	0.00000000	-2.66360000	-4.88510000
C	-3.31470000	1.91380000	0.07240000
H	0.00000000	0.00000000	-4.35090000
H	4.08680000	2.35950000	-2.74120000
C	2.30670000	1.33180000	-4.88510000
C	3.31470000	1.91380000	0.07240000
B	0.00000000	0.00000000	-3.15190000
N	0.00000000	1.74440000	1.33860000
N	0.00000000	1.46450000	2.66300000
N	-1.51070000	-0.87220000	1.33860000
N	-1.26830000	-0.73230000	2.66300000
N	1.51070000	-0.87220000	1.33860000
N	1.26830000	-0.73230000	2.66300000
C	0.00000000	3.08600000	1.22080000
C	0.00000000	3.66160000	2.49900000
C	0.00000000	2.60470000	3.39640000
C	-2.67260000	-1.54300000	1.22080000
C	-3.17100000	-1.83080000	2.49900000
C	-2.25580000	-1.30240000	3.39640000
C	2.67260000	-1.54300000	1.22080000
C	3.17100000	-1.83080000	2.49900000
C	2.25580000	-1.30240000	3.39640000
H	0.00000000	4.71900000	2.74120000
C	0.00000000	2.66360000	4.88510000
H	-4.08680000	-2.35950000	2.74120000
C	-3.31470000	-1.91380000	-0.07240000
C	-2.30670000	-1.33180000	4.88510000
C	0.00000000	3.82750000	-0.07240000
H	0.00000000	0.00000000	4.35090000
H	4.08680000	-2.35950000	2.74120000
C	2.30670000	-1.33180000	4.88510000
C	3.31470000	-1.91380000	-0.07240000
B	0.00000000	0.00000000	3.15190000
H	0.87670000	-3.59500000	0.68210000
H	0.00000000	-4.90310000	-0.12820000
H	-0.87670000	-3.59500000	0.68210000
H	-4.24620000	2.45150000	-0.12820000
H	-2.67500000	2.55680000	0.68210000
H	-3.55170000	1.03820000	0.68210000
H	4.24620000	2.45150000	-0.12820000
H	3.55170000	1.03820000	0.68210000
H	2.67500000	2.55680000	0.68210000
H	-3.55170000	-1.03820000	-0.68210000
H	-4.24620000	-2.45150000	0.12820000
H	-2.67500000	-2.55680000	-0.68210000
H	2.67500000	-2.55680000	-0.68210000
H	4.24620000	-2.45150000	0.12820000
H	3.55170000	-1.03820000	-0.68210000
H	0.87670000	3.59500000	-0.68210000
H	0.00000000	4.90310000	0.12820000
H	-0.87670000	3.59500000	-0.68210000
H	3.21310000	-1.85510000	5.20280000
H	1.44910000	-1.85660000	5.31970000
H	2.33240000	-0.32670000	5.31970000
H	-3.21310000	-1.85510000	5.20280000
H	-2.33240000	-0.32670000	5.31970000
H	-1.44910000	-1.85660000	5.31970000
H	-0.88330000	2.18330000	5.31970000
H	0.00000000	3.71010000	5.20280000
H	0.88330000	2.18330000	5.31970000
H	2.33240000	0.32670000	-5.31970000
H	3.21310000	1.85510000	-5.20280000
H	1.44910000	1.85660000	-5.31970000
H	0.88330000	-2.18330000	-5.31970000
H	-0.88330000	-2.18330000	-5.31970000
H	0.00000000	-3.71010000	-5.20280000
H	-2.33240000	0.32670000	-5.31970000
H	-1.44910000	1.85660000	-5.31970000
H	-3.21310000	1.85510000	-5.20280000

$[Co(Tb^{3,5\text{-}CH3})_2]$ ^2E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	-1.46740000	0.84720000	-1.22590000
N	-1.25790000	0.72620000	-2.55660000
N	0.00000000	-1.69440000	-1.22590000
N	0.00000000	-1.45250000	-2.55660000
N	1.46740000	0.84720000	-1.22590000
N	1.25790000	0.72620000	-2.55660000
C	-2.62690000	1.51660000	-1.06880000
C	-3.15280000	1.82030000	-2.33420000
C	-2.26080000	1.30530000	-3.26020000
C	0.00000000	-3.03330000	-1.06880000
C	0.00000000	-3.64050000	-2.33420000
C	0.00000000	-2.61060000	-3.26020000
C	2.62690000	1.51660000	-1.06880000

C	3.15280000	1.82030000	-2.33420000
C	2.26080000	1.30530000	-3.26020000
H	-4.07440000	2.35240000	-2.54460000
C	-2.33830000	1.35000000	-4.74730000
H	0.00000000	-4.70470000	-2.54460000
C	0.00000000	-3.76030000	0.23220000
C	0.00000000	-2.70010000	-4.74730000
C	-3.25660000	1.88020000	0.23220000
H	0.00000000	0.00000000	-4.26270000
H	4.07440000	2.35240000	-2.54460000
C	2.33830000	1.35000000	-4.74730000
C	3.25660000	1.88020000	0.23220000
B	0.00000000	0.00000000	-3.06350000
N	0.00000000	1.69440000	1.22590000
N	0.00000000	1.45250000	2.55660000
N	-1.46740000	-0.84720000	1.22590000
N	-1.25790000	-0.72620000	2.55660000
N	1.46740000	-0.84720000	1.22590000
N	1.25790000	-0.72620000	2.55660000
C	0.00000000	3.03330000	1.06880000
C	0.00000000	3.64050000	2.33420000
C	0.00000000	2.61060000	3.26020000
C	-2.62690000	-1.51660000	1.06880000
C	-3.15280000	-1.82030000	2.33420000
C	-2.26080000	-1.30530000	3.26020000
C	2.62690000	-1.51660000	1.06880000
C	3.15280000	-1.82030000	2.33420000
C	2.26080000	-1.30530000	3.26020000
H	0.00000000	4.70470000	2.54460000
C	0.00000000	2.70010000	4.74730000
H	-4.07440000	-2.35240000	2.54460000
C	-3.25660000	-1.88020000	-0.23220000
C	-2.33830000	-1.35000000	4.74730000
C	0.00000000	3.76030000	-0.23220000
H	0.00000000	0.00000000	4.26270000
H	4.07440000	-2.35240000	2.54460000
C	2.33830000	-1.35000000	4.74730000
C	3.25660000	-1.88020000	-0.23220000
B	0.00000000	0.00000000	3.06350000
H	0.87830000	-3.52570000	0.83850000
H	0.00000000	-4.83710000	0.03680000
H	-0.87830000	-3.52570000	0.83850000
H	-4.18900000	2.41850000	0.03680000
H	-2.61420000	2.52350000	0.83850000
H	-3.49250000	1.00220000	0.83850000
H	4.18900000	2.41850000	0.03680000
H	3.49250000	1.00220000	0.83850000
H	2.61420000	2.52350000	0.83850000
H	-3.49250000	-1.00220000	-0.83850000
H	-4.18900000	-2.41850000	-0.03680000
H	-2.61420000	-2.52350000	-0.83850000
H	2.61420000	-2.52350000	-0.83850000
H	4.18900000	-2.41850000	-0.03680000
H	3.49250000	-1.00220000	-0.83850000
H	0.87830000	3.52570000	-0.83850000
H	0.00000000	4.83710000	-0.03680000
H	-0.87830000	3.52570000	-0.83850000
H	3.25010000	-1.87640000	5.04370000
H	1.48800000	-1.87920000	5.19170000
H	2.37150000	-0.34910000	5.19170000
H	-3.25010000	-1.87640000	5.04370000
H	-2.37150000	-0.34910000	5.19170000
H	-1.48800000	-1.87920000	5.19170000
H	-0.88340000	2.22830000	5.19170000
H	0.00000000	3.75290000	5.04370000
H	0.88340000	2.22830000	5.19170000
H	2.37150000	0.34910000	-5.19170000
H	3.25010000	1.87640000	-5.04370000
H	1.48800000	1.87920000	-5.19170000
H	0.88340000	-2.22830000	-5.19170000
H	-0.88340000	-2.22830000	-5.19170000
H	0.00000000	-3.75290000	-5.04370000
H	-2.37150000	0.34910000	-5.19170000
H	-1.48800000	1.87920000	-5.19170000
H	-3.25010000	1.87640000	-5.04370000

$[Co(Tb^{3,5\text{-}CF3})_2]$ ^4E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.56658956	0.90447081	1.25295890
N	1.29455488	0.74741153	2.56571854
N	0.00000000	-1.80894162	1.25295890
N	0.00000000	-1.49482307	2.56571854
N	-1.56658956	0.90447081	1.25295890
N	-1.29455488	0.74741153	2.56571854
C	2.73712222	1.58027831	1.17104597
C	3.21388923	1.85553991	2.45013987
C	2.28228432	1.31767728	3.31130494
C	0.00000000	-3.16055663	1.17104597
C	0.00000000	-3.71107930	2.45013987
C	0.00000000	-2.63535509	3.31130494
C	-2.73712222	1.58027831	1.17104597
C	-3.21388923	1.85553991	2.45013987
C	-2.28228432	1.31767728	3.31130494
H	4.11920460	2.37822416	2.71910691
C	2.40158945	1.38655816	4.81291205
H	0.00000000	-4.75644778	2.71910691
C	0.00000000	-4.06630275	-0.06102525
C	0.00000000	-2.77311686	4.81291205
C	3.52152113	2.03315138	-0.06102525
H	0.00000000	0.00000000	4.22989155
H	-4.11920460	2.37822416	2.71910691
C	-2.40158945	1.38655816	4.81291205
C	-3.52152113	2.03315138	-0.06102525
B	0.00000000	0.00000000	3.04182460
N	0.00000000	1.80894162	-1.25295890
N	0.00000000	1.49482307	-2.56571854
N	1.56658956	-0.90447081	-1.25295890
N	1.29455488	-0.74741153	-2.56571854
N	-1.56658956	-0.90447081	-1.25295890
N	-1.29455488	-0.74741153	-2.56571854
C	0.00000000	3.16055663	-1.17104597
C	0.00000000	3.71107930	-2.45013987
C	0.00000000	2.63535509	-3.31130494
C	2.73712222	-1.58027831	-1.17104597
C	3.21388923	-1.85553991	-2.45013987
C	2.28228432	-1.31767728	-3.31130494
C	-2.73712222	-1.58027831	-1.17104597
C	-3.21388923	-1.85553991	-2.45013987
C	-2.28228432	-1.31767728	-3.31130494

H	0.00000000	4.75644778	-2.71910691
C	0.00000000	2.77311686	-4.81291205
H	4.11920460	-2.37822416	-2.71910691
C	3.52152113	-2.03315138	0.06102525
C	2.40158945	-1.38655816	-4.81291205
C	0.00000000	4.06630275	0.06102525
H	0.00000000	0.00000000	-4.22989155
H	-4.11920460	-2.37822416	-2.71910691
C	-2.40158945	-1.38655816	-4.81291205
C	-3.52152113	-2.03315138	0.06102525
B	0.00000000	0.00000000	-3.04182460
F	-1.07586709	-3.92982424	-0.85482393
F	0.00000000	-5.35479273	0.37131785
F	1.07586709	-3.92982424	-0.85482393
F	4.63738661	2.67739663	0.37131785
F	2.86539373	2.89664059	-0.85482393
F	3.94126135	1.03318365	-0.85482393
F	-4.63738661	2.67739663	0.37131785
F	-3.94126135	1.03318365	-0.85482393
F	-2.86539373	2.89664059	-0.85482393
F	3.94126135	-1.03318365	0.85482393
F	4.63738661	-2.67739663	-0.37131785
F	2.86539373	-2.89664059	0.85482393
F	-2.86539373	-2.89664059	0.85482393
F	-4.63738661	-2.67739663	-0.37131785
F	-3.94126135	-1.03318365	0.85482393
F	-1.07586709	3.92982424	0.85482393
F	0.00000000	5.35479273	-0.37131785
F	1.07586709	3.92982424	0.85482393
F	-3.54198706	-2.04496738	-5.13261131
F	-1.38433456	-2.05567263	-5.39075244
F	-2.47243199	-0.17103220	-5.39075244
F	3.54198706	-2.04496738	-5.13261131
F	2.47243199	-0.17103220	-5.39075244
F	1.38433456	-2.05567263	-5.39075244
F	1.08809743	2.22670484	-5.39075244
F	0.00000000	4.08993422	-5.13261131
F	-1.08809743	2.22670484	-5.39075244
F	-2.47243199	0.17103220	5.39075244
F	-3.54198706	2.04496738	5.13261131
F	-1.38433456	2.05567263	5.39075244
F	-1.08809743	-2.22670484	5.39075244
F	1.08809743	-2.22670484	5.39075244
F	0.00000000	-4.08993422	5.13261131
F	2.47243199	0.17103220	5.39075244
F	1.38433456	2.05567263	5.39075244
F	3.54198706	2.04496738	5.13261131

$[Co(Tb^{3,5\text{-}CF3})_2]$ ^2E_g D_{3d} OPBE

Co	0.00000000	0.00000000	0.00000000
N	1.52217253	0.87882635	1.17407127
N	1.28090475	0.73953050	2.49307785
N	0.00000000	-1.75765323	1.17407127
N	0.00000000	-1.47906099	2.49307785
N	-1.52217253	0.87882635	1.17407127
N	-1.28090475	0.73953050	2.49307785
C	2.69352278	1.55510588	1.05907947
C	3.19324973	1.84362337	2.32756179
C	2.28148632	1.31721689	3.21270810
C	0.00000000	-3.11021229	1.05907947
C	0.00000000	-3.68724727	2.32756179
C	0.00000000	-2.63443326	3.21270810
C	-2.69352278	1.55510588	1.05907947
C	-3.19324973	1.84362337	2.32756179
C	-2.28148632	1.31721689	3.21270810
H	4.10375263	2.36930276	2.57093887
C	2.42479123	1.39995376	4.71062051
H	0.00000000	-4.73860499	2.57093887
C	0.00000000	-4.01070898	-0.17572759
C	0.00000000	-2.79990751	4.71062051
C	3.47337552	2.00535423	-0.17572759
H	0.00000000	0.00000000	4.17385750
H	-4.10375263	2.36930276	2.57093887
C	-2.42479123	1.39995376	4.71062051
C	-3.47337552	2.00535423	-0.17572759
B	0.00000000	0.00000000	2.98597206
N	0.00000000	1.75765323	-1.17407127
N	0.00000000	1.47906099	-2.49307785
N	1.52217253	-0.87882635	-1.17407127
N	1.28090475	-0.73953050	-2.49307785
N	-1.52217253	-0.87882635	-1.17407127
N	-1.28090475	-0.73953050	-2.49307785
C	0.00000000	3.11021229	-1.05907947
C	0.00000000	3.68724727	-2.32756179
C	0.00000000	2.63443326	-3.21270810
C	2.69352278	-1.55510588	-1.05907947
C	3.19324973	-1.84362337	-2.32756179
C	2.28148632	-1.31721689	-3.21270810
C	-2.69352278	-1.55510588	-1.05907947
C	-3.19324973	-1.84362337	-2.32756179
C	-2.28148632	-1.31721689	-3.21270810
H	0.00000000	4.73860499	-2.57093887
C	0.00000000	2.79990751	-4.71062051
H	4.10375263	-2.36930276	-2.57093887
C	3.47337552	-2.00535423	0.17572759
C	2.42479123	-1.39995376	-4.71062051
C	0.00000000	4.01070898	0.17572759
H	0.00000000	0.00000000	-4.17385750
H	-4.10375263	-2.36930276	-2.57093887
C	-2.42479123	-1.39995376	-4.71062051
C	-3.47337552	-2.00535423	0.17572759
B	0.00000000	0.00000000	-2.98597206
F	-1.07803566	-3.87443367	-0.96668142
F	0.00000000	-5.30115268	0.25112583
F	1.07803566	-3.87443367	-0.96668142
F	4.59093278	2.65057634	0.25112583
F	2.81634006	2.87082309	-0.96668142
F	3.89437571	1.00361058	-0.96668142
F	-4.59093278	2.65057634	0.25112583
F	-3.89437571	1.00361058	-0.96668142
F	-2.81634006	2.87082309	-0.96668142
F	3.89437571	-1.00361058	0.96668142
F	4.59093278	-2.65057634	-0.25112583
F	2.81634006	-2.87082309	0.96668142
F	-2.81634006	-2.87082309	0.96668142
F	-4.59093278	-2.65057634	-0.25112583
F	-3.89437571	-1.00361058	0.96668142
F	-1.07803566	3.87443367	0.96668142
F	0.00000000	5.30115268	-0.25112583

F	1.07803566	3.87443367	0.96668142
F	-3.57011336	-2.06120571	-5.00458217
F	-1.41622172	-2.07402609	-5.29864121
F	-2.50426994	-0.18947086	-5.29864121
F	3.57011336	-2.06120571	-5.00458217
F	2.50426994	-0.18947086	-5.29864121
F	1.41622172	-2.07402609	-5.29864121
F	1.08804822	2.26349694	-5.29864121
F	0.00000000	4.12241195	-5.00458217
F	-1.08804822	2.26349694	-5.29864121
F	-2.50426994	0.18947086	5.29864121
F	-3.57011336	2.06120571	5.00458217
F	-1.41622172	2.07402609	5.29864121
F	-1.08804822	-2.26349694	5.29864121
F	1.08804822	-2.26349694	5.29864121
F	0.00000000	-4.12241195	5.00458217
F	2.50426994	0.18947086	5.29864121
F	1.41622172	2.07402609	5.29864121
F	3.57011336	2.06120571	5.00458217

$[Co(Tb^{3,5\text{-}NH2})_2]$ ^4E_g D_{3d} OPBE

Co	0.000000	0.000000	0.000000
N	0.000000	1.708400	1.365244
N	0.000000	1.455203	2.723324
N	1.479517	-0.854200	1.365244
N	1.260243	-0.727602	2.723324
N	-1.479517	-0.854200	1.365244
N	-1.260243	-0.727602	2.723324
C	0.000000	3.045013	1.238857
C	0.000000	3.672763	2.500299
C	0.000000	2.618621	3.407852
C	2.637058	-1.522506	1.238857
C	3.180706	-1.836381	2.500299
C	2.267792	-1.309310	3.407852
C	-2.637058	-1.522506	1.238857
C	-3.180706	-1.836381	2.500299
C	-2.267792	-1.309310	3.407852
H	0.000000	4.734011	2.721591
N	0.000000	2.679541	4.776808
H	4.099774	-2.367005	2.721591
N	3.157228	-1.822827	0.020768
N	2.320551	-1.339770	4.776808
N	0.000000	3.645653	0.020768
H	0.000000	0.000000	4.427665
H	-4.099774	-2.367005	2.721591
N	-2.320551	-1.339770	4.776808
N	-3.157228	-1.822827	0.020768
B	0.000000	0.000000	3.209694
N	-1.479517	0.854200	-1.365244
N	-1.260243	0.727602	-2.723324
N	1.479517	0.854200	-1.365244
N	1.260243	0.727602	-2.723324
N	0.000000	-1.708400	-1.365244
N	0.000000	-1.455203	-2.723324
C	-2.637058	1.522506	-1.238857
C	-3.180706	1.836381	-2.500299
C	-2.267792	1.309310	-3.407852
C	2.637058	1.522506	-1.238857
C	3.180706	1.836381	-2.500299
C	2.267792	1.309310	-3.407852
C	0.000000	-3.045013	-1.238857
C	0.000000	-3.672763	-2.500299
C	0.000000	-2.618621	-3.407852
H	-4.099774	2.367005	-2.721591
N	-2.320551	1.339770	-4.776808
H	4.099774	2.367005	-2.721591
N	3.157228	1.822827	-0.020768
N	2.320551	1.339770	-4.776808
N	-3.157228	1.822827	-0.020768
H	0.000000	0.000000	-4.427665
H	0.000000	-4.734011	-2.721591
N	0.000000	-2.679541	-4.776808
N	0.000000	-3.645653	-0.020768
B	0.000000	0.000000	-3.209694
H	0.000000	3.568631	5.235923
H	0.000000	1.842617	5.325536
H	3.090525	-1.784315	5.235923
H	1.595753	-0.921309	5.325536
H	-3.090525	-1.784315	5.235923
H	-1.595753	-0.921309	5.325536
H	-3.090525	1.784315	-5.235923
H	-1.595753	0.921309	-5.325536
H	3.090525	1.784315	-5.235923
H	1.595753	0.921309	-5.325536
H	0.000000	-3.568631	-5.235923
H	0.000000	-1.842617	-5.325536
H	0.000000	4.642940	-0.053226
H	4.020904	-2.321470	-0.053226
H	-4.020904	-2.321470	-0.053226
H	-4.020904	2.321470	0.053226
H	4.020904	2.321470	0.053226
H	0.000000	-4.642940	0.053226
H	2.670464	-1.541793	-0.812115
H	0.000000	3.083586	-0.812115
H	-2.670464	-1.541793	-0.812115
H	2.670464	1.541793	0.812115
H	-2.670464	1.541793	0.812115
H	0.000000	-3.083586	0.812115

$[Co(Tb^{3,5\text{-}NH2})_2]$ ^2E_g D_{3d} OPBE

Co	0.000000	0.000000	0.000000
N	0.000000	1.666061	1.268109
N	0.000000	1.445399	2.632554
N	1.442851	-0.833031	1.268109
N	1.251752	-0.722699	2.632554
N	-1.442851	-0.833031	1.268109
N	-1.251752	-0.722699	2.632554
C	0.000000	2.998093	1.107294
C	0.000000	3.653598	2.356823
C	0.000000	2.623836	3.289472
C	2.596425	-1.499047	1.107294
C	3.164109	-1.826799	2.356823
C	2.272309	-1.311918	3.289472
C	-2.596425	-1.499047	1.107294
C	-3.164109	-1.826799	2.356823
C	-2.272309	-1.311918	3.289472
H	0.000000	4.720418	2.549425
N	0.000000	2.711709	4.657923

H	4.088002	-2.360209	2.549425
N	3.101063	-1.790399	-0.118120
N	2.348409	-1.355854	4.657923
N	0.000000	3.580799	-0.118120
H	0.000000	0.000000	4.351421
H	-4.088002	-2.360209	2.549425
N	-2.348409	-1.355854	4.657923
N	-3.101063	-1.790399	-0.118120
B	0.000000	0.000000	3.134583
N	-1.442851	0.833031	-1.268109
N	-1.251752	0.722699	-2.632554
N	1.442851	0.833031	-1.268109
N	1.251752	0.722699	-2.632554
N	0.000000	-1.666061	-1.268109
N	0.000000	-1.445399	-2.632554
C	-2.596425	1.499047	-1.107294
C	-3.164109	1.826799	-2.356823
C	-2.272309	1.311918	-3.289472
C	2.596425	1.499047	-1.107294
C	3.164109	1.826799	-2.356823
C	2.272309	1.311918	-3.289472
C	0.000000	-2.998093	-1.107294
C	0.000000	-3.653598	-2.356823
C	0.000000	-2.623836	-3.289472
H	-4.088002	2.360209	-2.549425
N	-2.348409	1.355854	-4.657923
H	4.088002	2.360209	-2.549425
N	3.101063	1.790399	0.118120
N	2.348409	1.355854	-4.657923
N	-3.101063	1.790399	0.118120
H	0.000000	0.000000	-4.351421
H	0.000000	-4.720418	-2.549425
N	0.000000	-2.711709	-4.657923
N	0.000000	-3.580799	0.118120
B	0.000000	0.000000	-3.134583
H	0.000000	3.609844	5.098963
H	0.000000	1.886372	5.223882
H	3.126217	-1.804922	5.098963
H	1.633646	-0.943186	5.223882
H	-3.126217	-1.804922	5.098963
H	-1.633646	-0.943186	5.223882
H	-3.126217	1.804922	-5.098963
H	-1.633646	0.943186	-5.223882
H	3.126217	1.804922	-5.098963
H	1.633646	0.943186	-5.223882
H	0.000000	-3.609844	-5.098963
H	0.000000	-1.886372	-5.223882
H	0.000000	4.577084	-0.203583
H	3.963871	-2.288542	-0.203583
H	-3.963871	-2.288542	-0.203583
H	-3.963871	2.288542	0.203583
H	3.963871	2.288542	0.203583
H	0.000000	-4.577084	0.203583
H	2.603974	-1.503405	-0.941977
H	0.000000	3.006811	-0.941977
H	-2.603974	-1.503405	-0.941977
H	2.603974	1.503405	0.941977
H	-2.603974	1.503405	0.941977
H	0.000000	-3.006811	0.941977

$[Co(Tb^{3,5\text{-}NO2})_2]$ ^4E_g D_{3d} OPBE

Co	0.000000	0.000000	0.000000
N	0.000000	1.777462	1.379734
N	0.000000	1.476683	2.685274
N	1.539327	-0.888731	1.379734
N	1.278845	-0.738341	2.685274
N	-1.539327	-0.888731	1.379734
N	-1.278845	-0.738341	2.685274
C	0.000000	3.122285	1.313158
C	0.000000	3.710043	2.565494
C	0.000000	2.633627	3.418223
C	2.703978	-1.561142	1.313158
C	3.212992	-1.855022	2.565494
C	2.280788	-1.316814	3.418223
C	-2.703978	-1.561142	1.313158
C	-3.212992	-1.855022	2.565494
C	-2.280788	-1.316814	3.418223
H	0.000000	4.758431	2.817650
N	0.000000	2.807723	4.874644
H	4.120922	-2.379215	2.817650
N	3.385722	-1.954747	0.092700
N	2.431559	-1.403861	4.874644
N	0.000000	3.909495	0.092700
H	0.000000	0.000000	4.334863
H	-4.120922	-2.379215	2.817650
N	-2.431559	-1.403861	4.874644
N	-3.385722	-1.954747	0.092700
B	0.000000	0.000000	3.169537
N	-1.539327	0.888731	-1.379734
N	-1.278845	0.738341	-2.685274
N	1.539327	0.888731	-1.379734
N	1.278845	0.738341	-2.685274
N	0.000000	-1.777462	-1.379734
N	0.000000	-1.476683	-2.685274
C	-2.703978	1.561142	-1.313158
C	-3.212992	1.855022	-2.565494
C	-2.280788	1.316814	-3.418223
C	2.703978	1.561142	-1.313158
C	3.212992	1.855022	-2.565494
C	2.280788	1.316814	-3.418223
C	0.000000	-3.122285	-1.313158
C	0.000000	-3.710043	-2.565494
C	0.000000	-2.633627	-3.418223
H	-4.120922	2.379215	-2.817650
N	-2.431559	1.403861	-4.874644
H	4.120922	2.379215	-2.817650
N	3.385722	1.954747	-0.092700
N	2.431559	1.403861	-4.874644
N	-3.385722	1.954747	-0.092700
H	0.000000	0.000000	-4.334863
H	0.000000	-4.758431	-2.817650
N	0.000000	-2.807723	-4.874644
N	0.000000	-3.909495	-0.092700
B	0.000000	0.000000	-3.169537
O	0.000000	3.978668	5.233432
O	0.000000	1.835866	5.605104
O	3.445628	-1.989334	5.233432
O	1.589907	-0.917933	5.605104
O	-3.445628	-1.989334	5.233432

O	-1.589907	-0.917933	5.605104
O	-3.445628	1.989334	-5.233432
O	-1.589907	0.917933	-5.605104
O	3.445628	1.989334	-5.233432
O	1.589907	0.917933	-5.605104
O	0.000000	-3.978668	-5.233432
O	0.000000	-1.835866	-5.605104
O	0.000000	5.122905	0.252304
O	4.436565	-2.561452	0.252304
O	-4.436565	-2.561452	0.252304
O	-4.436565	2.561452	-0.252304
O	4.436565	2.561452	-0.252304
O	0.000000	-5.122905	-0.252304
O	2.883458	-1.664765	-0.981793
O	0.000000	3.329530	-0.981793
O	-2.883458	-1.664765	-0.981793
O	2.883458	1.664765	0.981793
O	-2.883458	1.664765	0.981793
O	0.000000	-3.329530	0.981793

$[Co(Tb^{3,5\text{-}NO2})_2]$ ^2E_g D_{3d} OPBE

Co	0.000000	0.000000	0.000000
N	0.000000	1.725519	1.210594
N	0.000000	1.465309	2.522978
N	1.494344	-0.862760	1.210594
N	1.268994	-0.732654	2.522978
N	-1.494344	-0.862760	1.210594
N	-1.268994	-0.732654	2.522978
C	0.000000	3.073096	1.100059
C	0.000000	3.689406	2.340553
C	0.000000	2.639769	3.222816
C	2.661379	-1.536548	1.100059
C	3.195120	-1.844703	2.340553
C	2.286107	-1.319885	3.222816
C	-2.661379	-1.536548	1.100059
C	-3.195120	-1.844703	2.340553
C	-2.286107	-1.319885	3.222816
H	0.000000	4.744562	2.562355
N	0.000000	2.844043	4.672665
H	4.108911	-2.372281	2.562355
N	3.345693	-1.931637	-0.123735
N	2.463014	-1.422022	4.672665
N	0.000000	3.863273	-0.123735
H	0.000000	0.000000	4.192133
H	-4.108911	-2.372281	2.562355
N	-2.463014	-1.422022	4.672665
N	-3.345693	-1.931637	-0.123735
B	0.000000	0.000000	3.026717
N	-1.494344	0.862760	-1.210594
N	-1.268994	0.732654	-2.522978
N	1.494344	0.862760	-1.210594
N	1.268994	0.732654	-2.522978
N	0.000000	-1.725519	-1.210594
N	0.000000	-1.465309	-2.522978
C	-2.661379	1.536548	-1.100059
C	-3.195120	1.844703	-2.340553
C	-2.286107	1.319885	-3.222816
C	2.661379	1.536548	-1.100059
C	3.195120	1.844703	-2.340553
C	2.286107	1.319885	-3.222816
C	0.000000	-3.073096	-1.100059
C	0.000000	-3.689406	-2.340553
C	0.000000	-2.639769	-3.222816
H	-4.108911	2.372281	-2.562355
N	-2.463014	1.422022	-4.672665
H	4.108911	2.372281	-2.562355
N	3.345693	1.931637	0.123735
N	2.463014	1.422022	-4.672665
N	-3.345693	1.931637	0.123735
H	0.000000	0.000000	-4.192133
H	0.000000	-4.744562	-2.562355
N	0.000000	-2.844043	-4.672665
N	0.000000	-3.863273	0.123735
B	0.000000	0.000000	-3.026717
O	0.000000	4.022446	5.006457
O	0.000000	1.886562	5.422629
O	3.483541	-2.011223	5.006457
O	1.633810	-0.943281	5.422629
O	-3.483541	-2.011223	5.006457
O	-1.633810	-0.943281	5.422629
O	-3.483541	2.011223	-5.006457
O	-1.633810	0.943281	-5.422629
O	3.483541	2.011223	-5.006457
O	1.633810	0.943281	-5.422629
O	0.000000	-4.022446	-5.006457
O	0.000000	-1.886562	-5.422629
O	0.000000	5.075377	0.047614
O	4.395406	-2.537689	0.047614
O	-4.395406	-2.537689	0.047614
O	-4.395406	2.537689	-0.047614
O	4.395406	2.537689	-0.047614
O	0.000000	-5.075377	-0.047614
O	2.857447	-1.649748	-1.205555
O	0.000000	3.299496	-1.205555
O	-2.857447	-1.649748	-1.205555
O	2.857447	1.649748	1.205555
O	-2.857447	1.649748	1.205555
O	0.000000	-3.299496	1.205555

$[Cr(Tb^{4NH2})_2]^+$ $^4A_{2g}$ D_{3d}

Cr	0.00000000	0.00000000	0.00000000
N	-1.41441882	-0.81661522	-1.24381154
N	-1.24409201	-0.71827662	-2.56733464
N	1.41441882	-0.81661522	-1.24381154
N	1.24409201	-0.71827662	-2.56733464
N	0.00000000	1.63322991	-1.24381154
N	0.00000000	1.43655324	-2.56733464
C	-2.56509305	-1.48095704	-1.02827712
C	-3.15700743	-1.82269917	-2.25423264
C	-2.27346135	-1.31258342	-3.20946795
C	2.56509305	-1.48095704	-1.02827712
C	3.15700743	-1.82269917	-2.25423264
C	2.27346135	-1.31258342	-3.20946795
C	0.00000000	2.96191407	-1.02827712
C	0.00000000	3.64539835	-2.25423264
C	0.00000000	2.62516684	-3.20946795

N	-4.32977111	-2.49979416	-2.46259089
H	-2.31126154	-1.33440775	-4.29123695
N	4.32977111	-2.49979416	-2.46259089
H	2.90604512	-1.67780568	-0.02054425
H	2.31126154	-1.33440775	-4.29123695
H	-2.90604512	-1.67780568	-0.02054425
H	0.00000000	0.00000000	-4.31959874
N	0.00000000	4.99958885	-2.46259089
H	0.00000000	2.66881496	-4.29123695
H	0.00000000	3.35561189	-0.02054425
B	0.00000000	0.00000000	-3.12038308
N	-1.41441882	0.81661522	1.24381154
N	-1.24409201	0.71827662	2.56733464
N	0.00000000	-1.63322991	1.24381154
N	0.00000000	-1.43655324	2.56733464
N	1.41441882	0.81661522	1.24381154
N	1.24409201	0.71827662	2.56733464
C	-2.56509305	1.48095704	1.02827712
C	-3.15700743	1.82269917	2.25423264
C	-2.27346135	1.31258342	3.20946795
C	0.00000000	-2.96191407	1.02827712
C	0.00000000	-3.64539835	2.25423264
C	0.00000000	-2.62516684	3.20946795
C	2.56509305	1.48095704	1.02827712
C	3.15700743	1.82269917	2.25423264
C	2.27346135	1.31258342	3.20946795
N	-4.32977111	2.49979416	2.46259089
H	-2.31126154	1.33440775	4.29123695
N	0.00000000	-4.99958885	2.46259089
H	0.00000000	-3.35561189	0.02054425
H	0.00000000	-2.66881496	4.29123695
H	-2.90604512	1.67780568	0.02054425
H	0.00000000	0.00000000	4.31959874
N	4.32977111	2.49979416	2.46259089
H	2.31126154	1.33440775	4.29123695
H	2.90604512	1.67780568	0.02054425
B	0.00000000	0.00000000	3.12038308
H	-4.66095140	-2.69100125	-3.38899821
H	-4.88431659	-2.81996121	-1.69158651
H	4.66095140	-2.69100125	-3.38899821
H	4.88431659	-2.81996121	-1.69158651
H	0.00000000	5.38200303	-3.38899821
H	0.00000000	5.63992296	-1.69158651
H	-4.66095140	2.69100125	3.38899821
H	-4.88431659	2.81996121	1.69158651
H	0.00000000	-5.38200303	3.38899821
H	0.00000000	-5.63992296	1.69158651
H	4.66095140	2.69100125	3.38899821
H	4.88431659	2.81996121	1.69158651

$[Cr(Tb^{4NH2})_2]^+$ $^2A_{2g}$ D_{3d}

Cr	0.00000000	0.00000000	0.00000000
N	-1.41238572	-0.81544150	-1.22015997
N	-1.24411053	-0.71828773	-2.54604425
N	1.41238572	-0.81544150	-1.22015997
N	1.24411053	-0.71828773	-2.54604425
N	0.00000000	1.63088247	-1.22015997
N	0.00000000	1.43657494	-2.54604425
C	-2.56337957	-1.47996800	-1.00497798
C	-3.15624648	-1.82225943	-2.22979946
C	-2.27342589	-1.31256278	-3.18700755
C	2.56337957	-1.47996800	-1.00497798
C	3.15624648	-1.82225943	-2.22979946
C	2.27342589	-1.31256278	-3.18700755
C	0.00000000	2.95993548	-1.00497798
C	0.00000000	3.64451938	-2.22979946
C	0.00000000	2.62512609	-3.18700755
N	-4.32869318	-2.49917238	-2.43838526
H	-2.31288982	-1.33534757	-4.26874004
N	4.32869318	-2.49917238	-2.43838526
H	2.90361197	-1.67640124	0.00291259
H	2.31288982	-1.33534757	-4.26874004
H	-2.90361197	-1.67640124	0.00291259
H	0.00000000	0.00000000	-4.29834751
N	0.00000000	4.99834423	-2.43838526
H	0.00000000	2.67069460	-4.26874004
H	0.00000000	3.35280196	0.00291259
B	0.00000000	0.00000000	-3.09870321
N	-1.41238572	0.81544150	1.22015997
N	-1.24411053	0.71828773	2.54604425
N	0.00000000	-1.63088247	1.22015997
N	0.00000000	-1.43657494	2.54604425
N	1.41238572	0.81544150	1.22015997
N	1.24411053	0.71828773	2.54604425
C	-2.56337957	1.47996800	1.00497798
C	-3.15624648	1.82225943	2.22979946
C	-2.27342589	1.31256278	3.18700755
C	0.00000000	-2.95993548	1.00497798
C	0.00000000	-3.64451938	2.22979946
C	0.00000000	-2.62512609	3.18700755
C	2.56337957	1.47996800	1.00497798
C	3.15624648	1.82225943	2.22979946
C	2.27342589	1.31256278	3.18700755
N	-4.32869318	2.49917238	2.43838526
H	-2.31288982	1.33534757	4.26874004
N	0.00000000	-4.99834423	2.43838526
H	0.00000000	-3.35280196	-0.00291259
H	0.00000000	-2.67069460	4.26874004
H	-2.90361197	1.67640124	-0.00291259
H	0.00000000	0.00000000	4.29834751
N	4.32869318	2.49917238	2.43838526
H	2.31288982	1.33534757	4.26874004
H	2.90361197	1.67640124	-0.00291259
B	0.00000000	0.00000000	3.09870321
H	-4.65997983	-2.69044085	-3.36481375
H	-4.88326935	-2.81935689	-1.66729834
H	4.65997983	-2.69044085	-3.36481375
H	4.88326935	-2.81935689	-1.66729834
H	0.00000000	5.38088117	-3.36481375
H	0.00000000	5.63871379	-1.66729834
H	-4.65997983	2.69044085	3.36481375
H	-4.88326935	2.81935689	1.66729834
H	0.00000000	-5.38088117	3.36481375
H	0.00000000	-5.63871379	1.66729834
H	4.65997983	2.69044085	3.36481375
H	4.88326935	2.81935689	1.66729834

$[Cr(Tb^{4NO2})_2]^+$ $^4A_{2g}$ D_{3d}

Cr	0.00000000	0.00000000	0.00000000
N	-1.41239789	-0.81544838	-1.24849688
N	-1.24248595	-0.71734950	-2.59039830
N	1.41239789	-0.81544838	-1.24849688
N	1.24248595	-0.71734950	-2.59039830
N	0.00000000	1.63089623	-1.24849688
N	0.00000000	1.43469901	-2.59039830
C	-2.55388878	-1.47448837	-1.02921535
C	-3.11942474	-1.80100079	-2.25915822
C	-2.26032664	-1.30500031	-3.22925283
C	2.55388878	-1.47448837	-1.02921535
C	3.11942474	-1.80100079	-2.25915822
C	2.26032664	-1.30500031	-3.22925283
C	0.00000000	2.94897674	-1.02921535
C	0.00000000	3.60200105	-2.25915822
C	0.00000000	2.61000009	-3.22925283
N	-4.35595057	-2.51490905	-2.48059720
H	-2.32327122	-1.34134103	-4.30892100
N	4.35595057	-2.51490905	-2.48059720
H	2.92091553	-1.68639158	-0.03469551
H	2.32327122	-1.34134103	-4.30892100
H	-2.92091553	-1.68639158	-0.03469551
H	0.00000000	0.00000000	-4.34439281
N	0.00000000	5.02981863	-2.48059720
H	0.00000000	2.68268205	-4.30892100
H	0.00000000	3.37278316	-0.03469551
B	0.00000000	0.00000000	-3.14959631
N	-1.41239789	0.81544838	1.24849688
N	-1.24248595	0.71734950	2.59039830
N	0.00000000	-1.63089623	1.24849688
N	0.00000000	-1.43469901	2.59039830
N	1.41239789	0.81544838	1.24849688
N	1.24248595	0.71734950	2.59039830
C	-2.55388878	1.47448837	1.02921535
C	-3.11942474	1.80100079	2.25915822
C	-2.26032664	1.30500031	3.22925283
C	0.00000000	-2.94897674	1.02921535
C	0.00000000	-3.60200105	2.25915822
C	0.00000000	-2.61000009	3.22925283
C	2.55388878	1.47448837	1.02921535
C	3.11942474	1.80100079	2.25915822
C	2.26032664	1.30500031	3.22925283
N	-4.35595057	2.51490905	2.48059720
H	-2.32327122	1.34134103	4.30892100
N	0.00000000	-5.02981863	2.48059720
H	0.00000000	-3.37278316	0.03469551
H	0.00000000	-2.68268205	4.30892100
H	-2.92091553	1.68639158	0.03469551
H	0.00000000	0.00000000	4.34439281
N	4.35595057	2.51490905	2.48059720
H	2.32327122	1.34134103	4.30892100
H	2.92091553	1.68639158	0.03469551
B	0.00000000	0.00000000	3.14959631
O	-4.67736912	-2.70048040	-3.64594922
O	-4.96679468	-2.86758029	-1.48086760
O	4.67736912	-2.70048040	-3.64594922
O	4.96679468	-2.86758029	-1.48086760
O	0.00000000	5.40096027	-3.64594922
O	0.00000000	5.73516005	-1.48086760
O	-4.67736912	2.70048040	3.64594922
O	-4.96679468	2.86758029	1.48086760
O	0.00000000	-5.40096027	3.64594922
O	0.00000000	-5.73516005	1.48086760
O	4.67736912	2.70048040	3.64594922
O	4.96679468	2.86758029	1.48086760

$[Cr(Tb^{4NO2})_2]^+$ $^2A_{2g}$ D_{3d}

Cr	0.00000000	0.00000000	0.00000000
N	-1.40880583	-0.81337454	-1.22533373
N	-1.24212294	-0.71713995	-2.56915819
N	1.40880583	-0.81337454	-1.22533373
N	1.24212294	-0.71713995	-2.56915819
N	0.00000000	1.62674907	-1.22533373
N	0.00000000	1.43428043	-2.56915819
C	-2.55113282	-1.47289714	-1.00474196
C	-3.11851667	-1.80047637	-2.23287028
C	-2.26076215	-1.30525167	-3.20540757
C	2.55113282	-1.47289714	-1.00474196
C	3.11851667	-1.80047637	-2.23287028
C	2.26076215	-1.30525167	-3.20540757
C	0.00000000	2.94579480	-1.00474196
C	0.00000000	3.60095275	-2.23287028
C	0.00000000	2.61050333	-3.20540757
N	-4.35537165	-2.51457514	-2.45220049
H	-2.32588482	-1.34285024	-4.28491223
N	4.35537165	-2.51457514	-2.45220049
H	2.91623708	-1.68369013	-0.00941883
H	2.32588482	-1.34285024	-4.28491223
H	-2.91623708	-1.68369013	-0.00941883
H	0.00000000	0.00000000	-4.32395598
N	0.00000000	5.02915028	-2.45220049
H	0.00000000	2.68570048	-4.28491223
H	0.00000000	3.36738026	-0.00941883
B	0.00000000	0.00000000	-3.12900232
N	-1.40880583	0.81337454	1.22533373
N	-1.24212294	0.71713995	2.56915819
N	0.00000000	-1.62674907	1.22533373
N	0.00000000	-1.43428043	2.56915819
N	1.40880583	0.81337454	1.22533373
N	1.24212294	0.71713995	2.56915819
C	-2.55113282	1.47289714	1.00474196
C	-3.11851667	1.80047637	2.23287028
C	-2.26076215	1.30525167	3.20540757
C	0.00000000	-2.94579480	1.00474196
C	0.00000000	-3.60095275	2.23287028
C	0.00000000	-2.61050333	3.20540757
C	2.55113282	1.47289714	1.00474196
C	3.11851667	1.80047637	2.23287028
C	2.26076215	1.30525167	3.20540757
N	-4.35537165	2.51457514	2.45220049
H	-2.32588482	1.34285024	4.28491223
N	0.00000000	-5.02915028	2.45220049
H	0.00000000	-3.36738026	0.00941883
H	0.00000000	-2.68570048	4.28491223
H	-2.91623708	1.68369013	0.00941883
H	0.00000000	0.00000000	4.32395598
N	4.35537165	2.51457514	2.45220049
H	2.32588482	1.34285024	4.28491223
H	2.91623708	1.68369013	0.00941883

B	0.00000000	0.00000000	3.12900232
O	-4.67829413	-2.70101434	-3.61708366
O	-4.96490605	-2.86648965	-1.45143953
O	4.67829413	-2.70101434	-3.61708366
O	4.96490605	-2.86648965	-1.45143953
O	0.00000000	5.40202868	-3.61708366
O	0.00000000	5.73297984	-1.45143953
O	-4.67829413	2.70101434	3.61708366
O	-4.96490605	2.86648965	1.45143953
O	0.00000000	-5.40202868	3.61708366
O	0.00000000	-5.73297984	1.45143953
O	4.67829413	2.70101434	3.61708366
O	4.96490605	2.86648965	1.45143953

$[Mn(Tb^{4NH2})_2]^{2+}$ $^4A_{2g}$ D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.39252517	-0.80397476	-1.16356234
N	-1.23877907	-0.71520951	-2.49518926
N	1.39252517	-0.80397476	-1.16356234
N	1.23877907	-0.71520951	-2.49518926
N	0.00000000	1.60794952	-1.16356234
N	0.00000000	1.43041849	-2.49518926
C	-2.53863101	-1.46567916	-0.92014292
C	-3.14690015	-1.81686341	-2.13645630
C	-2.27343595	-1.31256860	-3.11381810
C	2.53863101	-1.46567916	-0.92014292
C	3.14690015	-1.81686341	-2.13645630
C	2.27343595	-1.31256860	-3.11381810
C	0.00000000	2.93135885	-0.92014292
C	0.00000000	3.63372734	-2.13645630
C	0.00000000	2.62513773	-3.11381810
N	-4.31223206	-2.48966836	-2.33230374
H	-2.32940650	-1.34488334	-4.19494786
N	4.31223206	-2.48966836	-2.33230374
H	2.86701407	-1.65527120	0.09230703
H	2.32940650	-1.34488334	-4.19494786
H	-2.86701407	-1.65527120	0.09230703
H	0.00000000	0.00000000	-4.25892909
N	0.00000000	4.97933671	-2.33230374
H	0.00000000	2.68976668	-4.19494786
H	0.00000000	3.31054292	0.09230703
B	0.00000000	0.00000000	-3.06327533
N	-1.39252517	0.80397476	1.16356234
N	-1.23877907	0.71520951	2.49518926
N	0.00000000	-1.60794952	1.16356234
N	0.00000000	-1.43041849	2.49518926
N	1.39252517	0.80397476	1.16356234
N	1.23877907	0.71520951	2.49518926
C	-2.53863101	1.46567916	0.92014292
C	-3.14690015	1.81686341	2.13645630
C	-2.27343595	1.31256860	3.11381810
C	0.00000000	-2.93135885	0.92014292
C	0.00000000	-3.63372734	2.13645630
C	0.00000000	-2.62513773	3.11381810
C	2.53863101	1.46567916	0.92014292
C	3.14690015	1.81686341	2.13645630
C	2.27343595	1.31256860	3.11381810
N	-4.31223206	2.48966836	2.33230374
H	-2.32940650	1.34488334	4.19494786
N	0.00000000	-4.97933671	2.33230374
H	0.00000000	-3.31054292	-0.09230703
H	0.00000000	-2.68976668	4.19494786
H	-2.86701407	1.65527120	-0.09230703
H	0.00000000	0.00000000	4.25892909
N	4.31223206	2.48966836	2.33230374
H	2.32940650	1.34488334	4.19494786
H	2.86701407	1.65527120	-0.09230703
B	0.00000000	0.00000000	3.06327533
H	-4.65136588	-2.68546711	-3.25709496
H	-4.86561123	-2.80916177	-1.55781686
H	4.65136588	-2.68546711	-3.25709496
H	4.86561123	-2.80916177	-1.55781686
H	0.00000000	5.37093476	-3.25709496
H	0.00000000	5.61832406	-1.55781686
H	-4.65136588	2.68546711	3.25709496
H	-4.86561123	2.80916177	1.55781686
H	0.00000000	-5.37093476	3.25709496
H	0.00000000	-5.61832406	1.55781686
H	4.65136588	2.68546711	3.25709496
H	4.86561123	2.80916177	1.55781686

$[Mn(Tb^{4NH2})_2]^{2+}$ ^2E_g D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.38740961	-0.80102142	-1.17170532
N	-1.23936645	-0.71554871	-2.50608767
N	1.38740961	-0.80102142	-1.17170532
N	1.23936645	-0.71554871	-2.50608767
N	0.00000000	1.60204284	-1.17170532
N	0.00000000	1.43109690	-2.50608767
C	-2.53388694	-1.46294067	-0.93357874
C	-3.14364835	-1.81498641	-2.14932060
C	-2.26990528	-1.31053021	-3.12808049
C	2.53388694	-1.46294067	-0.93357874
C	3.14364835	-1.81498641	-2.14932060
C	2.26990528	-1.31053021	-3.12808049
C	0.00000000	2.92588080	-0.93357874
C	0.00000000	3.62997230	-2.14932060
C	0.00000000	2.62106095	-3.12808049
N	-4.30894534	-2.48777073	-2.34624598
H	-2.32710775	-1.34355616	-4.20911764
N	4.30894534	-2.48777073	-2.34624598
H	2.86438406	-1.65375299	0.07825526
H	2.32710775	-1.34355616	-4.20911764
H	-2.86438406	-1.65375299	0.07825526
H	0.00000000	0.00000000	-4.26615395
N	0.00000000	4.97554145	-2.34624598
H	0.00000000	2.68711285	-4.20911764
H	0.00000000	3.30750597	0.07825526
B	0.00000000	0.00000000	-3.06896927
N	-1.38740961	0.80102142	1.17170532
N	-1.23936645	0.71554871	2.50608767
N	0.00000000	-1.60204284	1.17170532
N	0.00000000	-1.43109690	2.50608767
N	1.38740961	0.80102142	1.17170532
N	1.23936645	0.71554871	2.50608767
C	-2.53388694	1.46294067	0.93357874
C	-3.14364835	1.81498641	2.14932060
C	-2.26990528	1.31053021	3.12808049

C	0.00000000	-2.92588080	0.93357874
C	0.00000000	-3.62997230	2.14932060
C	0.00000000	-2.62106095	3.12808049
C	2.53388694	1.46294067	0.93357874
C	3.14364835	1.81498641	2.14932060
C	2.26990528	1.31053021	3.12808049
N	-4.30894534	2.48777073	2.34624598
H	-2.32710775	1.34355616	4.20911764
N	0.00000000	-4.97554145	2.34624598
H	0.00000000	-3.30750597	-0.07825526
H	0.00000000	-2.68711285	4.20911764
H	-2.86438406	1.65375299	-0.07825526
H	0.00000000	0.00000000	4.26615395
N	4.30894534	2.48777073	2.34624598
H	2.32710775	1.34355616	4.20911764
H	2.86438406	1.65375299	-0.07825526
B	0.00000000	0.00000000	3.06896927
H	-4.64831041	-2.68370337	-3.27135840
H	-4.86277854	-2.80752661	-1.57165802
H	4.64831041	-2.68370337	-3.27135840
H	4.86277854	-2.80752661	-1.57165802
H	0.00000000	5.36740620	-3.27135840
H	0.00000000	5.61505322	-1.57165802
H	-4.64831041	2.68370337	3.27135840
H	-4.86277854	2.80752661	1.57165802
H	0.00000000	-5.36740620	3.27135840
H	0.00000000	-5.61505322	1.57165802
H	4.64831041	2.68370337	3.27135840
H	4.86277854	2.80752661	1.57165802

$[Mn(Tb^{4NO2})_2]^{2+}$ $^4A_{2g}$ D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.38149182	-0.79760452	-1.19169446
N	-1.23579080	-0.71348439	-2.53810289
N	1.38149182	-0.79760452	-1.19169446
N	1.23579080	-0.71348439	-2.53810289
N	0.00000000	1.59520905	-1.19169446
N	0.00000000	1.42696826	-2.53810289
C	-2.52255831	-1.45639951	-0.93831752
C	-3.10610535	-1.79331079	-2.15280470
C	-2.26503103	-1.30771658	-3.14828712
C	2.52255831	-1.45639951	-0.93831752
C	3.10610535	-1.79331079	-2.15280470
C	2.26503103	-1.30771658	-3.14828712
C	0.00000000	2.91279901	-0.93831752
C	0.00000000	3.58662157	-2.15280470
C	0.00000000	2.61543262	-3.14828712
N	-4.35097101	-2.51203403	-2.33499143
H	-2.34995286	-1.35674591	-4.22720174
N	4.35097101	-2.51203403	-2.33499143
H	2.87387538	-1.65923262	0.06375157
H	2.34995286	-1.35674591	-4.22720174
H	-2.87387538	-1.65923262	0.06375157
H	0.00000000	0.00000000	-4.30666459
N	0.00000000	5.02406859	-2.33499143
H	0.00000000	2.71349181	-4.22720174
H	0.00000000	3.31846576	0.06375157
B	0.00000000	0.00000000	-3.11428113
N	-1.38149182	0.79760452	1.19169446
N	-1.23579080	0.71348439	2.53810289
N	0.00000000	-1.59520905	1.19169446
N	0.00000000	-1.42696826	2.53810289
N	1.38149182	0.79760452	1.19169446
N	1.23579080	0.71348439	2.53810289
C	-2.52255831	1.45639951	0.93831752
C	-3.10610535	1.79331079	2.15280470
C	-2.26503103	1.30771658	3.14828712
C	0.00000000	-2.91279901	0.93831752
C	0.00000000	-3.58662157	2.15280470
C	0.00000000	-2.61543262	3.14828712
C	2.52255831	1.45639951	0.93831752
C	3.10610535	1.79331079	2.15280470
C	2.26503103	1.30771658	3.14828712
N	-4.35097101	2.51203403	2.33499143
H	-2.34995286	1.35674591	4.22720174
N	0.00000000	-5.02406859	2.33499143
H	0.00000000	-3.31846576	-0.06375157
H	0.00000000	-2.71349181	4.22720174
H	-2.87387538	1.65923262	-0.06375157
H	0.00000000	0.00000000	4.30666459
N	4.35097101	2.51203403	2.33499143
H	2.34995286	1.35674591	4.22720174
H	2.87387538	1.65923262	-0.06375157
B	0.00000000	0.00000000	3.11428113
O	-4.69802450	-2.71240541	-3.48916564
O	-4.93820694	-2.85107525	-1.31970509
O	4.69802450	-2.71240541	-3.48916564
O	4.93820694	-2.85107525	-1.31970509
O	0.00000000	5.42481135	-3.48916564
O	0.00000000	5.70215050	-1.31970509
O	-4.69802450	2.71240541	3.48916564
O	-4.93820694	2.85107525	1.31970509
O	0.00000000	-5.42481135	3.48916564
O	0.00000000	-5.70215050	1.31970509
O	4.69802450	2.71240541	3.48916564
O	4.93820694	2.85107525	1.31970509

$[Mn(Tb^{4NO2})_2]^{2+}$ ^2E_g D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.38624595	-0.80034937	-1.19263269
N	-1.23774558	-0.71461260	-2.53899085
N	1.38624595	-0.80034937	-1.19263269
N	1.23774558	-0.71461260	-2.53899085
N	0.00000000	1.60069873	-1.19263269
N	0.00000000	1.42922573	-2.53899085
C	-2.52595457	-1.45836064	-0.95179884
C	-3.10645936	-1.79351505	-2.17197256
C	-2.26085211	-1.30530353	-3.16164197
C	2.52595457	-1.45836064	-0.95179884
C	3.10645936	-1.79351505	-2.17197256
C	2.26085211	-1.30530353	-3.16164197
C	0.00000000	2.91672127	-0.95179884
C	0.00000000	3.58703062	-2.17197256
C	0.00000000	2.61060758	-3.16164197
N	-4.33937144	-2.50533729	-2.36868944
H	-2.33781830	-1.34974013	-4.24099951
N	4.33937144	-2.50533729	-2.36868944
H	2.88042765	-1.66301570	0.04881554

H	2.33781830	-1.34974013	-4.24099951
H	-2.88042765	-1.66301570	0.04881554
H	0.00000000	0.00000000	-4.30184537
N	0.00000000	5.01067459	-2.36868944
H	0.00000000	2.69947973	-4.24099951
H	0.00000000	3.32603141	0.04881554
B	0.00000000	0.00000000	-3.10818025
N	-1.38624595	0.80034937	1.19263269
N	-1.23774558	0.71461260	2.53899085
N	0.00000000	-1.60069873	1.19263269
N	0.00000000	-1.42922573	2.53899085
N	1.38624595	0.80034937	1.19263269
N	1.23774558	0.71461260	2.53899085
C	-2.52595457	1.45836064	0.95179884
C	-3.10645936	1.79351505	2.17197256
C	-2.26085211	1.30530353	3.16164197
C	0.00000000	-2.91672127	0.95179884
C	0.00000000	-3.58703062	2.17197256
C	0.00000000	-2.61060758	3.16164197
C	2.52595457	1.45836064	0.95179884
C	3.10645936	1.79351505	2.17197256
C	2.26085211	1.30530353	3.16164197
N	-4.33937144	2.50533729	2.36868944
H	-2.33781830	1.34974013	4.24099951
N	0.00000000	-5.01067459	2.36868944
H	0.00000000	-3.32603141	-0.04881554
H	0.00000000	-2.69947973	4.24099951
H	-2.88042765	1.66301570	-0.04881554
H	0.00000000	0.00000000	4.30184537
N	4.33937144	2.50533729	2.36868944
H	2.33781830	1.34974013	4.24099951
H	2.88042765	1.66301570	-0.04881554
B	0.00000000	0.00000000	3.10818025
O	-4.69604591	-2.71126345	-3.52170105
O	-4.95146071	-2.85872715	-1.36754006
O	4.69604591	-2.71126345	-3.52170105
O	4.95146071	-2.85872715	-1.36754006
O	0.00000000	5.42252689	-3.52170105
O	0.00000000	5.71745431	-1.36754006
O	-4.69604591	2.71126345	3.52170105
O	-4.95146071	2.85872715	1.36754006
O	0.00000000	-5.42252689	3.52170105
O	0.00000000	-5.71745431	1.36754006
O	4.69604591	2.71126345	3.52170105
O	4.95146071	2.85872715	1.36754006

$[Mn(Tb^{4NH2})_2]^+$ ^5E_g D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.48816760	-0.85919388	-1.41266724
N	-1.26057747	-0.72779493	-2.72674982
N	1.48816760	-0.85919388	-1.41266724
N	1.26057747	-0.72779493	-2.72674982
N	0.00000000	1.71838828	-1.41266724
N	0.00000000	1.45558934	-2.72674982
C	-2.64118080	-1.52488616	-1.27209501
C	-3.18148717	-1.83683244	-2.53407268
C	-2.25705527	-1.30311115	-3.43616854
C	2.64118080	-1.52488616	-1.27209501
C	3.18148717	-1.83683244	-2.53407268
C	2.25705527	-1.30311115	-3.43616854
C	0.00000000	3.04977284	-1.27209501
C	0.00000000	3.67366488	-2.53407268
C	0.00000000	2.60622282	-3.43616854
N	-4.34366678	-2.50781702	-2.80651747
H	-2.24842333	-1.29812788	-4.51878634
N	4.34366678	-2.50781702	-2.80651747
H	3.02986784	-1.74929488	-0.28591605
H	2.24842333	-1.29812788	-4.51878634
H	-3.02986784	-1.74929488	-0.28591605
H	0.00000000	0.00000000	-4.44709341
N	0.00000000	5.01563457	-2.80651747
H	0.00000000	2.59625577	-4.51878634
H	0.00000000	3.49859029	-0.28591605
B	0.00000000	0.00000000	-3.24521705
N	-1.48816760	0.85919388	1.41266724
N	-1.26057747	0.72779493	2.72674982
N	0.00000000	-1.71838828	1.41266724
N	0.00000000	-1.45558934	2.72674982
N	1.48816760	0.85919388	1.41266724
N	1.26057747	0.72779493	2.72674982
C	-2.64118080	1.52488616	1.27209501
C	-3.18148717	1.83683244	2.53407268
C	-2.25705527	1.30311115	3.43616854
C	0.00000000	-3.04977284	1.27209501
C	0.00000000	-3.67366488	2.53407268
C	0.00000000	-2.60622282	3.43616854
C	2.64118080	1.52488616	1.27209501
C	3.18148717	1.83683244	2.53407268
C	2.25705527	1.30311115	3.43616854
N	-4.34366678	2.50781702	2.80651747
H	-2.24842333	1.29812788	4.51878634
N	0.00000000	-5.01563457	2.80651747
H	0.00000000	-3.49859029	0.28591605
H	0.00000000	-2.59625577	4.51878634
H	-3.02986784	1.74929488	0.28591605
H	0.00000000	0.00000000	4.44709341
N	4.34366678	2.50781702	2.80651747
H	2.24842333	1.29812788	4.51878634
H	3.02986784	1.74929488	0.28591605
B	0.00000000	0.00000000	3.24521705
H	-4.63850158	-2.67804011	-3.74988704
H	-4.92908287	-2.84580729	-2.06574235
H	4.63850158	-2.67804011	-3.74988704
H	4.92908287	-2.84580729	-2.06574235
H	0.00000000	5.35608022	-3.74988704
H	0.00000000	5.69161458	-2.06574235
H	-4.63850158	2.67804011	3.74988704
H	-4.92908287	2.84580729	2.06574235
H	0.00000000	-5.35608022	3.74988704
H	0.00000000	-5.69161458	2.06574235
H	4.63850158	2.67804011	3.74988704
H	4.92908287	2.84580729	2.06574235

$[Mn(Tb^{4NH2})_2]^+$ $^3A_{2g}$ D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.38642164	-0.80045097	-1.18409548
N	-1.23866053	-0.71514125	-2.51178797
N	1.38642164	-0.80045097	-1.18409548

N	1.23866053	-0.71514125	-2.51178797
N	0.00000000	1.60090141	-1.18409548
N	0.00000000	1.43028196	-2.51178797
C	-2.53514162	-1.46366458	-0.94722516
C	-3.14488292	-1.81569869	-2.16020260
C	-2.27489489	-1.31341105	-3.13425863
C	2.53514162	-1.46366458	-0.94722516
C	3.14488292	-1.81569869	-2.16020260
C	2.27489489	-1.31341105	-3.13425863
C	0.00000000	2.92732916	-0.94722516
C	0.00000000	3.63139790	-2.16020260
C	0.00000000	2.62682263	-3.13425863
N	-4.31975061	-2.49400920	-2.34961101
H	-2.32894135	-1.34461505	-4.21518466
N	4.31975061	-2.49400920	-2.34961101
H	2.86201652	-1.65238612	0.06617944
H	2.32894135	-1.34461505	-4.21518466
H	-2.86201652	-1.65238612	0.06617944
H	0.00000000	0.00000000	-4.27175741
N	0.00000000	4.98801839	-2.34961101
H	0.00000000	2.68922956	-4.21518466
H	0.00000000	3.30477224	0.06617944
B	0.00000000	0.00000000	-3.07162839
N	-1.38642164	0.80045097	1.18409548
N	-1.23866053	0.71514125	2.51178797
N	0.00000000	-1.60090141	1.18409548
N	0.00000000	-1.43028196	2.51178797
N	1.38642164	0.80045097	1.18409548
N	1.23866053	0.71514125	2.51178797
C	-2.53514162	1.46366458	0.94722516
C	-3.14488292	1.81569869	2.16020260
C	-2.27489489	1.31341105	3.13425863
C	0.00000000	-2.92732916	0.94722516
C	0.00000000	-3.63139790	2.16020260
C	0.00000000	-2.62682263	3.13425863
C	2.53514162	1.46366458	0.94722516
C	3.14488292	1.81569869	2.16020260
C	2.27489489	1.31341105	3.13425863
N	-4.31975061	2.49400920	2.34961101
H	-2.32894135	1.34461505	4.21518466
N	0.00000000	-4.98801839	2.34961101
H	0.00000000	-3.30477224	-0.06617944
H	0.00000000	-2.68922956	4.21518466
H	-2.86201652	1.65238612	-0.06617944
H	0.00000000	0.00000000	4.27175741
N	4.31975061	2.49400920	2.34961101
H	2.32894135	1.34461505	4.21518466
H	2.86201652	1.65238612	-0.06617944
B	0.00000000	0.00000000	3.07162839
H	-4.66232197	-2.69179290	-3.27060062
H	-4.86489737	-2.80875007	-1.56953654
H	4.66232197	-2.69179290	-3.27060062
H	4.86489737	-2.80875007	-1.56953654
H	0.00000000	5.38358527	-3.27060062
H	0.00000000	5.61749960	-1.56953654
H	-4.66232197	2.69179290	3.27060062
H	-4.86489737	2.80875007	1.56953654
H	0.00000000	-5.38358527	3.27060062
H	0.00000000	-5.61749960	1.56953654
H	4.66232197	2.69179290	3.27060062
H	4.86489737	2.80875007	1.56953654

$[Mn(Tb^{4NO2})_2]^+$ ^5E_g D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.44553391	-0.83457920	-1.31666549
N	-1.24934039	-0.72130669	-2.65309575
N	1.44553391	-0.83457920	-1.31666549
N	1.24934039	-0.72130669	-2.65309575
N	0.00000000	1.66915892	-1.31666549
N	0.00000000	1.44261391	-2.65309575
C	-2.58929444	-1.49492996	-1.12618285
C	-3.13212658	-1.80833413	-2.37110302
C	-2.25476023	-1.30178661	-3.31914258
C	2.58929444	-1.49492996	-1.12618285
C	3.13212658	-1.80833413	-2.37110302
C	2.25476023	-1.30178661	-3.31914258
C	0.00000000	2.98985992	-1.12618285
C	0.00000000	3.61666825	-2.37110302
C	0.00000000	2.60357323	-3.31914258
N	-4.36266159	-2.51878369	-2.62300726
H	-2.29736587	-1.32638489	-4.40016121
N	4.36266159	-2.51878369	-2.62300726
H	2.97517419	-1.71771782	-0.14091778
H	2.29736587	-1.32638489	-4.40016121
H	-2.97517419	-1.71771782	-0.14091778
H	0.00000000	0.00000000	-4.39345389
N	0.00000000	5.03756738	-2.62300726
H	0.00000000	2.65276978	-4.40016121
H	0.00000000	3.43543510	-0.14091778
B	0.00000000	0.00000000	-3.19778636
N	-1.44553391	0.83457920	1.31666549
N	-1.24934039	0.72130669	2.65309575
N	0.00000000	-1.66915892	1.31666549
N	0.00000000	-1.44261391	2.65309575
N	1.44553391	0.83457920	1.31666549
N	1.24934039	0.72130669	2.65309575
C	-2.58929444	1.49492996	1.12618285
C	-3.13212658	1.80833413	2.37110302
C	-2.25476023	1.30178661	3.31914258
C	0.00000000	-2.98985992	1.12618285
C	0.00000000	-3.61666825	2.37110302
C	0.00000000	-2.60357323	3.31914258
C	2.58929444	1.49492996	1.12618285
C	3.13212658	1.80833413	2.37110302
C	2.25476023	1.30178661	3.31914258
N	-4.36266159	2.51878369	2.62300726
H	-2.29736587	1.32638489	4.40016121
N	0.00000000	-5.03756738	2.62300726
H	0.00000000	-3.43543510	0.14091778
H	0.00000000	-2.65276978	4.40016121
H	-2.97517419	1.71771782	0.14091778
H	0.00000000	0.00000000	4.39345389
N	4.36266159	2.51878369	2.62300726
H	2.29736587	1.32638489	4.40016121
H	2.97517419	1.71771782	0.14091778
B	0.00000000	0.00000000	3.19778636
O	-4.66154037	-2.69134151	-3.79776647
O	-4.99588250	-2.88437426	-1.64252437
O	4.66154037	-2.69134151	-3.79776647

O	4.99588250	-2.88437426	-1.64252437
O	0.00000000	5.38268302	-3.79776647
O	0.00000000	5.76874799	-1.64252437
O	-4.66154037	2.69134151	3.79776647
O	-4.99588250	2.88437426	1.64252437
O	0.00000000	-5.38268302	3.79776647
O	0.00000000	-5.76874799	1.64252437
O	4.66154037	2.69134151	3.79776647
O	4.99588250	2.88437426	1.64252437

$[Mn(Tb^{4NO2})_2]^+$ $^3A_{2g}$ D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.38430757	-0.79923016	-1.18850300
N	-1.23673115	-0.71402680	-2.53378004
N	1.38430757	-0.79923016	-1.18850300
N	1.23673115	-0.71402680	-2.53378004
N	0.00000000	1.59846031	-1.18850300
N	0.00000000	1.42805413	-2.53378004
C	-2.52447869	-1.45750813	-0.94767919
C	-3.10739495	-1.79405534	-2.16519751
C	-2.26193164	-1.30592690	-3.15313386
C	2.52447869	-1.45750813	-0.94767919
C	3.10739495	-1.79405534	-2.16519751
C	2.26193164	-1.30592690	-3.15313386
C	0.00000000	2.91501679	-0.94767919
C	0.00000000	3.58811015	-2.16519751
C	0.00000000	2.61185380	-3.15313386
N	-4.34674870	-2.50959664	-2.36620231
H	-2.34077957	-1.35144990	-4.23143251
N	4.34674870	-2.50959664	-2.36620231
H	2.87727323	-1.66119428	0.05329027
H	2.34077957	-1.35144990	-4.23143251
H	-2.87727323	-1.66119428	0.05329027
H	0.00000000	0.00000000	-4.29601225
N	0.00000000	5.01919275	-2.36620231
H	0.00000000	2.70289980	-4.23143251
H	0.00000000	3.32238908	0.05329027
B	0.00000000	0.00000000	-3.10088237
N	-1.38430757	0.79923016	1.18850300
N	-1.23673115	0.71402680	2.53378004
N	0.00000000	-1.59846031	1.18850300
N	0.00000000	-1.42805413	2.53378004
N	1.38430757	0.79923016	1.18850300
N	1.23673115	0.71402680	2.53378004
C	-2.52447869	1.45750813	0.94767919
C	-3.10739495	1.79405534	2.16519751
C	-2.26193164	1.30592690	3.15313386
C	0.00000000	-2.91501679	0.94767919
C	0.00000000	-3.58811015	2.16519751
C	0.00000000	-2.61185380	3.15313386
C	2.52447869	1.45750813	0.94767919
C	3.10739495	1.79405534	2.16519751
C	2.26193164	1.30592690	3.15313386
N	-4.34674870	2.50959664	2.36620231
H	-2.34077957	1.35144990	4.23143251
N	0.00000000	-5.01919275	2.36620231
H	0.00000000	-3.32238908	-0.05329027
H	0.00000000	-2.70289980	4.23143251
H	-2.87727323	1.66119428	-0.05329027
H	0.00000000	0.00000000	4.29601225
N	4.34674870	2.50959664	2.36620231
H	2.34077957	1.35144990	4.23143251
H	2.87727323	1.66119428	-0.05329027
B	0.00000000	0.00000000	3.10088237
O	-4.68152422	-2.70287916	-3.52662663
O	-4.94578105	-2.85544837	-1.35725656
O	4.68152422	-2.70287916	-3.52662663
O	4.94578105	-2.85544837	-1.35725656
O	0.00000000	5.40575832	-3.52662663
O	0.00000000	5.71089621	-1.35725656
O	-4.68152422	2.70287916	3.52662663
O	-4.94578105	2.85544837	1.35725656
O	0.00000000	-5.40575832	3.52662663
O	0.00000000	-5.71089621	1.35725656
O	4.68152422	2.70287916	3.52662663
O	4.94578105	2.85544837	1.35725656

$[Mn(Tb^{4NH2})_2]$ $^6A_{1g}$ D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.50484410	-0.86882226	-1.47782272
N	-1.26426054	-0.72992117	-2.78500271
N	1.50484410	-0.86882226	-1.47782272
N	1.26426054	-0.72992117	-2.78500271
N	0.00000000	1.73764451	-1.47782272
N	0.00000000	1.45984233	-2.78500271
C	-2.66132287	-1.53651535	-1.35952885
C	-3.18832467	-1.84078010	-2.62655910
C	-2.25718015	-1.30318364	-3.51166785
C	2.66132287	-1.53651535	-1.35952885
C	3.18832467	-1.84078010	-2.62655910
C	2.25718015	-1.30318364	-3.51166785
C	0.00000000	3.07303124	-1.35952885
C	0.00000000	3.68156020	-2.62655910
C	0.00000000	2.60636676	-3.51166785
N	-4.35743597	-2.51576685	-2.91301068
H	-2.23461709	-1.29015689	-4.59433857
N	4.35743597	-2.51576685	-2.91301068
H	3.05965258	-1.76649102	-0.37783097
H	2.23461709	-1.29015689	-4.59433857
H	-3.05965258	-1.76649102	-0.37783097
H	0.00000000	0.00000000	-4.49780288
N	0.00000000	5.03153370	-2.91301068
H	0.00000000	2.58031324	-4.59433857
H	0.00000000	3.53298258	-0.37783097
B	0.00000000	0.00000000	-3.29159838
N	-1.50484410	0.86882226	1.47782272
N	-1.26426054	0.72992117	2.78500271
N	0.00000000	-1.73764451	1.47782272
N	0.00000000	-1.45984233	2.78500271
N	1.50484410	0.86882226	1.47782272
N	1.26426054	0.72992117	2.78500271
C	-2.66132287	1.53651535	1.35952885
C	-3.18832467	1.84078010	2.62655910
C	-2.25718015	1.30318364	3.51166785
C	0.00000000	-3.07303124	1.35952885
C	0.00000000	-3.68156020	2.62655910
C	0.00000000	-2.60636676	3.51166785
C	2.66132287	1.53651535	1.35952885

C	3.18832467	1.84078010	2.62655910
C	2.25718015	1.30318364	3.51166785
N	-4.35743597	2.51576685	2.91301068
H	-2.23461709	1.29015689	4.59433857
N	0.00000000	-5.03153370	2.91301068
H	0.00000000	-3.53298258	0.37783097
H	0.00000000	-2.58031324	4.59433857
H	-3.05965258	1.76649102	0.37783097
H	0.00000000	0.00000000	4.49780288
N	4.35743597	2.51576685	2.91301068
H	2.23461709	1.29015689	4.59433857
H	3.05965258	1.76649102	0.37783097
B	0.00000000	0.00000000	3.29159838
H	-4.64425956	-2.68136440	-3.85791434
H	-4.94496400	-2.85497634	-2.17649279
H	4.64425956	-2.68136440	-3.85791434
H	4.94496400	-2.85497634	-2.17649279
H	0.00000000	5.36272880	-3.85791434
H	0.00000000	5.70995216	-2.17649279
H	-4.64425956	2.68136440	3.85791434
H	-4.94496400	2.85497634	2.17649279
H	0.00000000	-5.36272880	3.85791434
H	0.00000000	-5.70995216	2.17649279
H	4.64425956	2.68136440	3.85791434
H	4.94496400	2.85497634	2.17649279

$[Mn(Tb^{4NH2})_2]$ ^4E_g D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.46022493	-0.84306138	-1.32587953
N	-1.25609216	-0.72520514	-2.64073206
N	1.46022493	-0.84306138	-1.32587953
N	1.25609216	-0.72520514	-2.64073206
N	0.00000000	1.68612223	-1.32587953
N	0.00000000	1.45041028	-2.64073206
C	-2.61443777	-1.50944635	-1.16493556
C	-3.17354634	-1.83224765	-2.41270693
C	-2.26639154	-1.30850187	-3.33165074
C	2.61443777	-1.50944635	-1.16493556
C	3.17354634	-1.83224765	-2.41270693
C	2.26639154	-1.30850187	-3.33165074
C	0.00000000	3.01889270	-1.16493556
C	0.00000000	3.66449529	-2.41270693
C	0.00000000	2.61700322	-3.33165074
N	-4.34939618	-2.51112491	-2.66083285
H	-2.27216487	-1.31183516	-4.41461463
N	4.34939618	-2.51112491	-2.66083285
H	2.98549580	-1.72367688	-0.17033104
H	2.27216487	-1.31183516	-4.41461463
H	-2.98549580	-1.72367688	-0.17033104
H	0.00000000	0.00000000	-4.36731677
N	0.00000000	5.02225034	-2.66083285
H	0.00000000	2.62367032	-4.41461463
H	0.00000000	3.44735376	-0.17033104
B	0.00000000	0.00000000	-3.16040369
N	-1.46022493	0.84306138	1.32587953
N	-1.25609216	0.72520514	2.64073206
N	0.00000000	-1.68612223	1.32587953
N	0.00000000	-1.45041028	2.64073206
N	1.46022493	0.84306138	1.32587953
N	1.25609216	0.72520514	2.64073206
C	-2.61443777	1.50944635	1.16493556
C	-3.17354634	1.83224765	2.41270693
C	-2.26639154	1.30850187	3.33165074
C	0.00000000	-3.01889270	1.16493556
C	0.00000000	-3.66449529	2.41270693
C	0.00000000	-2.61700322	3.33165074
C	2.61443777	1.50944635	1.16493556
C	3.17354634	1.83224765	2.41270693
C	2.26639154	1.30850187	3.33165074
N	-4.34939618	2.51112491	2.66083285
H	-2.27216487	1.31183516	4.41461463
N	0.00000000	-5.02225034	2.66083285
H	0.00000000	-3.44735376	0.17033104
H	0.00000000	-2.62367032	4.41461463
H	-2.98549580	1.72367688	0.17033104
H	0.00000000	0.00000000	4.36731677
N	4.34939618	2.51112491	2.66083285
H	2.27216487	1.31183516	4.41461463
H	2.98549580	1.72367688	0.17033104
B	0.00000000	0.00000000	3.16040369
H	-4.65899768	-2.68987357	-3.59619492
H	-4.91861786	-2.83976514	-1.90533232
H	4.65899768	-2.68987357	-3.59619492
H	4.91861786	-2.83976514	-1.90533232
H	0.00000000	5.37974714	-3.59619492
H	0.00000000	5.67953082	-1.90533232
H	-4.65899768	2.68987357	3.59619492
H	-4.91861786	2.83976514	1.90533232
H	0.00000000	-5.37974714	3.59619492
H	0.00000000	-5.67953082	1.90533232
H	4.65899768	2.68987357	3.59619492
H	4.91861786	2.83976514	1.90533232

$[Mn(Tb^{4NH2})_2]$ ^2E_g D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.38658568	-0.80054569	-1.19683701
N	-1.24007608	-0.71595830	-2.52466391
N	1.38658568	-0.80054569	-1.19683701
N	1.24007608	-0.71595830	-2.52466391
N	0.00000000	1.60109085	-1.19683701
N	0.00000000	1.43191659	-2.52466391
C	-2.53568032	-1.46397574	-0.96969085
C	-3.14385473	-1.81510548	-2.18586294
C	-2.27850970	-1.31549813	-3.15686138
C	2.53568032	-1.46397574	-0.96969085
C	3.14385473	-1.81510548	-2.18586294
C	2.27850970	-1.31549813	-3.15686138
C	0.00000000	2.92795147	-0.96969085
C	0.00000000	3.63021043	-2.18586294
C	0.00000000	2.63099625	-3.15686138
N	-4.32869053	-2.49917079	-2.36855344
H	-2.32921599	-1.34477327	-4.23803876
N	4.32869053	-2.49917079	-2.36855344
H	2.86434754	-1.65373182	0.04319039
H	2.32921599	-1.34477327	-4.23803876
H	-2.86434754	-1.65373182	0.04319039
H	0.00000000	0.00000000	-4.28220284
N	0.00000000	4.99834158	-2.36855344

H	0.00000000	2.68954707	-4.23803876
H	0.00000000	3.30746364	0.04319039
B	0.00000000	0.00000000	-3.07643544
N	-1.38658568	0.80054569	1.19683701
N	-1.24007608	0.71595830	2.52466391
N	0.00000000	-1.60109085	1.19683701
N	0.00000000	-1.43191659	2.52466391
N	1.38658568	0.80054569	1.19683701
N	1.24007608	0.71595830	2.52466391
C	-2.53568032	1.46397574	0.96969085
C	-3.14385473	1.81510548	2.18586294
C	-2.27850970	1.31549813	3.15686138
C	0.00000000	-2.92795147	0.96969085
C	0.00000000	-3.63021043	2.18586294
C	0.00000000	-2.63099625	3.15686138
C	2.53568032	1.46397574	0.96969085
C	3.14385473	1.81510548	2.18586294
C	2.27850970	1.31549813	3.15686138
N	-4.32869053	2.49917079	2.36855344
H	-2.32921599	1.34477327	4.23803876
N	0.00000000	-4.99834158	2.36855344
H	0.00000000	-3.30746364	-0.04319039
H	0.00000000	-2.68954707	4.23803876
H	-2.86434754	1.65373182	-0.04319039
H	0.00000000	0.00000000	4.28220284
N	4.32869053	2.49917079	2.36855344
H	2.32921599	1.34477327	4.23803876
H	2.86434754	1.65373182	-0.04319039
B	0.00000000	0.00000000	3.07643544
H	-4.67575725	-2.69954958	-3.28610446
H	-4.86599806	-2.80938508	-1.58247810
H	4.67575725	-2.69954958	-3.28610446
H	4.86599806	-2.80938508	-1.58247810
H	0.00000000	5.39909969	-3.28610446
H	0.00000000	5.61877016	-1.58247810
H	-4.67575725	2.69954958	3.28610446
H	-4.86599806	2.80938508	1.58247810
H	0.00000000	-5.39909969	3.28610446
H	0.00000000	-5.61877016	1.58247810
H	4.67575725	2.69954958	3.28610446
H	4.86599806	2.80938508	1.58247810

$[Mn(Tb^{4NO2})_2]$ $^6A_{1g}$ D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.50250460	-0.86747127	-1.46433928
N	-1.26157126	-0.72836856	-2.79217200
N	1.50250460	-0.86747127	-1.46433928
N	1.26157126	-0.72836856	-2.79217200
N	0.00000000	1.73494253	-1.46433928
N	0.00000000	1.45673712	-2.79217200
C	-2.64872157	-1.52924023	-1.34109337
C	-3.15242899	-1.82005540	-2.61353023
C	-2.23855893	-1.29243235	-3.51376445
C	2.64872157	-1.52924023	-1.34109337
C	3.15242899	-1.82005540	-2.61353023
C	2.23855893	-1.29243235	-3.51376445
C	0.00000000	3.05847992	-1.34109337
C	0.00000000	3.64011134	-2.61353023
C	0.00000000	2.58486523	-3.51376445
N	-4.36321670	-2.51910437	-2.93396610
H	-2.23819380	-1.29222174	-4.59489738
N	4.36321670	-2.51910437	-2.93396610
H	3.06719759	-1.77084721	-0.37286940
H	2.23819380	-1.29222174	-4.59489738
H	-3.06719759	-1.77084721	-0.37286940
H	0.00000000	0.00000000	-4.50540716
N	0.00000000	5.03820821	-2.93396610
H	0.00000000	2.58444347	-4.59489738
H	0.00000000	3.54169495	-0.37286940
B	0.00000000	0.00000000	-3.30510351
N	-1.50250460	0.86747127	1.46433928
N	-1.26157126	0.72836856	2.79217200
N	0.00000000	-1.73494253	1.46433928
N	0.00000000	-1.45673712	2.79217200
N	1.50250460	0.86747127	1.46433928
N	1.26157126	0.72836856	2.79217200
C	-2.64872157	1.52924023	1.34109337
C	-3.15242899	1.82005540	2.61353023
C	-2.23855893	1.29243235	3.51376445
C	0.00000000	-3.05847992	1.34109337
C	0.00000000	-3.64011134	2.61353023
C	0.00000000	-2.58486523	3.51376445
C	2.64872157	1.52924023	1.34109337
C	3.15242899	1.82005540	2.61353023
C	2.23855893	1.29243235	3.51376445
N	-4.36321670	2.51910437	2.93396610
H	-2.23819380	1.29222174	4.59489738
N	0.00000000	-5.03820821	2.93396610
H	0.00000000	-3.54169495	0.37286940
H	0.00000000	-2.58444347	4.59489738
H	-3.06719759	1.77084721	0.37286940
H	0.00000000	0.00000000	4.50540716
N	4.36321670	2.51910437	2.93396610
H	2.23819380	1.29222174	4.59489738
H	3.06719759	1.77084721	0.37286940
B	0.00000000	0.00000000	3.30510351
O	-4.62262097	-2.66887159	-4.12522611
O	-5.04575745	-2.91316944	-1.99319162
O	4.62262097	-2.66887159	-4.12522611
O	5.04575745	-2.91316944	-1.99319162
O	0.00000000	5.33774317	-4.12522611
O	0.00000000	5.82633835	-1.99319162
O	-4.62262097	2.66887159	4.12522611
O	-5.04575745	2.91316944	1.99319162
O	0.00000000	-5.33774317	4.12522611
O	0.00000000	-5.82633835	1.99319162
O	4.62262097	2.66887159	4.12522611
O	5.04575745	2.91316944	1.99319162

$[Mn(Tb^{4NO2})_2]$ ^4E_g D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.45702499	-0.84121349	-1.31386667
N	-1.25340076	-0.72365095	-2.64953174
N	1.45702499	-0.84121349	-1.31386667
N	1.25340076	-0.72365095	-2.64953174
N	0.00000000	1.68242751	-1.31386667
N	0.00000000	1.44730242	-2.64953174
C	-2.60085485	-1.50160394	-1.14824689

C	-3.13704211	-1.81117211	-2.40200644
C	-2.24800475	-1.29788605	-3.33574975
C	2.60085485	-1.50160394	-1.14824689
C	3.13704211	-1.81117211	-2.40200644
C	2.24800475	-1.29788605	-3.33574975
C	0.00000000	3.00320842	-1.14824689
C	0.00000000	3.62234421	-2.40200644
C	0.00000000	2.59577210	-3.33574975
N	-4.35612520	-2.51501013	-2.67941544
H	-2.27631785	-1.31423286	-4.41638473
N	4.35612520	-2.51501013	-2.67941544
H	2.99338900	-1.72823363	-0.16671147
H	2.27631785	-1.31423286	-4.41638473
H	-2.99338900	-1.72823363	-0.16671147
H	0.00000000	0.00000000	-4.37688164
N	0.00000000	5.03001972	-2.67941544
H	0.00000000	2.62846573	-4.41638473
H	0.00000000	3.45646778	-0.16671147
B	0.00000000	0.00000000	-3.17641766
N	-1.45702499	0.84121349	1.31386667
N	-1.25340076	0.72365095	2.64953174
N	0.00000000	-1.68242751	1.31386667
N	0.00000000	-1.44730242	2.64953174
N	1.45702499	0.84121349	1.31386667
N	1.25340076	0.72365095	2.64953174
C	-2.60085485	1.50160394	1.14824689
C	-3.13704211	1.81117211	2.40200644
C	-2.24800475	1.29788605	3.33574975
C	0.00000000	-3.00320842	1.14824689
C	0.00000000	-3.62234421	2.40200644
C	0.00000000	-2.59577210	3.33574975
C	2.60085485	1.50160394	1.14824689
C	3.13704211	1.81117211	2.40200644
C	2.24800475	1.29788605	3.33574975
N	-4.35612520	2.51501013	2.67941544
H	-2.27631785	1.31423286	4.41638473
N	0.00000000	-5.03001972	2.67941544
H	0.00000000	-3.45646778	0.16671147
H	0.00000000	-2.62846573	4.41638473
H	-2.99338900	1.72823363	0.16671147
H	0.00000000	0.00000000	4.37688164
N	4.35612520	2.51501013	2.67941544
H	2.27631785	1.31423286	4.41638473
H	2.99338900	1.72823363	0.16671147
B	0.00000000	0.00000000	3.17641766
O	-4.64673135	-2.68279159	-3.86106983
O	-5.01289290	-2.89419526	-1.71475019
O	4.64673135	-2.68279159	-3.86106983
O	5.01289290	-2.89419526	-1.71475019
O	0.00000000	5.36558319	-3.86106983
O	0.00000000	5.78838999	-1.71475019
O	-4.64673135	2.68279159	3.86106983
O	-5.01289290	2.89419526	1.71475019
O	0.00000000	-5.36558319	3.86106983
O	0.00000000	-5.78838999	1.71475019
O	4.64673135	2.68279159	3.86106983
O	5.01289290	2.89419526	1.71475019

$[Mn(Tb^{4NO2})_2]$ ^2E_g D_{3d}

Mn	0.00000000	0.00000000	0.00000000
N	-1.38412501	-0.79912485	-1.18638787
N	-1.23772495	-0.71460043	-2.53456164
N	1.38412501	-0.79912485	-1.18638787
N	1.23772495	-0.71460043	-2.53456164
N	0.00000000	1.59825023	-1.18638787
N	0.00000000	1.42920138	-2.53456164
C	-2.52302557	-1.45666939	-0.95666251
C	-3.10738013	-1.79404687	-2.18142578
C	-2.25940481	-1.30446796	-3.16381953
C	2.52302557	-1.45666939	-0.95666251
C	3.10738013	-1.79404687	-2.18142578
C	2.25940481	-1.30446796	-3.16381953
C	0.00000000	2.91333877	-0.95666251
C	0.00000000	3.58809374	-2.18142578
C	0.00000000	2.60893591	-3.16381953
N	-4.33540526	-2.50304702	-2.39324115
H	-2.33144224	-1.34605864	-4.24167051
N	4.33540526	-2.50304702	-2.39324115
H	2.87556928	-1.66021054	0.04362855
H	2.33144224	-1.34605864	-4.24167051
H	-2.87556928	-1.66021054	0.04362855
H	0.00000000	0.00000000	-4.29292503
N	0.00000000	5.00609456	-2.39324115
H	0.00000000	2.69211728	-4.24167051
H	0.00000000	3.32042160	0.04362855
B	0.00000000	0.00000000	-3.09380621
N	-1.38412501	0.79912485	1.18638787
N	-1.23772495	0.71460043	2.53456164
N	0.00000000	-1.59825023	1.18638787
N	0.00000000	-1.42920138	2.53456164
N	1.38412501	0.79912485	1.18638787
N	1.23772495	0.71460043	2.53456164
C	-2.52302557	1.45666939	0.95666251
C	-3.10738013	1.79404687	2.18142578
C	-2.25940481	1.30446796	3.16381953
C	0.00000000	-2.91333877	0.95666251
C	0.00000000	-3.58809374	2.18142578
C	0.00000000	-2.60893591	3.16381953
C	2.52302557	1.45666939	0.95666251
C	3.10738013	1.79404687	2.18142578
C	2.25940481	1.30446796	3.16381953
N	-4.33540526	2.50304702	2.39324115
H	-2.33144224	1.34605864	4.24167051
N	0.00000000	-5.00609456	2.39324115
H	0.00000000	-3.32042160	-0.04362855
H	0.00000000	-2.69211728	4.24167051
H	-2.87556928	1.66021054	-0.04362855
H	0.00000000	0.00000000	4.29292503
N	4.33540526	2.50304702	2.39324115
H	2.33144224	1.34605864	4.24167051
H	2.87556928	1.66021054	-0.04362855
B	0.00000000	0.00000000	3.09380621
O	-4.67372733	-2.69837745	-3.55818359
O	-4.95216981	-2.85913674	-1.39370312
O	4.67372733	-2.69837745	-3.55818359
O	4.95216981	-2.85913674	-1.39370312
O	0.00000000	5.39675543	-3.55818359
O	0.00000000	5.71827294	-1.39370312
O	-4.67372733	2.69837745	3.55818359

O	-4.95216981	2.85913674	1.39370312
O	0.00000000	-5.39675543	3.55818359
O	0.00000000	-5.71827294	1.39370312
O	4.67372733	2.69837745	3.55818359
O	4.95216981	2.85913674	1.39370312

$[Fe(Tb^{4NH2})_2]^+$ $^6A_{1g}$ D_{3d}

Fe	0.00000000	0.00000000	0.00000000
N	-1.46141769	-0.84374984	-1.32991344
N	-1.25471312	-0.72440873	-2.64952698
N	1.46141769	-0.84374984	-1.32991344
N	1.25471312	-0.72440873	-2.64952698
N	0.00000000	1.68749968	-1.32991344
N	0.00000000	1.44881798	-2.64952698
C	-2.61461875	-1.50955060	-1.16220659
C	-3.17411362	-1.83257521	-2.40895242
C	-2.26348477	-1.30682332	-3.33228046
C	2.61461875	-1.50955060	-1.16220659
C	3.17411362	-1.83257521	-2.40895242
C	2.26348477	-1.30682332	-3.33228046
C	0.00000000	3.01910173	-1.16220659
C	0.00000000	3.66515095	-2.40895242
C	0.00000000	2.61364718	-3.33228046
N	-4.33933387	-2.50531560	-2.66226481
H	-2.27350157	-1.31260670	-4.41505755
N	4.33933387	-2.50531560	-2.66226481
H	2.98560534	-1.72373985	-0.16796880
H	2.27350157	-1.31260670	-4.41505755
H	-2.98560534	-1.72373985	-0.16796880
H	0.00000000	0.00000000	-4.38200249
N	0.00000000	5.01063120	-2.66226481
H	0.00000000	2.62521340	-4.41505755
H	0.00000000	3.44747970	-0.16796880
B	0.00000000	0.00000000	-3.18085481
N	-1.46141769	0.84374984	1.32991344
N	-1.25471312	0.72440873	2.64952698
N	0.00000000	-1.68749968	1.32991344
N	0.00000000	-1.44881798	2.64952698
N	1.46141769	0.84374984	1.32991344
N	1.25471312	0.72440873	2.64952698
C	-2.61461875	1.50955060	1.16220659
C	-3.17411362	1.83257521	2.40895242
C	-2.26348477	1.30682332	3.33228046
C	0.00000000	-3.01910173	1.16220659
C	0.00000000	-3.66515095	2.40895242
C	0.00000000	-2.61364718	3.33228046
C	2.61461875	1.50955060	1.16220659
C	3.17411362	1.83257521	2.40895242
C	2.26348477	1.30682332	3.33228046
N	-4.33933387	2.50531560	2.66226481
H	-2.27350157	1.31260670	4.41505755
N	0.00000000	-5.01063120	2.66226481
H	0.00000000	-3.44747970	0.16796880
H	0.00000000	-2.62521340	4.41505755
H	-2.98560534	1.72373985	0.16796880
H	0.00000000	0.00000000	4.38200249
N	4.33933387	2.50531560	2.66226481
H	2.27350157	1.31260670	4.41505755
H	2.98560534	1.72373985	0.16796880
B	0.00000000	0.00000000	3.18085481
H	-4.64512794	-2.68186606	-3.60060614
H	-4.91562536	-2.83803791	-1.91235609
H	4.64512794	-2.68186606	-3.60060614
H	4.91562536	-2.83803791	-1.91235609
H	0.00000000	5.36373159	-3.60060614
H	0.00000000	5.67607529	-1.91235609
H	-4.64512794	2.68186606	3.60060614
H	-4.91562536	2.83803791	1.91235609
H	0.00000000	-5.36373159	3.60060614
H	0.00000000	-5.67607529	1.91235609
H	4.64512794	2.68186606	3.60060614
H	4.91562536	2.83803791	1.91235609

$[Fe(Tb^{4NH2})_2]^+$ ^4E_g D_{3d}

Fe	0.00000000	0.00000000	0.00000000
N	-1.41848660	-0.81896371	-1.23176271
N	-1.24556312	-0.71912595	-2.55503921
N	1.41848660	-0.81896371	-1.23176271
N	1.24556312	-0.71912595	-2.55503921
N	0.00000000	1.63792741	-1.23176271
N	0.00000000	1.43825190	-2.55503921
C	-2.56832050	-1.48282027	-1.02129516
C	-3.15791497	-1.82322306	-2.24868051
C	-2.27089907	-1.31110437	-3.20266855
C	2.56832050	-1.48282027	-1.02129516
C	3.15791497	-1.82322306	-2.24868051
C	2.27089907	-1.31110437	-3.20266855
C	0.00000000	2.96564107	-1.02129516
C	0.00000000	3.64644612	-2.24868051
C	0.00000000	2.62220874	-3.20266855
N	-4.32901545	-2.49935812	-2.46486370
H	-2.30697520	-1.33193278	-4.28470585
N	4.32901545	-2.49935812	-2.46486370
H	2.91145490	-1.68092941	-0.01438092
H	2.30697520	-1.33193278	-4.28470585
H	-2.91145490	-1.68092941	-0.01438092
H	0.00000000	0.00000000	-4.30283387
N	0.00000000	4.99871677	-2.46486370
H	0.00000000	2.66386504	-4.28470585
H	0.00000000	3.36185883	-0.01438092
B	0.00000000	0.00000000	-3.10204021
N	-1.41848660	0.81896371	1.23176271
N	-1.24556312	0.71912595	2.55503921
N	0.00000000	-1.63792741	1.23176271
N	0.00000000	-1.43825190	2.55503921
N	1.41848660	0.81896371	1.23176271
N	1.24556312	0.71912595	2.55503921
C	-2.56832050	1.48282027	1.02129516
C	-3.15791497	1.82322306	2.24868051
C	-2.27089907	1.31110437	3.20266855
C	0.00000000	-2.96564107	1.02129516
C	0.00000000	-3.64644612	2.24868051
C	0.00000000	-2.62220874	3.20266855
C	2.56832050	1.48282027	1.02129516
C	3.15791497	1.82322306	2.24868051
C	2.27089907	1.31110437	3.20266855
N	-4.32901545	2.49935812	2.46486370
H	-2.30697520	1.33193278	4.28470585

N	0.00000000	-4.99871677	2.46486370
H	0.00000000	-3.36185883	0.01438092
H	0.00000000	-2.66386504	4.28470585
H	-2.91145490	1.68092941	0.01438092
H	0.00000000	0.00000000	4.30283387
N	4.32901545	2.49935812	2.46486370
H	2.30697520	1.33193278	4.28470585
H	2.91145490	1.68092941	0.01438092
B	0.00000000	0.00000000	3.10204021
H	-4.65641582	-2.68838288	-3.39332476
H	-4.88719108	-2.82162124	-1.69701852
H	4.65641582	-2.68838288	-3.39332476
H	4.88719108	-2.82162124	-1.69701852
H	0.00000000	5.37676576	-3.39332476
H	0.00000000	5.64324196	-1.69701852
H	-4.65641582	2.68838288	3.39332476
H	-4.88719108	2.82162124	1.69701852
H	0.00000000	-5.37676576	3.39332476
H	0.00000000	-5.64324196	1.69701852
H	4.65641582	2.68838288	3.39332476
H	4.88719108	2.82162124	1.69701852

$[Fe(Tb^{4NH2})_2]^+$ ^2E_g D_{3d}

Fe	0.00000000	0.00000000	0.00000000
N	-1.36853174	-0.79012196	-1.14890096
N	-1.23448691	-0.71273137	-2.47836090
N	1.36853174	-0.79012196	-1.14890096
N	1.23448691	-0.71273137	-2.47836090
N	0.00000000	1.58024445	-1.14890096
N	0.00000000	1.42546275	-2.47836090
C	-2.51181548	-1.45019755	-0.89425610
C	-3.13483014	-1.80989520	-2.10059555
C	-2.27748468	-1.31490651	-3.08810961
C	2.51181548	-1.45019755	-0.89425610
C	3.13483014	-1.80989520	-2.10059555
C	2.27748468	-1.31490651	-3.08810961
C	0.00000000	2.90039457	-0.89425610
C	0.00000000	3.61978987	-2.10059555
C	0.00000000	2.62981248	-3.08810961
N	-4.31194525	-2.48950272	-2.27010531
H	-2.34233800	-1.35234950	-4.16808735
N	4.31194525	-2.48950272	-2.27010531
H	2.82859633	-1.63309073	0.12305541
H	2.34233800	-1.35234950	-4.16808735
H	-2.82859633	-1.63309073	0.12305541
H	0.00000000	0.00000000	-4.24676437
N	0.00000000	4.97900545	-2.27010531
H	0.00000000	2.70469900	-4.16808735
H	0.00000000	3.26618199	0.12305541
B	0.00000000	0.00000000	-3.04678299
N	-1.36853174	0.79012196	1.14890096
N	-1.23448691	0.71273137	2.47836090
N	0.00000000	-1.58024445	1.14890096
N	0.00000000	-1.42546275	2.47836090
N	1.36853174	0.79012196	1.14890096
N	1.23448691	0.71273137	2.47836090
C	-2.51181548	1.45019755	0.89425610
C	-3.13483014	1.80989520	2.10059555
C	-2.27748468	1.31490651	3.08810961
C	0.00000000	-2.90039457	0.89425610
C	0.00000000	-3.61978987	2.10059555
C	0.00000000	-2.62981248	3.08810961
C	2.51181548	1.45019755	0.89425610
C	3.13483014	1.80989520	2.10059555
C	2.27748468	1.31490651	3.08810961
N	-4.31194525	2.48950272	2.27010531
H	-2.34233800	1.35234950	4.16808735
N	0.00000000	-4.97900545	2.27010531
H	0.00000000	-3.26618199	-0.12305541
H	0.00000000	-2.70469900	4.16808735
H	-2.82859633	1.63309073	-0.12305541
H	0.00000000	0.00000000	4.24676437
N	4.31194525	2.48950272	2.27010531
H	2.34233800	1.35234950	4.16808735
H	2.82859633	1.63309073	-0.12305541
B	0.00000000	0.00000000	3.04678299
H	-4.66620031	-2.69403238	-3.18536551
H	-4.84726042	-2.79856711	-1.48078929
H	4.66620031	-2.69403238	-3.18536551
H	4.84726042	-2.79856711	-1.48078929
H	0.00000000	5.38806422	-3.18536551
H	0.00000000	5.59713422	-1.48078929
H	-4.66620031	2.69403238	3.18536551
H	-4.84726042	2.79856711	1.48078929
H	0.00000000	-5.38806422	3.18536551
H	0.00000000	-5.59713422	1.48078929
H	4.66620031	2.69403238	3.18536551
H	4.84726042	2.79856711	1.48078929

$[Fe(Tb^{4NO2})_2]^+$ $^6A_{1g}$ D_{3d}

Fe	0.00000000	0.00000000	0.00000000
N	-1.44788028	-0.83593442	-1.32454071
N	-1.25048500	-0.72196816	-2.66228650
N	1.44788028	-0.83593442	-1.32454071
N	1.25048500	-0.72196816	-2.66228650
N	0.00000000	1.67186831	-1.32454071
N	0.00000000	1.44393579	-2.66228650
C	-2.59426024	-1.49779651	-1.14043836
C	-3.13499578	-1.80999098	-2.38438907
C	-2.25368388	-1.30116483	-3.33066330
C	2.59426024	-1.49779651	-1.14043836
C	3.13499578	-1.80999098	-2.38438907
C	2.25368388	-1.30116483	-3.33066330
C	0.00000000	2.99559356	-1.14043836
C	0.00000000	3.61998143	-2.38438907
C	0.00000000	2.60232966	-3.33066330
N	-4.36568055	-2.52052680	-2.64085271
H	-2.29489356	-1.32495770	-4.41174543
N	4.36568055	-2.52052680	-2.64085271
H	2.98198206	-1.72164801	-0.15601098
H	2.29489356	-1.32495770	-4.41174543
H	-2.98198206	-1.72164801	-0.15601098
H	0.00000000	0.00000000	-4.40119363
N	0.00000000	5.04105413	-2.64085271
H	0.00000000	2.64991487	-4.41174543
H	0.00000000	3.44329603	-0.15601098
B	0.00000000	0.00000000	-3.20516786
N	-1.44788028	0.83593442	1.32454071

N	-1.25048500	0.72196816	2.66228650
N	0.00000000	-1.67186831	1.32454071
N	0.00000000	-1.44393579	2.66228650
N	1.44788028	0.83593442	1.32454071
N	1.25048500	0.72196816	2.66228650
C	-2.59426024	1.49779651	1.14043836
C	-3.13499578	1.80999098	2.38438907
C	-2.25368388	1.30116483	3.33066330
C	0.00000000	-2.99559356	1.14043836
C	0.00000000	-3.61998143	2.38438907
C	0.00000000	-2.60232966	3.33066330
C	2.59426024	1.49779651	1.14043836
C	3.13499578	1.80999098	2.38438907
C	2.25368388	1.30116483	3.33066330
N	-4.36568055	2.52052680	2.64085271
H	-2.29489356	1.32495770	4.41174543
N	0.00000000	-5.04105413	2.64085271
H	0.00000000	-3.44329603	0.15601098
H	0.00000000	-2.64991487	4.41174543
H	-2.98198206	1.72164801	0.15601098
H	0.00000000	0.00000000	4.40119363
N	4.36568055	2.52052680	2.64085271
H	2.29489356	1.32495770	4.41174543
H	2.98198206	1.72164801	0.15601098
B	0.00000000	0.00000000	3.20516786
O	-4.66256751	-2.69193472	-3.81574421
O	-4.99941317	-2.88641265	-1.66048624
O	4.66256751	-2.69193472	-3.81574421
O	4.99941317	-2.88641265	-1.66048624
O	0.00000000	5.38386943	-3.81574421
O	0.00000000	5.77282477	-1.66048624
O	-4.66256751	2.69193472	3.81574421
O	-4.99941317	2.88641265	1.66048624
O	0.00000000	-5.38386943	3.81574421
O	0.00000000	-5.77282477	1.66048624
O	4.66256751	2.69193472	3.81574421
O	4.99941317	2.88641265	1.66048624

$[Fe(Tb^{4NO2})_2]^+$ ^4E_g D_{3d}

Fe	0.00000000	0.00000000	0.00000000
N	-1.42043397	-0.82008768	-1.24283627
N	-1.24443015	-0.71847189	-2.58250033
N	1.42043397	-0.82008768	-1.24283627
N	1.24443015	-0.71847189	-2.58250033
N	0.00000000	1.64017589	-1.24283627
N	0.00000000	1.43694431	-2.58250033
C	-2.56287368	-1.47967590	-1.03067059
C	-3.12257387	-1.80281851	-2.26396050
C	-2.25774902	-1.30351226	-3.22959574
C	2.56287368	-1.47967590	-1.03067059
C	3.12257387	-1.80281851	-2.26396050
C	2.25774902	-1.30351226	-3.22959574
C	0.00000000	2.95935179	-1.03067059
C	0.00000000	3.60563756	-2.26396050
C	0.00000000	2.60702452	-3.22959574
N	-4.35682688	-2.51541495	-2.49639420
H	-2.31586908	-1.33706792	-4.30968936
N	4.35682688	-2.51541495	-2.49639420
H	2.93351683	-1.69366671	-0.03780072
H	2.31586908	-1.33706792	-4.30968936
H	-2.93351683	-1.69366671	-0.03780072
H	0.00000000	0.00000000	-4.33075221
N	0.00000000	5.03083042	-2.49639420
H	0.00000000	2.67413531	-4.30968936
H	0.00000000	3.38733342	-0.03780072
B	0.00000000	0.00000000	-3.13492645
N	-1.42043397	0.82008768	1.24283627
N	-1.24443015	0.71847189	2.58250033
N	0.00000000	-1.64017589	1.24283627
N	0.00000000	-1.43694431	2.58250033
N	1.42043397	0.82008768	1.24283627
N	1.24443015	0.71847189	2.58250033
C	-2.56287368	1.47967590	1.03067059
C	-3.12257387	1.80281851	2.26396050
C	-2.25774902	1.30351226	3.22959574
C	0.00000000	-2.95935179	1.03067059
C	0.00000000	-3.60563756	2.26396050
C	0.00000000	-2.60702452	3.22959574
C	2.56287368	1.47967590	1.03067059
C	3.12257387	1.80281851	2.26396050
C	2.25774902	1.30351226	3.22959574
N	-4.35682688	2.51541495	2.49639420
H	-2.31586908	1.33706792	4.30968936
N	0.00000000	-5.03083042	2.49639420
H	0.00000000	-3.38733342	0.03780072
H	0.00000000	-2.67413531	4.30968936
H	-2.93351683	1.69366671	0.03780072
H	0.00000000	0.00000000	4.33075221
N	4.35682688	2.51541495	2.49639420
H	2.31586908	1.33706792	4.30968936
H	2.93351683	1.69366671	0.03780072
B	0.00000000	0.00000000	3.13492645
O	-4.66874036	-2.69549873	-3.66629503
O	-4.97729250	-2.87364096	-1.50530236
O	4.66874036	-2.69549873	-3.66629503
O	4.97729250	-2.87364096	-1.50530236
O	0.00000000	5.39099692	-3.66629503
O	0.00000000	5.74728244	-1.50530236
O	-4.66874036	2.69549873	3.66629503
O	-4.97729250	2.87364096	1.50530236
O	0.00000000	-5.39099692	3.66629503
O	0.00000000	-5.74728244	1.50530236
O	4.66874036	2.69549873	3.66629503
O	4.97729250	2.87364096	1.50530236

$[Fe(Tb^{4NO2})_2]^+$ ^2E_g D_{3d}

[Fe	0.00000000	0.00000000	0.00000000
N	-1.36538049	-0.78830318	-1.15174687
N	-1.23214318	-0.71137827	-2.49791982
N	1.36538049	-0.78830318	-1.15174687
N	1.23214318	-0.71137827	-2.49791982
N	0.00000000	1.57660582	-1.15174687
N	0.00000000	1.42275653	-2.49791982
C	-2.50143726	-1.44420515	-0.89169383
C	-3.09779991	-1.78851538	-2.10186504
C	-2.26459340	-1.30746363	-3.10270274
C	2.50143726	-1.44420515	-0.89169383
C	3.09779991	-1.78851538	-2.10186504

C	2.26459340	-1.30746363	-3.10270274
C	0.00000000	2.88841082	-0.89169383
C	0.00000000	3.57703129	-2.10186504
C	0.00000000	2.61492726	-3.10270274
N	-4.33902854	-2.50513938	-2.28482490
H	-2.35455776	-1.35940449	-4.17979117
N	4.33902854	-2.50513938	-2.28482490
H	2.84340906	-1.64164276	0.11386360
H	2.35455776	-1.35940449	-4.17979117
H	-2.84340906	-1.64164276	0.11386360
H	0.00000000	0.00000000	-4.26935441
N	0.00000000	5.01027823	-2.28482490
H	0.00000000	2.71880951	-4.17979117
H	0.00000000	3.28328606	0.11386360
B	0.00000000	0.00000000	-3.07463623
N	-1.36538049	0.78830318	1.15174687
N	-1.23214318	0.71137827	2.49791982
N	0.00000000	-1.57660582	1.15174687
N	0.00000000	-1.42275653	2.49791982
N	1.36538049	0.78830318	1.15174687
N	1.23214318	0.71137827	2.49791982
C	-2.50143726	1.44420515	0.89169383
C	-3.09779991	1.78851538	2.10186504
C	-2.26459340	1.30746363	3.10270274
C	0.00000000	-2.88841082	0.89169383
C	0.00000000	-3.57703129	2.10186504
C	0.00000000	-2.61492726	3.10270274
C	2.50143726	1.44420515	0.89169383
C	3.09779991	1.78851538	2.10186504
C	2.26459340	1.30746363	3.10270274
N	-4.33902854	2.50513938	2.28482490
H	-2.35455776	1.35940449	4.17979117
N	0.00000000	-5.01027823	2.28482490
H	0.00000000	-3.28328606	-0.11386360
H	0.00000000	-2.71880951	4.17979117
H	-2.84340906	1.64164276	-0.11386360
H	0.00000000	0.00000000	4.26935441
N	4.33902854	2.50513938	2.28482490
H	2.35455776	1.35940449	4.17979117
H	2.84340906	1.64164276	-0.11386360
B	0.00000000	0.00000000	3.07463623
O	-4.68573806	-2.70531179	-3.44069142
O	-4.92773558	-2.84502940	-1.26791451
O	4.68573806	-2.70531179	-3.44069142
O	4.92773558	-2.84502940	-1.26791451
O	0.00000000	5.41062411	-3.44069142
O	0.00000000	5.69005880	-1.26791451
O	-4.68573806	2.70531179	3.44069142
O	-4.92773558	2.84502940	1.26791451
O	0.00000000	-5.41062411	3.44069142
O	0.00000000	-5.69005880	1.26791451
O	4.68573806	2.70531179	3.44069142
O	4.92773558	2.84502940	1.26791451

$Fe(Tb^{4NH2})_2]$ $^5A_{1g}$ D_{3d}

Fe	0.00000000	0.00000000	0.00000000
N	-1.48746486	-0.85878800	-1.37393835
N	-1.26137335	-0.72825426	-2.68442516
N	1.48746486	-0.85878800	-1.37393835
N	1.26137335	-0.72825426	-2.68442516
N	0.00000000	1.71757600	-1.37393835
N	0.00000000	1.45650799	-2.68442516
C	-2.64306097	-1.52597203	-1.23856105
C	-3.18293977	-1.83767118	-2.49772296
C	-2.26091562	-1.30534004	-3.39671838
C	2.64306097	-1.52597203	-1.23856105
C	3.18293977	-1.83767118	-2.49772296
C	2.26091562	-1.30534004	-3.39671838
C	0.00000000	3.05194405	-1.23856105
C	0.00000000	3.67534237	-2.49772296
C	0.00000000	2.61068008	-3.39671838
N	-4.35464244	-2.51415392	-2.76972801
H	-2.24986110	-1.29895763	-4.47961029
N	4.35464244	-2.51415392	-2.76972801
H	3.02961754	-1.74915041	-0.25109937
H	2.24986110	-1.29895763	-4.47961029
H	-3.02961754	-1.74915041	-0.25109937
H	0.00000000	0.00000000	-4.40155506
N	0.00000000	5.02830836	-2.76972801
H	0.00000000	2.59791580	-4.47961029
H	0.00000000	3.49830083	-0.25109937
B	0.00000000	0.00000000	-3.19469861
N	-1.48746486	0.85878800	1.37393835
N	-1.26137335	0.72825426	2.68442516
N	0.00000000	-1.71757600	1.37393835
N	0.00000000	-1.45650799	2.68442516
N	1.48746486	0.85878800	1.37393835
N	1.26137335	0.72825426	2.68442516
C	-2.64306097	1.52597203	1.23856105
C	-3.18293977	1.83767118	2.49772296
C	-2.26091562	1.30534004	3.39671838
C	0.00000000	-3.05194405	1.23856105
C	0.00000000	-3.67534237	2.49772296
C	0.00000000	-2.61068008	3.39671838
C	2.64306097	1.52597203	1.23856105
C	3.18293977	1.83767118	2.49772296
C	2.26091562	1.30534004	3.39671838
N	-4.35464244	2.51415392	2.76972801
H	-2.24986110	1.29895763	4.47961029
N	0.00000000	-5.02830836	2.76972801
H	0.00000000	-3.49830083	0.25109937
H	0.00000000	-2.59791580	4.47961029
H	-3.02961754	1.74915041	0.25109937
H	0.00000000	0.00000000	4.40155506
N	4.35464244	2.51415392	2.76972801
H	2.24986110	1.29895763	4.47961029
H	3.02961754	1.74915041	0.25109937
B	0.00000000	0.00000000	3.19469861
H	-4.65022709	-2.68480987	-3.71105125
H	-4.93520280	-2.84934061	-2.02582756
H	4.65022709	-2.68480987	-3.71105125
H	4.93520280	-2.84934061	-2.02582756
H	0.00000000	5.36961975	-3.71105125
H	0.00000000	5.69868121	-2.02582756
H	-4.65022709	2.68480987	3.71105125
H	-4.93520280	2.84934061	2.02582756
H	0.00000000	-5.36961975	3.71105125
H	0.00000000	-5.69868121	2.02582756
H	4.65022709	2.68480987	3.71105125

H	4.93520280	2.84934061	2.02582756

$[Fe(Tb^{4NH2})_2]$ ^3E_g D_{3d}

Fe	0.00000000	0.00000000	0.00000000
N	-1.42487060	-0.82264943	-1.26532048
N	-1.24813016	-0.72060818	-2.58549389
N	1.42487060	-0.82264943	-1.26532048
N	1.24813016	-0.72060818	-2.58549389
N	0.00000000	1.64529832	-1.26532048
N	0.00000000	1.44121635	-2.58549389
C	-2.57531569	-1.48685895	-1.07004720
C	-3.15946917	-1.82412054	-2.30282381
C	-2.27286602	-1.31223998	-3.24791691
C	2.57531569	-1.48685895	-1.07004720
C	3.15946917	-1.82412054	-2.30282381
C	2.27286602	-1.31223998	-3.24791691
C	0.00000000	2.97371843	-1.07004720
C	0.00000000	3.64824109	-2.30282381
C	0.00000000	2.62447944	-3.24791691
N	-4.34017103	-2.50579927	-2.51820106
H	-2.30079759	-1.32836613	-4.33038125
N	4.34017103	-2.50579927	-2.51820106
H	2.92400487	-1.68817491	-0.06516024
H	2.30079759	-1.32836613	-4.33038125
H	-2.92400487	-1.68817491	-0.06516024
H	0.00000000	0.00000000	-4.32885193
N	0.00000000	5.01159800	-2.51820106
H	0.00000000	2.65673226	-4.33038125
H	0.00000000	3.37634982	-0.06516024
B	0.00000000	0.00000000	-3.12272098
N	-1.42487060	0.82264943	1.26532048
N	-1.24813016	0.72060818	2.58549389
N	0.00000000	-1.64529832	1.26532048
N	0.00000000	-1.44121635	2.58549389
N	1.42487060	0.82264943	1.26532048
N	1.24813016	0.72060818	2.58549389
C	-2.57531569	1.48685895	1.07004720
C	-3.15946917	1.82412054	2.30282381
C	-2.27286602	1.31223998	3.24791691
C	0.00000000	-2.97371843	1.07004720
C	0.00000000	-3.64824109	2.30282381
C	0.00000000	-2.62447944	3.24791691
C	2.57531569	1.48685895	1.07004720
C	3.15946917	1.82412054	2.30282381
C	2.27286602	1.31223998	3.24791691
N	-4.34017103	2.50579927	2.51820106
H	-2.30079759	1.32836613	4.33038125
N	0.00000000	-5.01159800	2.51820106
H	0.00000000	-3.37634982	0.06516024
H	0.00000000	-2.65673226	4.33038125
H	-2.92400487	1.68817491	0.06516024
H	0.00000000	0.00000000	4.32885193
N	4.34017103	2.50579927	2.51820106
H	2.30079759	1.32836613	4.33038125
H	2.92400487	1.68817491	0.06516024
B	0.00000000	0.00000000	3.12272098
H	-4.66883508	-2.69555323	-3.44477085
H	-4.89346659	-2.82524452	-1.74706704
H	4.66883508	-2.69555323	-3.44477085
H	4.89346659	-2.82524452	-1.74706704
H	0.00000000	5.39110593	-3.44477085
H	0.00000000	5.65048851	-1.74706704
H	-4.66883508	2.69555323	3.44477085
H	-4.89346659	2.82524452	1.74706704
H	0.00000000	-5.39110593	3.44477085
H	0.00000000	-5.65048851	1.74706704
H	4.66883508	2.69555323	3.44477085
H	4.89346659	2.82524452	1.74706704

$[Fe(Tb^{4NH2})_2]$ $^1A_{1g}$ D_{3d}

Fe	0.00000000	0.00000000	0.00000000
N	-1.37041932	-0.79121206	-1.15965014
N	-1.23592786	-0.71356324	-2.48717805
N	1.37041932	-0.79121206	-1.15965014
N	1.23592786	-0.71356324	-2.48717805
N	0.00000000	1.58242360	-1.15965014
N	0.00000000	1.42712648	-2.48717805
C	-2.51496832	-1.45201739	-0.91505171
C	-3.13551490	-1.81029050	-2.12449372
C	-2.28129370	-1.31710577	-3.10652340
C	2.51496832	-1.45201739	-0.91505171
C	3.13551490	-1.81029050	-2.12449372
C	2.28129370	-1.31710577	-3.10652340
C	0.00000000	2.90403531	-0.91505171
C	0.00000000	3.62058099	-2.12449372
C	0.00000000	2.63421153	-3.10652340
N	-4.32275634	-2.49574437	-2.28786450
H	-2.34102564	-1.35159172	-4.18692395
N	4.32275634	-2.49574437	-2.28786450
H	2.83383307	-1.63611445	0.10165177
H	2.34102564	-1.35159172	-4.18692395
H	-2.83383307	-1.63611445	0.10165177
H	0.00000000	0.00000000	-4.25306528
N	0.00000000	4.99148874	-2.28786450
H	0.00000000	2.70318344	-4.18692395
H	0.00000000	3.27222837	0.10165177
B	0.00000000	0.00000000	-3.04807683
N	-1.37041932	0.79121206	1.15965014
N	-1.23592786	0.71356324	2.48717805
N	0.00000000	-1.58242360	1.15965014
N	0.00000000	-1.42712648	2.48717805
N	1.37041932	0.79121206	1.15965014
N	1.23592786	0.71356324	2.48717805
C	-2.51496832	1.45201739	0.91505171
C	-3.13551490	1.81029050	2.12449372
C	-2.28129370	1.31710577	3.10652340
C	0.00000000	-2.90403531	0.91505171
C	0.00000000	-3.62058099	2.12449372
C	0.00000000	-2.63421153	3.10652340
C	2.51496832	1.45201739	0.91505171
C	3.13551490	1.81029050	2.12449372
C	2.28129370	1.31710577	3.10652340
N	-4.32275634	2.49574437	2.28786450
H	-2.34102564	1.35159172	4.18692395
N	0.00000000	-4.99148874	2.28786450
H	0.00000000	-3.27222837	-0.10165177
H	0.00000000	-2.70318344	4.18692395
H	-2.83383307	1.63611445	-0.10165177

H	0.00000000	0.00000000	4.25306528
N	4.32275634	2.49574437	2.28786450
H	2.34102564	1.35159172	4.18692395
H	2.83383307	1.63611445	-0.10165177
B	0.00000000	0.00000000	3.04807683
H	-4.68079608	-2.70245899	-3.19970992
H	-4.85037410	-2.80036472	-1.49313023
H	4.68079608	-2.70245899	-3.19970992
H	4.85037410	-2.80036472	-1.49313023
H	0.00000000	5.40491746	-3.19970992
H	0.00000000	5.60072945	-1.49313023
H	-4.68079608	2.70245899	3.19970992
H	-4.85037410	2.80036472	1.49313023
H	0.00000000	-5.40491746	3.19970992
H	0.00000000	-5.60072945	1.49313023
H	4.68079608	2.70245899	3.19970992
H	4.85037410	2.80036472	1.49313023

$[Fe(Tb^{4NO2})_2]$ $^5A_{1g}$ D_{3d}

Fe	0.00000000	0.00000000	0.00000000
N	-1.48496502	-0.85734493	-1.36049989
N	-1.25873910	-0.72673340	-2.69146005
N	1.48496502	-0.85734493	-1.36049989
N	1.25873910	-0.72673340	-2.69146005
N	0.00000000	1.71468986	-1.36049989
N	0.00000000	1.45346628	-2.69146005
C	-2.63043585	-1.51868261	-1.22030073
C	-3.14695783	-1.81689674	-2.48515818
C	-2.24251295	-1.29471522	-3.39902347
C	2.63043585	-1.51868261	-1.22030073
C	3.14695783	-1.81689674	-2.48515818
C	2.24251295	-1.29471522	-3.39902347
C	0.00000000	3.03736575	-1.22030073
C	0.00000000	3.63379349	-2.48515818
C	0.00000000	2.58943097	-3.39902347
N	-4.36121271	-2.51794706	-2.78910648
H	-2.25363784	-1.30113837	-4.48003364
N	4.36121271	-2.51794706	-2.78910648
H	3.03776105	-1.75385215	-0.24620395
H	2.25363784	-1.30113837	-4.48003364
H	-3.03776105	-1.75385215	-0.24620395
H	0.00000000	0.00000000	-4.40910907
N	0.00000000	5.03589465	-2.78910648
H	0.00000000	2.60227675	-4.48003364
H	0.00000000	3.50770431	-0.24620395
B	0.00000000	0.00000000	-3.20850696
N	-1.48496502	0.85734493	1.36049989
N	-1.25873910	0.72673340	2.69146005
N	0.00000000	-1.71468986	1.36049989
N	0.00000000	-1.45346628	2.69146005
N	1.48496502	0.85734493	1.36049989
N	1.25873910	0.72673340	2.69146005
C	-2.63043585	1.51868261	1.22030073
C	-3.14695783	1.81689674	2.48515818
C	-2.24251295	1.29471522	3.39902347
C	0.00000000	-3.03736575	1.22030073
C	0.00000000	-3.63379349	2.48515818
C	0.00000000	-2.58943097	3.39902347
C	2.63043585	1.51868261	1.22030073
C	3.14695783	1.81689674	2.48515818
C	2.24251295	1.29471522	3.39902347
N	-4.36121271	2.51794706	2.78910648
H	-2.25363784	1.30113837	4.48003364
N	0.00000000	-5.03589465	2.78910648
H	0.00000000	-3.50770431	0.24620395
H	0.00000000	-2.60227675	4.48003364
H	-3.03776105	1.75385215	0.24620395
H	0.00000000	0.00000000	4.40910907
N	4.36121271	2.51794706	2.78910648
H	2.25363784	1.30113837	4.48003364
H	3.03776105	1.75385215	0.24620395
B	0.00000000	0.00000000	3.20850696
O	-4.63235043	-2.67448880	-3.97690567
O	-5.03395680	-2.90635628	-1.83920051
O	4.63235043	-2.67448880	-3.97690567
O	5.03395680	-2.90635628	-1.83920051
O	0.00000000	5.34897760	-3.97690567
O	0.00000000	5.81271256	-1.83920051
O	-4.63235043	2.67448880	3.97690567
O	-5.03395680	2.90635628	1.83920051
O	0.00000000	-5.34897760	3.97690567
O	0.00000000	-5.81271256	1.83920051
O	4.63235043	2.67448880	3.97690567
O	5.03395680	2.90635628	1.83920051

$[Fe(Tb^{4NO2})_2]$ ^3E_g D_{3d}

Fe	0.00000000	0.00000000	0.00000000
N	-1.42245967	-0.82125769	-1.25386168
N	-1.24571605	-0.71921432	-2.59443593
N	1.42245967	-0.82125769	-1.25386168
N	1.24571605	-0.71921432	-2.59443593
N	0.00000000	1.64251485	-1.25386168
N	0.00000000	1.43842918	-2.59443593
C	-2.56281494	-1.47964203	-1.05533501
C	-3.12313321	-1.80314184	-2.29553122
C	-2.25405113	-1.30137703	-3.25338543
C	2.56281494	-1.47964203	-1.05533501
C	3.12313321	-1.80314184	-2.29553122
C	2.25405113	-1.30137703	-3.25338543
C	0.00000000	2.95928353	-1.05533501
C	0.00000000	3.60628368	-2.29553122
C	0.00000000	2.60275406	-3.25338543
N	-4.34704134	-2.50976545	-2.54059532
H	-2.30346835	-1.32990815	-4.33302396
N	4.34704134	-2.50976545	-2.54059532
H	2.93462810	-1.69430807	-0.06354202
H	2.30346835	-1.32990815	-4.33302396
H	-2.93462810	-1.69430807	-0.06354202
H	0.00000000	0.00000000	-4.33832473
N	0.00000000	5.01953090	-2.54059532
H	0.00000000	2.65981630	-4.33302396
H	0.00000000	3.38861667	-0.06354202
B	0.00000000	0.00000000	-3.13866403
N	-1.42245967	0.82125769	1.25386168
N	-1.24571605	0.71921432	2.59443593
N	0.00000000	-1.64251485	1.25386168
N	0.00000000	-1.43842918	2.59443593
N	1.42245967	0.82125769	1.25386168

N	1.24571605	0.71921432	2.59443593
C	-2.56281494	1.47964203	1.05533501
C	-3.12313321	1.80314184	2.29553122
C	-2.25405113	1.30137703	3.25338543
C	0.00000000	-2.95928353	1.05533501
C	0.00000000	-3.60628368	2.29553122
C	0.00000000	-2.60275406	3.25338543
C	2.56281494	1.47964203	1.05533501
C	3.12313321	1.80314184	2.29553122
C	2.25405113	1.30137703	3.25338543
N	-4.34704134	2.50976545	2.54059532
H	-2.30346835	1.32990815	4.33302396
N	0.00000000	-5.01953090	2.54059532
H	0.00000000	-3.38861667	0.06354202
H	0.00000000	-2.65981630	4.33302396
H	-2.93462810	1.69430807	0.06354202
H	0.00000000	0.00000000	4.33832473
N	4.34704134	2.50976545	2.54059532
H	2.30346835	1.32990815	4.33302396
H	2.93462810	1.69430807	0.06354202
B	0.00000000	0.00000000	3.13866403
O	-4.66130489	-2.69120551	-3.71430781
O	-4.98415064	-2.87760079	-1.55841641
O	4.66130489	-2.69120551	-3.71430781
O	4.98415064	-2.87760079	-1.55841641
O	0.00000000	5.38241102	-3.71430781
O	0.00000000	5.75520158	-1.55841641
O	-4.66130489	2.69120551	3.71430781
O	-4.98415064	2.87760079	1.55841641
O	0.00000000	-5.38241102	3.71430781
O	0.00000000	-5.75520158	1.55841641
O	4.66130489	2.69120551	3.71430781
O	4.98415064	2.87760079	1.55841641

$[Fe(Tb^{4NO2})_2]$ $^1A_{1g}$ D_{3d}

Fe	0.00000000	0.00000000	0.00000000
N	-1.36795388	-0.78978858	-1.14659374
N	-1.23368732	-0.71226940	-2.49477068
N	1.36795388	-0.78978858	-1.14659374
N	1.23368732	-0.71226940	-2.49477068
N	0.00000000	1.57957715	-1.14659374
N	0.00000000	1.42453933	-2.49477068
C	-2.50235750	-1.44473697	-0.89993894
C	-3.09883657	-1.78911388	-2.11850396
C	-2.26189248	-1.30590414	-3.11161673
C	2.50235750	-1.44473697	-0.89993894
C	3.09883657	-1.78911388	-2.11850396
C	2.26189248	-1.30590414	-3.11161673
C	0.00000000	2.88947341	-0.89993894
C	0.00000000	3.57822829	-2.11850396
C	0.00000000	2.61180829	-3.11161673
N	-4.32887574	-2.49927769	-2.31342376
H	-2.34303069	-1.35274956	-4.18849401
N	4.32887574	-2.49927769	-2.31342376
H	2.84570780	-1.64296994	0.10428337
H	2.34303069	-1.35274956	-4.18849401
H	-2.84570780	-1.64296994	0.10428337
H	0.00000000	0.00000000	-4.26138712
N	0.00000000	4.99855484	-2.31342376
H	0.00000000	2.70549859	-4.18849401
H	0.00000000	3.28593988	0.10428337
B	0.00000000	0.00000000	-3.06282658
N	-1.36795388	0.78978858	1.14659374
N	-1.23368732	0.71226940	2.49477068
N	0.00000000	-1.57957715	1.14659374
N	0.00000000	-1.42453933	2.49477068
N	1.36795388	0.78978858	1.14659374
N	1.23368732	0.71226940	2.49477068
C	-2.50235750	1.44473697	0.89993894
C	-3.09883657	1.78911388	2.11850396
C	-2.26189248	1.30590414	3.11161673
C	0.00000000	-2.88947341	0.89993894
C	0.00000000	-3.57822829	2.11850396
C	0.00000000	-2.61180829	3.11161673
C	2.50235750	1.44473697	0.89993894
C	3.09883657	1.78911388	2.11850396
C	2.26189248	1.30590414	3.11161673
N	-4.32887574	2.49927769	2.31342376
H	-2.34303069	1.35274956	4.18849401
N	0.00000000	-4.99855484	2.31342376
H	0.00000000	-3.28593988	-0.10428337
H	0.00000000	-2.70549859	4.18849401
H	-2.84570780	1.64296994	-0.10428337
H	0.00000000	0.00000000	4.26138712
N	4.32887574	2.49927769	2.31342376
H	2.34303069	1.35274956	4.18849401
H	2.84570780	1.64296994	-0.10428337
B	0.00000000	0.00000000	3.06282658
O	-4.67875028	-2.70127787	-3.47364434
O	-4.93571928	-2.84963906	-1.30594489
O	4.67875028	-2.70127787	-3.47364434
O	4.93571928	-2.84963906	-1.30594489
O	0.00000000	5.40255574	-3.47364434
O	0.00000000	5.69927813	-1.30594489
O	-4.67875028	2.70127787	3.47364434
O	-4.93571928	2.84963906	1.30594489
O	0.00000000	-5.40255574	3.47364434
O	0.00000000	-5.69927813	1.30594489
O	4.67875028	2.70127787	3.47364434
O	4.93571928	2.84963906	1.30594489

$[Co(Tb^{4NH2})_2]^+$ $^5A_{1g}$ D_{3d}

Co	0.00000000	0.00000000	0.00000000
N	-1.45092146	-0.83768970	-1.28805023
N	-1.25305204	-0.72344986	-2.60990378
N	1.45092146	-0.83768970	-1.28805023
N	1.25305204	-0.72344986	-2.60990378
N	0.00000000	1.67537940	-1.28805023
N	0.00000000	1.44690025	-2.60990378
C	-2.60153537	-1.50199712	-1.11293278
C	-3.16864457	-1.82941761	-2.35608867
C	-2.26306513	-1.30658149	-3.28781635
C	2.60153537	-1.50199712	-1.11293278
C	3.16864457	-1.82941761	-2.35608867
C	2.26306513	-1.30658149	-3.28781635
C	0.00000000	3.00399425	-1.11293278
C	0.00000000	3.65883574	-2.35608867
C	0.00000000	2.61316298	-3.28781635

N	-4.33459827	-2.50258134	-2.60210265
H	-2.27941777	-1.31602254	-4.37054580
N	4.33459827	-2.50258134	-2.60210265
H	2.96751435	-1.71329548	-0.11629305
H	2.27941777	-1.31602254	-4.37054580
H	-2.96751435	-1.71329548	-0.11629305
H	0.00000000	0.00000000	-4.34396947
N	0.00000000	5.00516321	-2.60210265
H	0.00000000	2.63204508	-4.37054580
H	0.00000000	3.42659043	-0.11629305
B	0.00000000	0.00000000	-3.14163589
N	-1.45092146	0.83768970	1.28805023
N	-1.25305204	0.72344986	2.60990378
N	0.00000000	-1.67537940	1.28805023
N	0.00000000	-1.44690025	2.60990378
N	1.45092146	0.83768970	1.28805023
N	1.25305204	0.72344986	2.60990378
C	-2.60153537	1.50199712	1.11293278
C	-3.16864457	1.82941761	2.35608867
C	-2.26306513	1.30658149	3.28781635
C	0.00000000	-3.00399425	1.11293278
C	0.00000000	-3.65883574	2.35608867
C	0.00000000	-2.61316298	3.28781635
C	2.60153537	1.50199712	1.11293278
C	3.16864457	1.82941761	2.35608867
C	2.26306513	1.30658149	3.28781635
N	-4.33459827	2.50258134	2.60210265
H	-2.27941777	1.31602254	4.37054580
N	0.00000000	-5.00516321	2.60210265
H	0.00000000	-3.42659043	0.11629305
H	0.00000000	-2.63204508	4.37054580
H	-2.96751435	1.71329548	0.11629305
H	0.00000000	0.00000000	4.34396947
N	4.33459827	2.50258134	2.60210265
H	2.27941777	1.31602254	4.37054580
H	2.96751435	1.71329548	0.11629305
B	0.00000000	0.00000000	3.14163589
H	-4.64539465	-2.68202005	-3.53853418
H	-4.90729399	-2.83322716	-1.84815842
H	4.64539465	-2.68202005	-3.53853418
H	4.90729399	-2.83322716	-1.84815842
H	0.00000000	5.36404010	-3.53853418
H	0.00000000	5.66645485	-1.84815842
H	-4.64539465	2.68202005	3.53853418
H	-4.90729399	2.83322716	1.84815842
H	0.00000000	-5.36404010	3.53853418
H	0.00000000	-5.66645485	1.84815842
H	4.64539465	2.68202005	3.53853418
H	4.90729399	2.83322716	1.84815842

$[Co(Tb^{4NH2})_2]^+$ ^3E_g D_{3d}

Co	0.00000000	0.00000000	0.00000000
N	-1.40534078	-0.81137372	-1.20889854
N	-1.24270133	-0.71747386	-2.53335988
N	1.40534078	-0.81137372	-1.20889854
N	1.24270133	-0.71747386	-2.53335988
N	0.00000000	1.62274743	-1.20889854
N	0.00000000	1.43494772	-2.53335988
C	-2.55022105	-1.47237061	-0.98583234
C	-3.15005563	-1.81868536	-2.20959336
C	-2.27254587	-1.31205477	-3.17357439
C	2.55022105	-1.47237061	-0.98583234
C	3.15005563	-1.81868536	-2.20959336
C	2.27254587	-1.31205477	-3.17357439
C	0.00000000	2.94474121	-0.98583234
C	0.00000000	3.63737126	-2.20959336
C	0.00000000	2.62411007	-3.17357439
N	-4.32342204	-2.49612908	-2.40970174
H	-2.31615167	-1.33723091	-4.25513013
N	4.32342204	-2.49612908	-2.40970174
H	2.88665395	-1.66661041	0.02386960
H	2.31615167	-1.33723091	-4.25513013
H	-2.88665395	-1.66661041	0.02386960
H	0.00000000	0.00000000	-4.28732422
N	0.00000000	4.99225763	-2.40970174
H	0.00000000	2.67446128	-4.25513013
H	0.00000000	3.33322081	0.02386960
B	0.00000000	0.00000000	-3.08643054
N	-1.40534078	0.81137372	1.20889854
N	-1.24270133	0.71747386	2.53335988
N	0.00000000	-1.62274743	1.20889854
N	0.00000000	-1.43494772	2.53335988
N	1.40534078	0.81137372	1.20889854
N	1.24270133	0.71747386	2.53335988
C	-2.55022105	1.47237061	0.98583234
C	-3.15005563	1.81868536	2.20959336
C	-2.27254587	1.31205477	3.17357439
C	0.00000000	-2.94474121	0.98583234
C	0.00000000	-3.63737126	2.20959336
C	0.00000000	-2.62411007	3.17357439
C	2.55022105	1.47237061	0.98583234
C	3.15005563	1.81868536	2.20959336
C	2.27254587	1.31205477	3.17357439
N	-4.32342204	2.49612908	2.40970174
H	-2.31615167	1.33723091	4.25513013
N	0.00000000	-4.99225763	2.40970174
H	0.00000000	-3.33322081	-0.02386960
H	0.00000000	-2.67446128	4.25513013
H	-2.88665395	1.66661041	-0.02386960
H	0.00000000	0.00000000	4.28732422
N	4.32342204	2.49612908	2.40970174
H	2.31615167	1.33723091	4.25513013
H	2.88665395	1.66661041	-0.02386960
B	0.00000000	0.00000000	3.08643054
H	-4.66048043	-2.69072978	-3.33379603
H	-4.87382935	-2.81390690	-1.63414962
H	4.66048043	-2.69072978	-3.33379603
H	4.87382935	-2.81390690	-1.63414962
H	0.00000000	5.38145956	-3.33379603
H	0.00000000	5.62781380	-1.63414962
H	-4.66048043	2.69072978	3.33379603
H	-4.87382935	2.81390690	1.63414962
H	0.00000000	-5.38145956	3.33379603
H	0.00000000	-5.62781380	1.63414962
H	4.66048043	2.69072978	3.33379603
H	4.87382935	2.81390690	1.63414962

$[Co(Tb^{4NH2})_2]^+$ $^1A_{1g}$ D_{3d}

Co	0.00000000	0.00000000	0.00000000
N	-1.35981990	-0.78509213	-1.13240015
N	-1.23095095	-0.71068981	-2.45715041
N	1.35981990	-0.78509213	-1.13240015
N	1.23095095	-0.71068981	-2.45715041
N	0.00000000	1.57018479	-1.13240015
N	0.00000000	1.42137961	-2.45715041
C	-2.50012331	-1.44344684	-0.86028187
C	-3.13070944	-1.80751602	-2.06221908
C	-2.28135403	-1.31714016	-3.05562924
C	2.50012331	-1.44344684	-0.86028187
C	3.13070944	-1.80751602	-2.06221908
C	2.28135403	-1.31714016	-3.05562924
C	0.00000000	2.88689420	-0.86028187
C	0.00000000	3.61503151	-2.06221908
C	0.00000000	2.63428086	-3.05562924
N	-4.31042122	-2.48862270	-2.21504124
H	-2.35092390	-1.35730630	-4.13509844
N	4.31042122	-2.48862270	-2.21504124
H	2.80836006	-1.62140756	0.16027668
H	2.35092390	-1.35730630	-4.13509844
H	-2.80836006	-1.62140756	0.16027668
H	0.00000000	0.00000000	-4.23206171
N	0.00000000	4.97724593	-2.21504124
H	0.00000000	2.71461314	-4.13509844
H	0.00000000	3.24281458	0.16027668
B	0.00000000	0.00000000	-3.03360489
N	-1.35981990	0.78509213	1.13240015
N	-1.23095095	0.71068981	2.45715041
N	0.00000000	-1.57018479	1.13240015
N	0.00000000	-1.42137961	2.45715041
N	1.35981990	0.78509213	1.13240015
N	1.23095095	0.71068981	2.45715041
C	-2.50012331	1.44344684	0.86028187
C	-3.13070944	1.80751602	2.06221908
C	-2.28135403	1.31714016	3.05562924
C	0.00000000	-2.88689420	0.86028187
C	0.00000000	-3.61503151	2.06221908
C	0.00000000	-2.63428086	3.05562924
C	2.50012331	1.44344684	0.86028187
C	3.13070944	1.80751602	2.06221908
C	2.28135403	1.31714016	3.05562924
N	-4.31042122	2.48862270	2.21504124
H	-2.35092390	1.35730630	4.13509844
N	0.00000000	-4.97724593	2.21504124
H	0.00000000	-3.24281458	-0.16027668
H	0.00000000	-2.71461314	4.13509844
H	-2.80836006	1.62140756	-0.16027668
H	0.00000000	0.00000000	4.23206171
N	4.31042122	2.48862270	2.21504124
H	2.35092390	1.35730630	4.13509844
H	2.80836006	1.62140756	-0.16027668
B	0.00000000	0.00000000	3.03360489
H	-4.67332303	-2.69814408	-3.12544783
H	-4.83744207	-2.79289856	-1.41877712
H	4.67332303	-2.69814408	-3.12544783
H	4.83744207	-2.79289856	-1.41877712
H	0.00000000	5.39628817	-3.12544783
H	0.00000000	5.58579659	-1.41877712
H	-4.67332303	2.69814408	3.12544783
H	-4.83744207	2.79289856	1.41877712
H	0.00000000	-5.39628817	3.12544783
H	0.00000000	-5.58579659	1.41877712
H	4.67332303	2.69814408	3.12544783
H	4.83744207	2.79289856	1.41877712

$[Co(Tb^{4NO2})_2]^+$ $^5A_{1g}$ D_{3d}

Co	0.00000000	0.00000000	0.00000000
N	-1.43748883	-0.82993461	-1.27588339
N	-1.24841380	-0.72077222	-2.61456795
N	1.43748883	-0.82993461	-1.27588339
N	1.24841380	-0.72077222	-2.61456795
N	0.00000000	1.65986922	-1.27588339
N	0.00000000	1.44154444	-2.61456795
C	-2.58312582	-1.49136860	-1.08374760
C	-3.13112114	-1.80775362	-2.32281348
C	-2.25391301	-1.30129766	-3.27710368
C	2.58312582	-1.49136860	-1.08374760
C	3.13112114	-1.80775362	-2.32281348
C	2.25391301	-1.30129766	-3.27710368
C	0.00000000	2.98273667	-1.08374760
C	0.00000000	3.61550724	-2.32281348
C	0.00000000	2.60259478	-3.27710368
N	-4.36184825	-2.51831431	-2.57526013
H	-2.30155272	-1.32880217	-4.35796462
N	4.36184825	-2.51831431	-2.57526013
H	2.96446788	-1.71153650	-0.09612346
H	2.30155272	-1.32880217	-4.35796462
H	-2.96446788	-1.71153650	-0.09612346
H	0.00000000	0.00000000	-4.35600666
N	0.00000000	5.03662862	-2.57526013
H	0.00000000	2.65760434	-4.35796462
H	0.00000000	3.42307246	-0.09612346
B	0.00000000	0.00000000	-3.15950938
N	-1.43748883	0.82993461	1.27588339
N	-1.24841380	0.72077222	2.61456795
N	0.00000000	-1.65986922	1.27588339
N	0.00000000	-1.44154444	2.61456795
N	1.43748883	0.82993461	1.27588339
N	1.24841380	0.72077222	2.61456795
C	-2.58312582	1.49136860	1.08374760
C	-3.13112114	1.80775362	2.32281348
C	-2.25391301	1.30129766	3.27710368
C	0.00000000	-2.98273667	1.08374760
C	0.00000000	-3.61550724	2.32281348
C	0.00000000	-2.60259478	3.27710368
C	2.58312582	1.49136860	1.08374760
C	3.13112114	1.80775362	2.32281348
C	2.25391301	1.30129766	3.27710368
N	-4.36184825	2.51831431	2.57526013
H	-2.30155272	1.32880217	4.35796462
N	0.00000000	-5.03662862	2.57526013
H	0.00000000	-3.42307246	0.09612346
H	0.00000000	-2.65760434	4.35796462
H	-2.96446788	1.71153650	0.09612346
H	0.00000000	0.00000000	4.35600666
N	4.36184825	2.51831431	2.57526013
H	2.30155272	1.32880217	4.35796462
H	2.96446788	1.71153650	0.09612346

B	0.00000000	0.00000000	3.15950938
O	-4.66073497	-2.69087636	-3.75017809
O	-4.99486277	-2.88378528	-1.59450154
O	4.66073497	-2.69087636	-3.75017809
O	4.99486277	-2.88378528	-1.59450154
O	0.00000000	5.38175273	-3.75017809
O	0.00000000	5.76757057	-1.59450154
O	-4.66073497	2.69087636	3.75017809
O	-4.99486277	2.88378528	1.59450154
O	0.00000000	-5.38175273	3.75017809
O	0.00000000	-5.76757057	1.59450154
O	4.66073497	2.69087636	3.75017809
O	4.99486277	2.88378528	1.59450154

$[Co(Tb^{4NO2})_2]^+$ ^3E_g D_{3d}

Co	0.00000000	0.00000000	0.00000000
N	-1.40227632	-0.80960468	-1.21385059
N	-1.24032956	-0.71610435	-2.55470900
N	1.40227632	-0.80960468	-1.21385059
N	1.24032956	-0.71610435	-2.55470900
N	0.00000000	1.61920935	-1.21385059
N	0.00000000	1.43220923	-2.55470900
C	-2.54074825	-1.46690209	-0.98336955
C	-3.11409486	-1.79792362	-2.20965792
C	-2.26045999	-1.30507704	-3.18840352
C	2.54074825	-1.46690209	-0.98336955
C	3.11409486	-1.79792362	-2.20965792
C	2.26045999	-1.30507704	-3.18840352
C	0.00000000	2.93380365	-0.98336955
C	0.00000000	3.59584725	-2.20965792
C	0.00000000	2.61015408	-3.18840352
N	-4.35017248	-2.51157312	-2.42391226
H	-2.32951445	-1.34494578	-4.26764888
N	4.35017248	-2.51157312	-2.42391226
H	2.90034006	-1.67451208	0.01457460
H	2.32951445	-1.34494578	-4.26764888
H	-2.90034006	-1.67451208	0.01457460
H	0.00000000	0.00000000	-4.31154360
N	0.00000000	5.02314624	-2.42391226
H	0.00000000	2.68989156	-4.26764888
H	0.00000000	3.34902416	0.01457460
B	0.00000000	0.00000000	-3.11590571
N	-1.40227632	0.80960468	1.21385059
N	-1.24032956	0.71610435	2.55470900
N	0.00000000	-1.61920935	1.21385059
N	0.00000000	-1.43220923	2.55470900
N	1.40227632	0.80960468	1.21385059
N	1.24032956	0.71610435	2.55470900
C	-2.54074825	1.46690209	0.98336955
C	-3.11409486	1.79792362	2.20965792
C	-2.26045999	1.30507704	3.18840352
C	0.00000000	-2.93380365	0.98336955
C	0.00000000	-3.59584725	2.20965792
C	0.00000000	-2.61015408	3.18840352
C	2.54074825	1.46690209	0.98336955
C	3.11409486	1.79792362	2.20965792
C	2.26045999	1.30507704	3.18840352
N	-4.35017248	2.51157312	2.42391226
H	-2.32951445	1.34494578	4.26764888
N	0.00000000	-5.02314624	2.42391226
H	0.00000000	-3.34902416	-0.01457460
H	0.00000000	-2.68989156	4.26764888
H	-2.90034006	1.67451208	-0.01457460
H	0.00000000	0.00000000	4.31154360
N	4.35017248	2.51157312	2.42391226
H	2.32951445	1.34494578	4.26764888
H	2.90034006	1.67451208	-0.01457460
B	0.00000000	0.00000000	3.11590571
O	-4.67536566	-2.69932362	-3.58913675
O	-4.96030221	-2.86383213	-1.42411758
O	4.67536566	-2.69932362	-3.58913675
O	4.96030221	-2.86383213	-1.42411758
O	0.00000000	5.39864724	-3.58913675
O	0.00000000	5.72766372	-1.42411758
O	-4.67536566	2.69932362	3.58913675
O	-4.96030221	2.86383213	1.42411758
O	0.00000000	-5.39864724	3.58913675
O	0.00000000	-5.72766372	1.42411758
O	4.67536566	2.69932362	3.58913675
O	4.96030221	2.86383213	1.42411758

$[Co(Tb^{4NO2})_2]^+$ $^1A_{1g}$ D_{3d}

Co	0.00000000	0.00000000	0.00000000
N	-1.36079147	-0.78565359	-1.13259119
N	-1.23016459	-0.71023577	-2.47633468
N	1.36079147	-0.78565359	-1.13259119
N	1.23016459	-0.71023577	-2.47633468
N	0.00000000	1.57130664	-1.13259119
N	0.00000000	1.42047155	-2.47633468
C	-2.49207770	-1.43880172	-0.86158417
C	-3.09333894	-1.78593988	-2.07119023
C	-2.26655082	-1.30859395	-3.07570252
C	2.49207770	-1.43880172	-0.86158417
C	3.09333894	-1.78593988	-2.07119023
C	2.26655082	-1.30859395	-3.07570252
C	0.00000000	2.87760343	-0.86158417
C	0.00000000	3.57187975	-2.07119023
C	0.00000000	2.61718737	-3.07570252
N	-4.33559576	-2.50315761	-2.24484133
H	-2.35951033	-1.36226417	-4.15243111
N	4.33559576	-2.50315761	-2.24484133
H	2.82998965	-1.63389508	0.14564016
H	2.35951033	-1.36226417	-4.15243111
H	-2.82998965	-1.63389508	0.14564016
H	0.00000000	0.00000000	-4.25156771
N	0.00000000	5.00631470	-2.24484133
H	0.00000000	2.72452780	-4.15243111
H	0.00000000	3.26779069	0.14564016
B	0.00000000	0.00000000	-3.05727710
N	-1.36079147	0.78565359	1.13259119
N	-1.23016459	0.71023577	2.47633468
N	0.00000000	-1.57130664	1.13259119
N	0.00000000	-1.42047155	2.47633468
N	1.36079147	0.78565359	1.13259119
N	1.23016459	0.71023577	2.47633468
C	-2.49207770	1.43880172	0.86158417
C	-3.09333894	1.78593988	2.07119023
C	-2.26655082	1.30859395	3.07570252

C	0.00000000	-2.87760343	0.86158417
C	0.00000000	-3.57187975	2.07119023
C	0.00000000	-2.61718737	3.07570252
C	2.49207770	1.43880172	0.86158417
C	3.09333894	1.78593988	2.07119023
C	2.26655082	1.30859395	3.07570252
N	-4.33559576	2.50315761	2.24484133
H	-2.35951033	1.36226417	4.15243111
N	0.00000000	-5.00631470	2.24484133
H	0.00000000	-3.26779069	-0.14564016
H	0.00000000	-2.72452780	4.15243111
H	-2.82998965	1.63389508	-0.14564016
H	0.00000000	0.00000000	4.25156771
N	4.33559576	2.50315761	2.24484133
H	2.35951033	1.36226417	4.15243111
H	2.82998965	1.63389508	-0.14564016
B	0.00000000	0.00000000	3.05727710
O	-4.68789922	-2.70655959	-3.39832496
O	-4.91937775	-2.84020436	-1.22428490
O	4.68789922	-2.70655959	-3.39832496
O	4.91937775	-2.84020436	-1.22428490
O	0.00000000	5.41311971	-3.39832496
O	0.00000000	5.68040819	-1.22428490
O	-4.68789922	2.70655959	3.39832496
O	-4.91937775	2.84020436	1.22428490
O	0.00000000	-5.41311971	3.39832496
O	0.00000000	-5.68040819	1.22428490
O	4.68789922	2.70655959	3.39832496
O	4.91937775	2.84020436	1.22428490

$[Co(Tb^{4NH2})_2]$ ^4E_g D_{3d}

[Co	0.00000000	0.00000000	0.00000000
N	-1.45988414	-0.84286453	-1.33428974
N	-1.25532803	-0.72476433	-2.64895706
N	1.45988414	-0.84286453	-1.33428974
N	1.25532803	-0.72476433	-2.64895706
N	0.00000000	1.68572905	-1.33428974
N	0.00000000	1.44952814	-2.64895706
C	-2.61261899	-1.50839646	-1.17314574
C	-3.17236204	-1.83156395	-2.42108910
C	-2.26559778	-1.30804361	-3.34052399
C	2.61261899	-1.50839646	-1.17314574
C	3.17236204	-1.83156395	-2.42108910
C	2.26559778	-1.30804361	-3.34052399
C	0.00000000	3.01679293	-1.17314574
C	0.00000000	3.66312790	-2.42108910
C	0.00000000	2.61608721	-3.34052399
N	-4.34817219	-2.51041845	-2.66811380
H	-2.27131448	-1.31134409	-4.42351592
N	4.34817219	-2.51041845	-2.66811380
H	2.98388604	-1.72274765	-0.17853329
H	2.27131448	-1.31134409	-4.42351592
H	-2.98388604	-1.72274765	-0.17853329
H	0.00000000	0.00000000	-4.37880626
N	0.00000000	5.02083691	-2.66811380
H	0.00000000	2.62268817	-4.42351592
H	0.00000000	3.44549476	-0.17853329
B	0.00000000	0.00000000	-3.17226785
N	-1.45988414	0.84286453	1.33428974
N	-1.25532803	0.72476433	2.64895706
N	0.00000000	-1.68572905	1.33428974
N	0.00000000	-1.44952814	2.64895706
N	1.45988414	0.84286453	1.33428974
N	1.25532803	0.72476433	2.64895706
C	-2.61261899	1.50839646	1.17314574
C	-3.17236204	1.83156395	2.42108910
C	-2.26559778	1.30804361	3.34052399
C	0.00000000	-3.01679293	1.17314574
C	0.00000000	-3.66312790	2.42108910
C	0.00000000	-2.61608721	3.34052399
C	2.61261899	1.50839646	1.17314574
C	3.17236204	1.83156395	2.42108910
C	2.26559778	1.30804361	3.34052399
N	-4.34817219	2.51041845	2.66811380
H	-2.27131448	1.31134409	4.42351592
N	0.00000000	-5.02083691	2.66811380
H	0.00000000	-3.44549476	0.17853329
H	0.00000000	-2.62268817	4.42351592
H	-2.98388604	1.72274765	0.17853329
H	0.00000000	0.00000000	4.37880626
N	4.34817219	2.51041845	2.66811380
H	2.27131448	1.31134409	4.42351592
H	2.98388604	1.72274765	0.17853329
B	0.00000000	0.00000000	3.17226785
H	-4.65861614	-2.68965343	-3.60304141
H	-4.91676627	-2.83869621	-1.91194121
H	4.65861614	-2.68965343	-3.60304141
H	4.91676627	-2.83869621	-1.91194121
H	0.00000000	5.37930634	-3.60304141
H	0.00000000	5.67739241	-1.91194121
H	-4.65861614	2.68965343	3.60304141
H	-4.91676627	2.83869621	1.91194121
H	0.00000000	-5.37930634	3.60304141
H	0.00000000	-5.67739241	1.91194121
H	4.65861614	2.68965343	3.60304141
H	4.91676627	2.83869621	1.91194121

$Co(Tb^{4NH2})_2]$ ^2E_g D_{3d}

Co	0.00000000	0.00000000	0.00000000
N	-1.45597669	-0.84060864	-1.31977652
N	-1.25246624	-0.72311171	-2.65479388
N	1.45597669	-0.84060864	-1.31977652
N	1.25246624	-0.72311171	-2.65479388
N	0.00000000	1.68121729	-1.31977652
N	0.00000000	1.44622343	-2.65479388
C	-2.59865611	-1.50033498	-1.15277771
C	-3.13593824	-1.81053498	-2.40638538
C	-2.24756500	-1.29763257	-3.34073619
C	2.59865611	-1.50033498	-1.15277771
C	3.13593824	-1.81053498	-2.40638538
C	2.24756500	-1.29763257	-3.34073619
C	0.00000000	3.00066942	-1.15277771
C	0.00000000	3.62106995	-2.40638538
C	0.00000000	2.59526462	-3.34073619
N	-4.35501022	-2.51436612	-2.68213912
H	-2.27599293	-1.31404501	-4.42138968
N	4.35501022	-2.51436612	-2.68213912
H	2.99045472	-1.72653973	-0.17081842

H	2.27599293	-1.31404501	-4.42138968
H	-2.99045472	-1.72653973	-0.17081842
H	0.00000000	0.00000000	-4.38591735
N	0.00000000	5.02873276	-2.68213912
H	0.00000000	2.62809054	-4.42138968
H	0.00000000	3.45307999	-0.17081842
B	0.00000000	0.00000000	-3.18574493
N	-1.45597669	0.84060864	1.31977652
N	-1.25246624	0.72311171	2.65479388
N	0.00000000	-1.68121729	1.31977652
N	0.00000000	-1.44622343	2.65479388
N	1.45597669	0.84060864	1.31977652
N	1.25246624	0.72311171	2.65479388
C	-2.59865611	1.50033498	1.15277771
C	-3.13593824	1.81053498	2.40638538
C	-2.24756500	1.29763257	3.34073619
C	0.00000000	-3.00066942	1.15277771
C	0.00000000	-3.62106995	2.40638538
C	0.00000000	-2.59526462	3.34073619
C	2.59865611	1.50033498	1.15277771
C	3.13593824	1.81053498	2.40638538
C	2.24756500	1.29763257	3.34073619
N	-4.35501022	2.51436612	2.68213912
H	-2.27599293	1.31404501	4.42138968
N	0.00000000	-5.02873276	2.68213912
H	0.00000000	-3.45307999	0.17081842
H	0.00000000	-2.62809054	4.42138968
H	-2.99045472	1.72653973	0.17081842
H	0.00000000	0.00000000	4.38591735
N	4.35501022	2.51436612	2.68213912
H	2.27599293	1.31404501	4.42138968
H	2.99045472	1.72653973	0.17081842
B	0.00000000	0.00000000	3.18574493
O	-4.64709172	-2.68299956	-3.86334317
O	-5.01072539	-2.89294375	-1.71643350
O	4.64709172	-2.68299956	-3.86334317
O	5.01072539	-2.89294375	-1.71643350
O	0.00000000	5.36599912	-3.86334317
O	0.00000000	5.78588751	-1.71643350
O	-4.64709172	2.68299956	3.86334317
O	-5.01072539	2.89294375	1.71643350
O	0.00000000	-5.36599912	3.86334317
O	0.00000000	-5.78588751	1.71643350
O	4.64709172	2.68299956	3.86334317
O	5.01072539	2.89294375	1.71643350

$[Co(Tb^{4NO2})_2]$ ^4E_g D_{3d}

Co	0.00000000	0.00000000	0.00000000
N	-1.45597669	-0.84060864	-1.31977652
N	-1.25246624	-0.72311171	-2.65479388
N	1.45597669	-0.84060864	-1.31977652
N	1.25246624	-0.72311171	-2.65479388
N	0.00000000	1.68121729	-1.31977652
N	0.00000000	1.44622343	-2.65479388
C	-2.59865611	-1.50033498	-1.15277771
C	-3.13593824	-1.81053498	-2.40638538
C	-2.24756500	-1.29763257	-3.34073619
C	2.59865611	-1.50033498	-1.15277771
C	3.13593824	-1.81053498	-2.40638538
C	2.24756500	-1.29763257	-3.34073619
C	0.00000000	3.00066942	-1.15277771
C	0.00000000	3.62106995	-2.40638538
C	0.00000000	2.59526462	-3.34073619
N	-4.35501022	-2.51436612	-2.68213912
H	-2.27599293	-1.31404501	-4.42138968
N	4.35501022	-2.51436612	-2.68213912
H	2.99045472	-1.72653973	-0.17081842
H	2.27599293	-1.31404501	-4.42138968
H	-2.99045472	-1.72653973	-0.17081842
H	0.00000000	0.00000000	-4.38591735
N	0.00000000	5.02873276	-2.68213912
H	0.00000000	2.62809054	-4.42138968
H	0.00000000	3.45307999	-0.17081842
B	0.00000000	0.00000000	-3.18574493
N	-1.45597669	0.84060864	1.31977652
N	-1.25246624	0.72311171	2.65479388
N	0.00000000	-1.68121729	1.31977652
N	0.00000000	-1.44622343	2.65479388
N	1.45597669	0.84060864	1.31977652
N	1.25246624	0.72311171	2.65479388
C	-2.59865611	1.50033498	1.15277771
C	-3.13593824	1.81053498	2.40638538
C	-2.24756500	1.29763257	3.34073619
C	0.00000000	-3.00066942	1.15277771
C	0.00000000	-3.62106995	2.40638538
C	0.00000000	-2.59526462	3.34073619
C	2.59865611	1.50033498	1.15277771
C	3.13593824	1.81053498	2.40638538
C	2.24756500	1.29763257	3.34073619
N	-4.35501022	2.51436612	2.68213912
H	-2.27599293	1.31404501	4.42138968
N	0.00000000	-5.02873276	2.68213912
H	0.00000000	-3.45307999	0.17081842
H	0.00000000	-2.62809054	4.42138968
H	-2.99045472	1.72653973	0.17081842
H	0.00000000	0.00000000	4.38591735
N	4.35501022	2.51436612	2.68213912
H	2.27599293	1.31404501	4.42138968
H	2.99045472	1.72653973	0.17081842
B	0.00000000	0.00000000	3.18574493
O	-4.64709172	-2.68299956	-3.86334317
O	-5.01072539	-2.89294375	-1.71643350
O	4.64709172	-2.68299956	-3.86334317
O	5.01072539	-2.89294375	-1.71643350
O	0.00000000	5.36599912	-3.86334317
O	0.00000000	5.78588751	-1.71643350
O	-4.64709172	2.68299956	3.86334317
O	-5.01072539	2.89294375	1.71643350
O	0.00000000	-5.36599912	3.86334317
O	0.00000000	-5.78588751	1.71643350
O	4.64709172	2.68299956	3.86334317
O	5.01072539	2.89294375	1.71643350

$[Co(Tb^{4NO2})_2]$ ^2E_g D_{3d}

Co	0.00000000	0.00000000	0.00000000
N	-1.40661451	-0.81210927	-1.21422736
N	-1.24201075	-0.71707539	-2.55545144
N	1.40661451	-0.81210927	-1.21422736

N	1.24201075	-0.71707539	-2.55545144
N	0.00000000	1.62421855	-1.21422736
N	0.00000000	1.43415025	-2.55545144
C	-2.54310362	-1.46826154	-0.99899563
C	-3.11559138	-1.79878724	-2.23306978
C	-2.25690128	-1.30302224	-3.20211979
C	2.54310362	-1.46826154	-0.99899563
C	3.11559138	-1.79878724	-2.23306978
C	2.25690128	-1.30302224	-3.20211979
C	0.00000000	2.93652362	-0.99899563
C	0.00000000	3.59757501	-2.23306978
C	0.00000000	2.60604502	-3.20211979
N	-4.34181042	-2.50674544	-2.46103987
H	-2.31577807	-1.33701500	-4.28111062
N	4.34181042	-2.50674544	-2.46103987
H	2.90508308	-1.67725057	-0.00262313
H	2.31577807	-1.33701500	-4.28111062
H	-2.90508308	-1.67725057	-0.00262313
H	0.00000000	0.00000000	-4.30732077
N	0.00000000	5.01349087	-2.46103987
H	0.00000000	2.67403053	-4.28111062
H	0.00000000	3.35450115	-0.00262313
B	0.00000000	0.00000000	-3.10804213
N	-1.40661451	0.81210927	1.21422736
N	-1.24201075	0.71707539	2.55545144
N	0.00000000	-1.62421855	1.21422736
N	0.00000000	-1.43415025	2.55545144
N	1.40661451	0.81210927	1.21422736
N	1.24201075	0.71707539	2.55545144
C	-2.54310362	1.46826154	0.99899563
C	-3.11559138	1.79878724	2.23306978
C	-2.25690128	1.30302224	3.20211979
C	0.00000000	-2.93652362	0.99899563
C	0.00000000	-3.59757501	2.23306978
C	0.00000000	-2.60604502	3.20211979
C	2.54310362	1.46826154	0.99899563
C	3.11559138	1.79878724	2.23306978
C	2.25690128	1.30302224	3.20211979
N	-4.34181042	2.50674544	2.46103987
H	-2.31577807	1.33701500	4.28111062
N	0.00000000	-5.01349087	2.46103987
H	0.00000000	-3.35450115	0.00262313
H	0.00000000	-2.67403053	4.28111062
H	-2.90508308	1.67725057	0.00262313
H	0.00000000	0.00000000	4.30732077
N	4.34181042	2.50674544	2.46103987
H	2.31577807	1.33701500	4.28111062
H	2.90508308	1.67725057	0.00262313
B	0.00000000	0.00000000	3.10804213
O	-4.66840486	-2.69530505	-3.63015381
O	-4.96863357	-2.86864182	-1.47010361
O	4.66840486	-2.69530505	-3.63015381
O	4.96863357	-2.86864182	-1.47010361
O	0.00000000	5.39060957	-3.63015381
O	0.00000000	5.73728416	-1.47010361
O	-4.66840486	2.69530505	3.63015381
O	-4.96863357	2.86864182	1.47010361
O	0.00000000	-5.39060957	3.63015381
O	0.00000000	-5.73728416	1.47010361
O	4.66840486	2.69530505	3.63015381
O	4.96863357	2.86864182	1.47010361