Supplementary data for article:

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Supporting Information for

Computational study of the spin-state energies and UV-Vis spectra of bis(1,4,7-triazacyclononane) complexes of some first-row transition metal cations†

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Table S1 M-N bond lengths from geometry optimizations at different level of theory (LDA, OPBE and SSB-D) and comparison with experimental data

M^{n+}	d^n	Symm.	Spin state	State	LDA	OPBE	SSB-D	exp.	Ref. code
Cr^{3+}	d^3	D_3	HS	$^4A_2$	2.076	2.137	2.111		
			LS	$^2A_2$	2.061	2.109	2.095		
Mn^{2+}	d^5	D_3	HS	$^6A_1$	2.250	2.344	2.313	2.278[a]	CEXNUP[1]
			IS	^4E	2.124	2.210	2.192		
			LS	^2E	2.018	2.077	2.079		
		C_2	IS	^4B	2.052/2.310[c]	2.112/2.443[c]	2.119/2.373[c]		
			LS	^2A	2.020[b]	2.080[b]	2.085[b]		
Fe^{3+}	d^5	D_3	HS	$^6A_1$	2.162	2.233	2.189		
			IS	^4E	2.075	2.149	2.121		
			LS	^2E	1.981	2.032	2.023	2.005[a]	DETTUR[2]
		C_2	IS	^4B	2.015/2.205[c]	2.079/2.283[c]	2.066/2.225[c]		
			LS	^2A	1.983[b]	2.034[b]	2.026[b]		
Fe^{2+}	d^6	D_3	HS	^5E	2.171	2.258	2.236		
			IS	^3E	2.084	2.167	2.154		
			LS	$^1A_1$	1.975	2.029	2.036	2.034[a]	DETTOL[2]
		C_2	HS	^5B	2.185[b]	2.277[b]	2.249[b]		
			IS	^3B	1.971/2.125[d]	2.025/2.229[d]	2.031/2.203[d]		
Co^{3+}	d^6	D_3	HS	$^5A_1$	2.128	2.200	2.164		
			IS	^3E	1.992	2.114	2.097		
			LS	$^1A_1$	1.951	1.997	1.993	1.977[a]	XACPAS[3]
		C_2	IS	^3B	1.951/2.092[c]	2.001/2.161[c]	1.994/2.132[c]		
Co^{2+}	d^7	D_3	HS	^4E	2.126	2.211	2.190		
			LS	^2E	2.032	2.103	2.102		
		C_2	HS	^4B	2.129[b]	2.215[b]	2.195[b]	2.161[a]	DOTZUH[4]
			LS	^2A	1.958/2.204[c]	2.016/2.324[c]	2.021/2.276[c]		
Ni^{3+}	d^7	D_3	HS	^4E	2.109	2.191	2.150		
			LS	^2E	2.013	2.078	2.063		
		C_2	HS	^4B	2.111[b]	2.190[b]	2.149[b]		
			LS	^2A	1.952/2.148[c]	2.007/2.231[c]	2.002/2.173[c]	1.971/2.109[c]	DORTIN[5]

[a] Average of six similar bond lengths.

[b] Average of three pairs of similar bond lengths.

[c] Elongated octahedron – four short and two long bond distances

[d] Compressed octahedron – four long and two short bond lengths

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Cartesian coordinates (Å)

49
Cr^3+ ^4A D_3 LDA

Cr	0.000000	0.000000	0.000000
N	0.025587	-1.573381	1.353695
N	-1.375382	0.764532	1.353695
N	1.349795	0.808849	1.353695
C	1.085392	-1.376493	2.384648
C	2.080116	-0.345504	1.925793
C	0.649382	1.628224	2.384648
C	-0.740843	1.974185	1.925793
C	-1.339273	-1.628681	1.925793
C	-1.734774	-0.251731	2.384648
H	1.589945	-2.328759	2.616826
H	-0.728747	2.753771	1.143506
H	-1.336512	2.384791	2.761678
H	-2.242989	1.062796	0.884846
H	2.749209	-0.745772	1.143506
H	0.595598	-1.059298	3.319919
H	-2.811737	-0.212553	2.616826
H	1.221792	2.541312	2.616826
H	0.201086	-2.473884	0.884846
H	-1.215178	0.013846	3.319919
H	2.733546	-0.034942	2.761678
H	2.041903	1.411088	0.884846
H	-1.397034	-2.349849	2.761678
H	0.619580	1.045452	3.319919
H	-2.020462	-2.007999	1.143506
N	-1.375382	-0.764532	-1.353695
N	1.349795	-0.808849	-1.353695
N	0.025587	1.573381	-1.353695
C	-1.734774	0.251731	-2.384648
C	-0.740843	-1.974185	-1.925793
H	-2.242989	-1.062796	-0.884846
C	2.080116	0.345504	-1.925793
C	0.649382	-1.628224	-2.384648
H	2.041903	-1.411088	-0.884846
C	-1.339273	1.628681	-1.925793
C	1.085392	1.376493	-2.384648
H	0.201086	2.473884	-0.884846
H	-2.811737	0.212553	-2.616826
H	-1.215178	-0.013846	-3.319919
H	-1.336512	-2.384791	-2.761678
H	-0.728747	-2.753771	-1.143506
H	2.749209	0.745772	-1.143506
H	2.733546	0.034942	-2.761678
H	1.221792	-2.541312	-2.616826
H	0.619580	-1.045452	-3.319919
H	-2.020462	2.007999	-1.143506
H	-1.397034	2.349849	-2.761678
H	1.589945	2.328759	-2.616826
H	0.595598	1.059298	-3.319919

49
Cr^3+ ^2A D_3 LDA

Cr	0.000000	0.000000	0.000000
N	-0.040200	1.566100	1.339200
N	1.376400	-0.748200	1.339200
N	-1.336200	-0.817900	1.339200
C	-1.099100	1.366500	2.372300
C	-2.083100	0.325900	1.913400
C	-0.633900	-1.635100	2.372300
C	0.759300	-1.967000	1.913400
C	1.323800	1.641000	1.913400
C	1.733000	0.268500	2.372300
H	-1.610400	2.316000	2.601000
H	0.756800	-2.747300	1.131800
H	1.361800	-2.368200	2.749000
H	2.246600	-1.038200	0.868400
H	-2.757600	0.718300	1.131800
H	-0.606400	1.055600	3.308100
H	2.810900	0.236600	2.601000
H	-1.200500	-2.552600	2.601000
H	-0.224200	2.464700	0.868400
H	1.217400	-0.002600	3.308100
H	-2.731900	0.004800	2.749000
H	-2.022400	-1.426500	0.868400
H	1.370100	2.363500	2.749000
H	-0.611000	-1.053000	3.308100
H	2.000800	2.029000	1.131800
N	1.376400	0.748200	-1.339200
N	-1.336200	0.817900	-1.339200
N	-0.040200	-1.566100	-1.339200
C	1.733000	-0.268500	-2.372300
C	0.759300	1.967000	-1.913400
H	2.246600	1.038200	-0.868400
C	-2.083100	-0.325900	-1.913400
C	-0.633900	1.635100	-2.372300
H	-2.022400	1.426500	-0.868400
C	1.323800	-1.641000	-1.913400
C	-1.099100	-1.366500	-2.372300
H	-0.224200	-2.464700	-0.868400
H	2.810900	-0.236600	-2.601000
H	1.217400	0.002600	-3.308100
H	1.361800	2.368200	-2.749000
H	0.756800	2.747300	-1.131800
H	-2.757600	-0.718300	-1.131800
H	-2.731900	-0.004800	-2.749000
H	-1.200500	2.552600	-2.601000
H	-0.611000	1.053000	-3.308100
H	2.000800	-2.029000	-1.131800
H	1.370100	-2.363500	-2.749000
H	-1.610400	-2.316000	-2.601000
H	-0.606400	-1.055600	-3.308100

49
Cr^3+ ^2A D_3 OPBE

Cr	0.000000	0.000000	0.000000
N	0.040600	-1.577900	1.399700
N	-1.386800	0.753800	1.399700
N	1.346200	0.824100	1.399700
C	1.120400	-1.390600	2.429300
C	2.096600	-0.320900	1.989000
C	0.644100	1.665600	2.429300
C	-0.770400	1.976200	1.989000
C	-1.326200	-1.655300	1.989000
C	-1.764500	-0.275000	2.429300
H	1.646600	-2.336300	2.603500
H	-0.792100	2.762800	1.226700
H	-1.363500	2.351600	2.834000
H	-2.253500	1.054200	0.954300
H	2.788700	-0.695400	1.226700
H	0.649700	-1.126400	3.380200
H	-2.846600	-0.257800	2.603500
H	1.200000	2.594200	2.603500
H	0.213700	-2.478700	0.954300
H	-1.300300	0.000600	3.380200
H	2.718300	0.005000	2.834000
H	2.039700	1.424400	0.954300
H	-1.354800	-2.356600	2.834000
H	0.650700	1.125800	3.380200
H	-1.996600	-2.067400	1.226700
N	-1.386800	-0.753800	-1.399700
N	1.346200	-0.824100	-1.399700
N	0.040600	1.577900	-1.399700
C	-1.764500	0.275000	-2.429300
C	-0.770400	-1.976200	-1.989000
H	-2.253500	-1.054200	-0.954300
C	2.096600	0.320900	-1.989000
C	0.644100	-1.665600	-2.429300
H	2.039700	-1.424400	-0.954300
C	-1.326200	1.655300	-1.989000
C	1.120400	1.390600	-2.429300
H	0.213700	2.478700	-0.954300

```
H    -2.846600    0.257800   -2.603500
H    -1.300300   -0.000600   -3.380200
H    -1.363500   -2.351600   -2.834000
H    -0.792100   -2.762800   -1.226700
H     2.788700    0.695400   -1.226700
H     2.718300   -0.005000   -2.834000
H     1.200000   -2.594200   -2.603500
H     0.650700   -1.125800   -3.380200
H    -1.996600    2.067400   -1.226700
H    -1.354800    2.356600   -2.834000
H     1.646600    2.336300   -2.603500
H     0.649700    1.126400   -3.380200

 49
Cr^3+ ^4A D_3 OPBE
Cr    0.000000    0.000000    0.000000
N     0.031900   -1.580700    1.438000
N    -1.384900    0.762800    1.438000
N     1.353000    0.818000    1.438000
C     1.111600   -1.396100    2.465100
C     2.094300   -0.333300    2.022300
C     0.653200    1.660700    2.465100
C    -0.758500    1.980400    2.022300
C    -1.335800   -1.647100    2.022300
C    -1.764900   -0.264600    2.465100
H     1.633300   -2.344000    2.641400
H    -0.771900    2.763900    1.256300
H    -1.348600    2.365300    2.865100
H    -2.248600    1.066500    0.989700
H     2.779600   -0.713500    1.256300
H     0.643900   -1.126800    3.416100
H    -2.846600   -0.242500    2.641400
H     1.213300    2.586500    2.641400
H     0.200600   -2.480600    0.989700
H    -1.297800    0.005800    3.416100
H     2.722700   -0.014700    2.865100
H     2.047900    1.414000    0.989700
H    -1.374100   -2.350500    2.865100
H     0.653900    1.121100    3.416100
H    -2.007700   -2.050400    1.256300
N    -1.384900   -0.762800   -1.438000
N     1.353000   -0.818000   -1.438000
N     0.031900    1.580700   -1.438000
C    -1.764900    0.264600   -2.465100
C    -0.758500   -1.980400   -2.022300
H    -2.248600   -1.066500   -0.989700
C     2.094300    0.333300   -2.022300
C     0.653200   -1.660700   -2.465100
H     2.047900   -1.414000   -0.989700
C    -1.335800    1.647100   -2.022300
C     1.111600    1.396100   -2.465100
H     0.200600    2.480600   -0.989700
H    -2.846600    0.242500   -2.641400
H    -1.297800   -0.005800   -3.416100
H    -1.348600   -2.365300   -2.865100
H    -0.771900   -2.763900   -1.256300
H     2.779600    0.713500   -1.256300
H     2.722700    0.014700   -2.865100
H     1.213300   -2.586500   -2.641400
H     0.653900   -1.121100   -3.416100
H    -2.007700    2.050400   -1.256300
H    -1.374100    2.350500   -2.865100
H     1.633300    2.344000   -2.641400
H     0.643900    1.126800   -3.416100

 49
Cr^3+ ^4A D_3 SSB-D
Cr    0.000000    0.000000    0.000000
N    -0.027298    1.589612    1.388060
N     1.390293   -0.771165    1.388060
N    -1.362995   -0.818447    1.388060
C    -1.092669    1.389457    2.408460
C    -2.084619    0.343343    1.950719
C    -0.656971   -1.641007    2.408460
C     0.744966   -1.977004    1.950719
C     1.339653    1.633661    1.950719
C     1.749640    0.251550    2.408460
H    -1.608663    2.327151    2.609756
H     0.731773   -2.732521    1.164998
H     1.323364   -2.387462    2.780401
H     2.249161   -1.075906    0.946549
H    -2.732319    0.732527    1.164998
H    -0.624771    1.085522    3.341670
H     2.819704    0.229568    2.609756
H    -1.211041   -2.556719    2.609756
H    -0.192819    2.485784    0.946549
H     1.252475   -0.001693    3.341670
H    -2.729285    0.047664    2.780401
H    -2.056342   -1.409878    0.946549
H     1.405921    2.339798    2.780401
H    -0.627704   -1.083829    3.341670
H     2.000547    1.999994    1.164998
N     1.390293    0.771165   -1.388060
N    -1.362995    0.818447   -1.388060
N    -0.027298   -1.589612   -1.388060
C     1.749640   -0.251550   -2.408460
C     0.744966    1.977004   -1.950719
H     2.249161    1.075906   -0.946549
C    -2.084619   -0.343343   -1.950719
C    -0.656971    1.641007   -2.408460
H    -2.056342    1.409878   -0.946549
C     1.339653   -1.633661   -1.950719
C    -1.092669   -1.389457   -2.408460
H    -0.192819   -2.485784   -0.946549
H     2.819704   -0.229568   -2.609756
H     1.252475    0.001693   -3.341670
H     1.323364    2.387462   -2.780401
H     0.731773    2.732521   -1.164998
H    -2.732319   -0.732527   -1.164998
H    -2.729285   -0.047664   -2.780401
H    -1.211041    2.556719   -2.609756
H    -0.627704    1.083829   -3.341670
H     2.000547   -1.999994   -1.164998
H     1.405921   -2.339798   -2.780401
H    -1.608663   -2.327151   -2.609756
H    -0.624771   -1.085522   -3.341670

 49
Cr^3+ ^2A D_3 SSB-D
Cr    0.000000000    0.000000000    0.000000000
N     0.040555789   -1.588299186    1.365819071
N    -1.395785338    0.759027249    1.365819071
N     1.355229549    0.829271937    1.365819071
C     1.105736918   -1.380848718    2.387134034
C     2.088335530   -0.324693149    1.931778558
C     0.642981609    1.648020620    2.387134034
C    -0.762975249    1.970898196    1.931778558
C    -1.325360281   -1.646205046    1.931778558
C    -1.748718528   -0.267171902    2.387134034
H     1.629395118   -2.314656398    2.586330885
H    -0.760803070    2.729104037    1.148746296
H    -1.344955436    2.371109037    2.763917808
H    -2.258189198    1.057724616    0.926504477
H     2.743874961   -0.705677232    1.148746296
H     0.634409770   -1.082804587    3.320528201
H    -2.819248801   -0.253769366    2.586330885
H     1.189853683    2.568425764    2.586330885
H     0.213078211   -2.484511520    0.926504477
H    -1.254941164   -0.008012683    3.320528201
H     2.725918380   -0.020788944    2.763917808
H     2.045110986    1.426786904    0.926504477
H    -1.380962943   -2.350320093    2.763917808
H     0.620531395    1.090817270    3.320528201
H    -1.983071891   -2.023426805    1.148746296
N    -1.395785338   -0.759027249   -1.365819071
N     1.355229549   -0.829271937   -1.365819071
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N 0.040555789 1.588299186 -1.365819071
C -1.748718528 0.267171902 -2.387134034
C -0.762975249 -1.970898196 -1.931778558
H -2.258189198 -1.057724616 -0.926504477
C 2.088335530 0.324693149 -1.931778558
C 0.642981609 -1.648020620 -2.387134034
H 2.045110986 -1.426786904 -0.926504477
C -1.325360281 1.646205046 -1.931778558
C 1.105736918 1.380848718 -2.387134034
H 0.213078211 2.484511520 -0.926504477
H -2.819248801 0.253769366 -2.586330885
H -1.254941164 0.008012683 -3.320528201
H -1.344955436 -2.371109037 -2.763917808
H -0.760803070 -2.729104037 -1.148746296
H 2.743874961 0.705677232 -1.148746296
H 2.725918380 0.020788944 -2.763917808
H 1.189853683 -2.568425764 -2.586330885
H 0.620531395 -1.090817270 -3.320528201
H -1.983071891 2.023426805 -1.148746296
H -1.380962943 2.350320093 -2.763917808
H 1.629395118 2.314656398 -2.586330885
H 0.634409770 1.082804587 -3.320528201

49
Mn^2+ ^2E D_3 LDA
Mn 0.000000 0.000000 0.000000
N -1.362000 -0.754200 1.284500
N 1.334200 -0.802500 1.284500
N 0.027900 1.556600 1.284500
C -1.729100 0.249000 2.315000
C -1.324600 1.625800 1.863700
C 1.080200 1.372900 2.315000
C 2.070300 0.334200 1.863700
C -0.745700 -1.960000 1.863700
C 0.648900 -1.622000 2.315000
H -2.806200 0.216300 2.546800
H 2.739700 0.734200 1.081900
H 2.717300 0.026900 2.706600
H 2.026800 -1.402300 0.813100
H -2.005700 2.005500 1.081900
H -1.210400 -0.014100 3.251600
H 1.215800 -2.538400 2.546800
H 1.590400 2.322100 2.546800
H -2.227900 -1.054100 0.813100
H 0.617400 -1.041200 3.251600
H -1.382000 2.339800 2.706600
H 0.201000 2.456400 0.813100
H -1.335300 -2.366700 2.706600
H 0.593000 1.055300 3.251600
H -0.734000 -2.739700 1.081900
N 0.027900 -1.556600 -1.284500
N -1.362000 0.754200 -1.284500
N 1.334200 0.802500 -1.284500
C 1.080200 -1.372900 -2.315000
C -1.324600 -1.625800 -1.863700
H 0.201000 -2.456400 -0.813100
C -0.745700 1.960000 -1.863700
C -1.729100 -0.249000 -2.315000
H -2.227900 1.054100 -0.813100
C 2.070300 -0.334200 -1.863700
C 0.648900 1.622000 -2.315000
H 2.026800 1.402300 -0.813100
H 1.590400 -2.322100 -2.546800
H 0.593000 -1.055300 -3.251600
H -1.382000 -2.339800 -2.706600
H -2.005700 -2.005500 -1.081900
H -0.734000 2.739700 -1.081900
H -1.335300 2.366700 -2.706600
H -2.806200 -0.216300 -2.546800
H -1.210400 0.014100 -3.251600
H 2.739700 -0.734200 -1.081900
H 2.717300 -0.026900 -2.706600
H 1.215800 2.538400 -2.546800
H 0.617400 1.041200 -3.251600

49
Mn^2+ ^6A_1 D_3 LDA
Mn 0.000000 0.000000 0.000000
N -1.513900 -0.622900 1.544000
N 1.296400 -0.999700 1.544000
N 0.217500 1.622600 1.544000
C -1.692500 0.438200 2.546400
C -1.141400 1.764700 2.077500
C 1.225700 1.246600 2.546400
C 2.099000 0.106100 2.077500
C -0.957600 -1.870800 2.077500
C 0.466700 -1.684800 2.546400
H -2.753700 0.565500 2.816400
H 2.766400 0.449200 1.266400
H 2.751400 -0.214400 2.911800
H 1.936900 -1.677400 1.119100
H -1.772200 2.171200 1.266400
H -1.189300 0.128100 3.477500
H 0.887100 -2.667500 2.816400
H 1.866600 2.102000 2.816400
H -2.421100 -0.838800 1.119100
H 0.483700 -1.094000 3.477500
H -1.190000 2.489900 2.911800
H 0.484200 2.516100 1.119100
H -1.561300 -2.275600 2.911800
H 0.705600 0.965900 3.477500
H -0.994200 -2.620400 1.266400
N 0.217500 -1.622600 -1.544000
N -1.513900 0.622900 -1.544000
N 1.296400 0.999700 -1.544000
C 1.225700 -1.246600 -2.546400
C -1.141400 -1.764700 -2.077500
H 0.484200 -2.516100 -1.119100
C -0.957600 1.870800 -2.077500
C -1.692500 -0.438200 -2.546400
H -2.421100 0.838800 -1.119100
C 2.099000 -0.106100 -2.077500
C 0.466700 1.684800 -2.546400
H 1.936900 1.677400 -1.119100
H 1.866600 -2.102000 -2.816400
H 0.705600 -0.965900 -3.477500
H -1.190000 -2.489900 -2.911800
H -1.772200 -2.171200 -1.266400
H -0.994200 2.620400 -1.266400
H -1.561300 2.275600 -2.911800
H -2.753700 -0.565500 -2.816400
H -1.189300 -0.128100 -3.477500
H 2.766400 -0.449200 -1.266400
H 2.751400 0.214400 -2.911800
H 0.887100 2.667500 -2.816400
H 0.483700 1.094000 -3.477500

49
Mn^2+ ^2A C_2 LDA
Mn 0.000000 0.000000 0.003600
N -1.294700 -1.548800 0.025300
N -1.281900 0.731800 -1.371500
N -1.285900 0.793700 1.348700
C -2.323900 -1.376500 1.080500
C -1.870800 -0.345100 2.076300
C -2.304900 1.611900 0.646400
C -1.847000 1.943300 -0.750100
C -1.882000 -1.635800 -1.322200
C -2.326100 -0.260600 -1.734400
H -2.556300 -2.328800 1.584800
H -1.058700 2.717000 -0.739200
H -2.686100 2.358000 -1.339100
H -0.810200 1.028600 -2.237900
H -1.091400 -0.750600 2.744900
H -3.261200 -1.055100 0.597100
H -2.555500 -0.227400 -2.811700

H -2.537600 2.533600 1.204600
H -0.812700 -2.442300 0.201600
H -3.260400 0.012700 -1.216800
H -2.712900 -0.037000 2.724100
H -0.823300 1.394500 2.046400
H -2.728000 -2.347100 -1.369700
H -3.243300 1.034300 0.612100
H -1.102800 -2.022200 -2.002200
N 1.281900 -0.731800 -1.371500
N 1.285900 -0.793700 1.348700
N 1.294700 1.548800 0.025300
C 2.326100 0.260600 -1.734400
C 1.847000 -1.943300 -0.750100
H 0.810200 -1.028600 -2.237900
C 1.870800 0.345100 2.076300
C 2.304900 -1.611900 0.646400
H 0.823300 -1.394500 2.046400
C 1.882000 1.635800 -1.322200
C 2.323900 1.376500 1.080500
H 0.812700 2.442300 0.201600
H 2.555500 0.227400 -2.811700
H 3.260400 -0.012700 -1.216800
H 2.686100 -2.358000 -1.339100
H 1.058700 -2.717000 -0.739200
H 1.091400 0.750600 2.744900
H 2.712900 0.037000 2.724100
H 2.537600 -2.533600 1.204600
H 3.243300 -1.034300 0.612100
H 1.102800 2.022200 -2.002200
H 2.728000 2.347100 -1.369700
H 2.556300 2.328800 1.584800
H 3.261200 1.055100 0.597100

49
Mn^2+ ^2E D_3 OPBE
Mn 0.000000 0.000000 0.000000
N -0.025600 -1.565700 1.364900
N 1.368700 0.760700 1.364900
N -1.343100 0.805000 1.364900
C -1.098300 -1.399200 2.392200
C -2.082000 -0.332400 1.960400
C -0.662600 1.650700 2.392200
C 0.753100 1.969300 1.960400
C 1.328900 -1.636900 1.960400
C 1.760900 -0.251500 2.392200
H -1.621200 -2.346500 2.568800
H 0.764300 2.756800 1.199000
H 1.334000 2.351100 2.812300
H 2.227900 1.071300 0.916800
H -2.769600 -0.716500 1.199000
H -0.635400 -1.130300 3.346200
H 2.842700 -0.230800 2.568800
H -1.221500 2.577200 2.568800
H -0.186200 -2.465100 0.916800
H 1.296600 0.014900 3.346200
H -2.703100 -0.020300 2.812300
H -2.041700 1.393800 0.916800
H 1.369100 -2.330800 2.812300
H -0.661200 1.115500 3.346200
H 2.005300 -2.040300 1.199000
N 1.368700 -0.760700 -1.364900
N -1.343100 -0.805000 -1.364900
N -0.025600 1.565700 -1.364900
C 1.760900 0.251500 -2.392200
C 0.753100 -1.969300 -1.960400
H 2.227900 -1.071300 -0.916800
C -2.082000 0.332400 -1.960400
C -0.662600 -1.650700 -2.392200
H -2.041700 -1.393800 -0.916800
C 1.328900 1.636900 -1.960400
C -1.098300 1.399200 -2.392200
H -0.186200 2.465100 -0.916800
H 2.842700 0.230800 -2.568800
H 1.296600 -0.014900 -3.346200
H 1.334000 -2.351100 -2.812300
H 0.764300 -2.756800 -1.199000
H -2.769600 0.716500 -1.199000
H -2.703100 0.020300 -2.812300
H -1.221500 -2.577200 -2.568800
H -0.661200 -1.115500 -3.346200
H 2.005300 2.040300 -1.199000
H 1.369100 2.330800 -2.812300
H -1.621200 2.346500 -2.568800
H -0.635400 1.130300 -3.346200

49
Mn^2+ ^6A_1 D_3 OPBE
Mn 0.000000 0.000000 0.000000
N -0.190200 1.638500 -1.665900
N 1.514100 -0.654500 -1.665900
N -1.323800 -0.984000 -1.665900
C -1.227700 1.293500 -2.666800
C -2.109900 0.136000 -2.219500
C -0.506400 -1.710000 -2.666800
C 0.937100 -1.895200 -2.219500
C 1.172800 1.759200 -2.219500
C 1.734100 0.416500 -2.666800
H -1.869800 2.157400 -2.876600
H 0.992000 -2.656000 -1.430800
H 1.522400 -2.283100 -3.066400
H 2.418000 -0.903200 -1.274200
H -2.796100 0.468900 -1.430800
H -0.743000 1.054500 -3.618200
H 2.803200 0.540600 -2.876600
H -0.933400 -2.698000 -2.876600
H -0.426800 2.545600 -1.274200
H 1.284700 0.116200 -3.618200
H -2.738400 -0.176900 -3.066400
H -1.991200 -1.642500 -1.274200
H 1.216000 2.460000 -3.066400
H -0.541700 -1.170700 -3.618200
H 1.804100 2.187100 -1.430800
N 1.514100 0.654500 1.665900
N -1.323800 0.984000 1.665900
N -0.190200 -1.638500 1.665900
C 1.734100 -0.416500 2.666800
C 0.937100 1.895200 2.219500
H 2.418000 0.903200 1.274200
C -2.109900 -0.136000 2.219500
C -0.506400 1.710000 2.666800
H -1.991200 1.642500 1.274200
C 1.172800 -1.759200 2.219500
C -1.227700 -1.293500 2.666800
H -0.426800 -2.545600 1.274200
H 2.803200 -0.540600 2.876600
H 1.284700 -0.116200 3.618200
H 1.522400 2.283100 3.066400
H 0.992000 2.656000 1.430800
H -2.796100 -0.468900 1.430800
H -2.738400 0.176900 3.066400
H -0.933400 2.698000 2.876600
H -0.541700 1.170700 3.618200
H 1.804100 -2.187100 1.430800
H 1.216000 -2.460000 3.066400
H -1.869800 -2.157400 2.876600
H -0.743000 -1.054500 3.618200

49
Mn^2+ ^2A_ C_2 SSB-D
Mn 0.000000 0.000000 -0.002800
N -1.403300 -1.533200 -0.022900
N -1.352400 0.763500 1.380000
N -1.359100 0.817900 -1.360000
C -2.427800 -1.363300 -1.096800
C -1.979900 -0.311400 -2.088400
C -2.361000 1.678200 -0.660700

C	-1.915600	1.984700	0.755900
C	-2.004400	-1.612400	1.328100
C	-2.406800	-0.222500	1.769100
H	-2.620200	-2.311700	-1.612200
H	-1.134800	2.753500	0.764200
H	-2.756200	2.391000	1.336000
H	-0.900600	1.066500	2.239600
H	-1.228700	-0.713100	-2.776800
H	-3.377200	-1.075600	-0.635900
H	-2.578900	-0.200400	2.851400
H	-2.524900	2.612300	-1.210900
H	-0.956000	-2.432200	-0.187500
H	-3.355300	0.068800	1.308400
H	-2.828300	0.014100	-2.707800
H	-0.912000	1.400000	-2.064500
H	-2.869700	-2.290300	1.360300
H	-3.325200	1.161700	-0.654500
H	-1.251000	-2.034400	2.001600
N	1.352400	-0.763500	1.380000
N	1.359100	-0.817900	-1.360000
N	1.403300	1.533200	-0.022900
C	2.406800	0.222500	1.769100
C	1.915600	-1.984700	0.755900
H	0.900600	-1.066500	2.239600
C	1.979900	0.311400	-2.088400
C	2.361000	-1.678200	-0.660700
H	0.912000	-1.400000	-2.064500
C	2.004400	1.612400	1.328100
C	2.427800	1.363300	-1.096800
H	0.956000	2.432200	-0.187500
H	2.578900	0.200400	2.851400
H	3.355300	-0.068800	1.308400
H	2.756200	-2.391000	1.336000
H	1.134800	-2.753500	0.764200
H	1.228700	0.713100	-2.776800
H	2.828300	-0.014100	-2.707800
H	2.524900	-2.612300	-1.210900
H	3.325200	-1.161700	-0.654500
H	1.251000	2.034400	2.001600
H	2.869700	2.290300	1.360300
H	2.620200	2.311700	-1.612200
H	3.377200	1.075600	-0.635900

49

Mn^2+ ^2E D_3 SSB-D

Mn	0.000000000	0.000000000	0.000000000
N	-0.026152096	-1.578215754	1.353389783
N	1.379850984	0.766459497	1.353389783
N	-1.353698888	0.811756257	1.353389783
C	-1.084654405	-1.388447175	2.373592846
C	-2.074833249	-0.336921760	1.923956724
C	-0.660103323	1.633561856	2.373592846
C	0.745633822	1.965319182	1.923956724
C	1.329199428	-1.628397423	1.923956724
C	1.744757728	-0.245114681	2.373592846
H	-1.605602249	-2.322984403	2.577346304
H	0.730348819	2.721924446	1.140083377
H	1.314875206	2.374667206	2.762000098
H	2.238172867	1.076200243	0.917343098
H	-2.722430127	-0.728461592	1.140083377
H	-0.621018771	-1.083750750	3.309156337
H	2.814564630	-0.229000134	2.577346304
H	-1.208962381	2.551984537	2.577346304
H	-0.187069684	-2.476414682	0.917343098
H	1.249065066	0.004057343	3.309156337
H	-2.713959729	-0.048618272	2.762000098
H	-2.051103183	1.400214440	0.917343098
H	1.399084524	-2.326048934	2.762000098
H	-0.628046295	1.079693406	3.309156337
H	1.992081308	-1.993462854	1.140083377
N	1.379850984	-0.766459497	-1.353389783
N	-1.353698888	-0.811756257	-1.353389783
N	-0.026152096	1.578215754	-1.353389783
C	1.744757728	0.245114681	-2.373592846
C	0.745633822	-1.965319182	-1.923956724
H	2.238172867	-1.076200243	-0.917343098
C	-2.074833249	0.336921760	-1.923956724
C	-0.660103323	-1.633561856	-2.373592846
H	-2.051103183	-1.400214440	-0.917343098
C	1.329199428	1.628397423	-1.923956724
C	-1.084654405	1.388447175	-2.373592846
H	-0.187069684	2.476414682	-0.917343098
H	2.814564630	0.229000134	-2.577346304
H	1.249065066	-0.004057343	-3.309156337
H	1.314875206	-2.374667206	-2.762000098
H	0.730348819	-2.721924446	-1.140083377
H	-2.722430127	0.728461592	-1.140083377
H	-2.713959729	0.048618272	-2.762000098
H	-1.208962381	-2.551984537	-2.577346304
H	-0.628046295	-1.079693406	-3.309156337
H	1.992081308	1.993462854	-1.140083377
H	1.399084524	2.326048934	-2.762000098
H	-1.605602249	2.322984403	-2.577346304
H	-0.621018771	1.083750750	-3.309156337

49

Mn^2+ ^6A_1 D_3 SSB-D

Mn	0.000000000	0.000000000	0.000000000
N	-0.270065245	-1.625807828	1.623012041
N	1.543023503	0.579020551	1.623012041
N	-1.272958259	1.046787277	1.623012041
C	-1.273140495	-1.219704896	2.620253128
C	-2.104614997	-0.035818520	2.159355850
C	-0.419725178	1.712424460	2.620253128
C	1.021287750	1.840559312	2.159355850
C	1.083327247	-1.804740792	2.159355850
C	1.692865673	-0.492719563	2.620253128
H	-1.948975747	-2.041792648	2.852990324
H	1.089992036	2.576910295	1.357019348
H	1.619565159	2.214782236	2.994041483
H	2.454123496	0.779360405	1.239882279
H	-2.776665797	-0.344494354	1.357019348
H	-0.770655202	-0.972566110	3.553181798
H	2.742732176	-0.666966184	2.852990324
H	-0.793756429	2.708758832	2.852990324
H	-0.552115838	-2.515013495	1.239882279
H	1.227594559	-0.181123927	3.553181798
H	-2.727840260	0.295193453	2.994041483
H	-1.902007658	1.735653089	1.239882279
H	1.108275101	-2.509975689	2.994041483
H	-0.456939357	1.153690037	3.553181798
H	1.686673761	-2.232415940	1.357019348
N	1.543023503	-0.579020551	-1.623012041
N	-1.272958259	-1.046787277	-1.623012041
N	-0.270065245	1.625807828	-1.623012041
C	1.692865673	0.492719563	-2.620253128
C	1.021287750	-1.840559312	-2.159355850
H	2.454123496	-0.779360405	-1.239882279
C	-2.104614997	0.035818520	-2.159355850
C	-0.419725178	-1.712424460	-2.620253128
H	-1.902007658	-1.735653089	-1.239882279
C	1.083327247	1.804740792	-2.159355850
C	-1.273140495	1.219704896	-2.620253128
H	-0.552115838	2.515013495	-1.239882279
H	2.742732176	0.666966184	-2.852990324
H	1.227594559	0.181123927	-3.553181798
H	1.619565159	-2.214782236	-2.994041483
H	1.089992036	-2.576910295	-1.357019348
H	-2.776665797	0.344494354	-1.357019348
H	-2.727840260	-0.295193453	-2.994041483
H	-0.793756429	-2.708758832	-2.852990324
H	-0.456939357	-1.153690037	-3.553181798
H	1.686673761	2.232415940	-1.357019348
H	1.108275101	2.509975689	-2.994041483
H	-1.948975747	2.041792648	-2.852990324
H	-0.770655202	0.972566110	-3.553181798

49
Mn^2+ ^2A_ C_2 SSB-D
Mn 0.000000000 0.000000000 0.006578162
N 1.390822107 1.549038402 0.024394322
N 1.337999596 -0.769223406 -1.388205250
N 1.346767735 -0.823550797 1.370210337
C 2.409408260 1.353098151 1.081423585
C 1.943325460 0.317966933 2.080043335
C 2.340332715 -1.661734738 0.658946066
C 1.875866861 -1.980656073 -0.747224225
C 1.962928562 1.605830500 -1.329368155
C 2.383317479 0.216900621 -1.752912198
H 2.632301919 2.287419655 1.595343655
H 1.072465847 -2.717066188 -0.729547763
H 2.701218474 -2.414532559 -1.316239897
H 0.895231643 -1.071545591 -2.245508821
H 1.169627548 0.728866826 2.727903383
H 3.338102371 1.028119109 0.617814122
H 2.581450085 0.198108136 -2.823581750
H 2.530218700 -2.588073609 1.199584678
H 0.957322409 2.447577161 0.190297955
H 3.314993797 -0.055171704 -1.261747116
H 2.777706901 0.016944868 2.718308452
H 0.910976343 -1.403842315 2.074511853
H 2.813677039 2.288665008 -1.394962122
H 3.287119933 -1.127823788 0.621025812
H 1.184227710 1.988552779 -1.988219178
N -1.337999596 0.769223406 -1.388205250
N -1.346767735 0.823550797 1.370210337
N -1.390822107 -1.549038402 0.024394322
C -2.383317479 -0.216900621 -1.752912198
C -1.875866861 1.980656073 -0.747224225
H -0.895231643 1.071545591 -2.245508821
C -1.943325460 -0.317966933 2.080043335
C -2.340332715 1.661734738 0.658946066
H -0.910976343 1.403842315 2.074511853
C -1.962928562 -1.605830500 -1.329368155
C -2.409408260 -1.353098151 1.081423585
H -0.957322409 -2.447577161 0.190297955
H -2.581450085 -0.198108136 -2.823581750
H -3.314993797 0.055171704 -1.261747116
H -2.701218474 2.414532559 -1.316239897
H -1.072465847 2.717066188 -0.729547763
H -1.169627548 -0.728866826 2.727903383
H -2.777706901 -0.016944868 2.718308452
H -2.530218700 2.588073609 1.199584678
H -3.287119933 1.127823788 0.621025812
H -1.184227710 -1.988552779 -1.988219178
H -2.813677039 -2.288665008 -1.394962122
H -2.632301919 -2.287419655 1.595343655
H -3.338102371 -1.028119109 0.617814122

49
Fe^3+ ^2E D_3 LDA
Fe 0.000000 0.000000 0.000000
N -1.316551 -0.797204 -1.247160
N -0.032124 1.538769 -1.247160
N 1.348675 -0.741564 -1.247160
C -0.637919 -1.629125 -2.284495
C 0.755041 -1.963963 -1.833096
C 1.729823 0.262108 -2.284495
C 1.323321 1.635866 -1.833096
C -2.078362 0.328097 -1.833096
C -1.091904 1.367016 -2.284495
H -1.220380 -2.539903 -2.500524
H 2.005557 2.041363 -1.065459
H 1.345938 2.354431 -2.672694
H -0.215950 2.421051 -0.746543
H 0.765093 -2.757545 -1.065459
H -0.616984 -1.051341 -3.222861
H -1.589431 2.326832 -2.500524
H 2.809811 0.213072 -2.500524
H -1.988716 -1.397543 -0.746543
H -0.601996 1.059994 -3.222861
H 1.366028 -2.342832 -2.672694
H 2.204667 -1.023507 -0.746543
H -2.711966 -0.011599 -2.672694
H 1.218980 -0.008653 -3.222861
H -2.770651 0.716182 -1.065459
N -1.316551 0.797204 1.247160
N -0.032124 -1.538769 1.247160
N 1.348675 0.741564 1.247160
C -0.637919 1.629125 2.284495
C -2.078362 -0.328097 1.833096
H -1.988716 1.397543 0.746543
C 1.323321 -1.635866 1.833096
C -1.091904 -1.367016 2.284495
H -0.215950 -2.421051 0.746543
C 0.755041 1.963963 1.833096
C 1.729823 -0.262108 2.284495
H 2.204667 1.023507 0.746543
H -1.220380 2.539903 2.500524
H -0.616984 1.051341 3.222861
H -2.711966 0.011599 2.672694
H -2.770651 -0.716182 1.065459
H 2.005557 -2.041363 1.065459
H 1.345938 -2.354431 2.672694
H -1.589431 -2.326832 2.500524
H -0.601996 -1.059994 3.222861
H 0.765093 2.757545 1.065459
H 1.366028 2.342832 2.672694
H 2.809811 -0.213072 2.500524
H 1.218980 0.008653 3.222861

49
Fe^3+ ^6A_1 D_3 LDA
Fe 0.000000 0.000000 0.000000
N -0.568972 -1.492907 -1.456769
N -1.008409 1.239198 -1.456769
N 1.577382 0.253709 -1.456769
C 0.491546 -1.674657 -2.476347
C 1.796284 -1.100254 -1.993931
C 1.204523 1.263020 -2.476347
C 0.054705 2.105754 -1.993931
C -1.850990 -1.005501 -1.993931
C -1.696068 0.411637 -2.476347
H 0.617853 -2.741728 -2.723687
H 0.381901 2.785844 -1.186044
H -0.319437 2.749009 -2.812135
H -1.714847 1.834481 -1.003711
H 2.221661 -1.723658 -1.186044
H 0.165676 -1.187034 -3.409294
H -2.683332 0.835787 -2.723687
H 2.065479 1.905940 -2.723687
H -0.731284 -2.402342 -1.003711
H -1.110840 0.450037 -3.409294
H 2.540430 -1.097864 -2.812135
H 2.446131 0.567861 -1.003711
H -2.220993 -1.651145 -2.812135
H 0.945163 0.736997 -3.409294
H -2.603563 -1.062186 -1.186044
N -0.568972 1.492907 1.456769
N -1.008409 -1.239198 1.456769
N 1.577382 -0.253709 1.456769
C 0.491546 1.674657 2.476347
C -1.850990 1.005501 1.993931
H -0.731284 2.402342 1.003711
C 0.054705 -2.105754 1.993931
C -1.696068 -0.411637 2.476347
H -1.714847 -1.834481 1.003711
C 1.796284 1.100254 1.993931
C 1.204523 -1.263020 2.476347
H 2.446131 -0.567861 1.003711
H 0.617853 2.741728 2.723687
H 0.165676 1.187034 3.409294
H -2.220993 1.651145 2.812135

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H    -2.603563   1.062186   1.186044
H     0.381901  -2.785844   1.186044
H    -0.319437  -2.749009   2.812135
H    -2.683332  -0.835787   2.723687
H    -1.110840  -0.450037   3.409294
H     2.221661   1.723658   1.186044
H     2.540430   1.097864   2.812135
H     2.065479  -1.905940   2.723687
H     0.945163  -0.736997   3.409294

 49
Fe^3+ ^2A_ C_2 LDA
Fe    0.000000   0.000000  -0.008500
N    -1.244300  -0.722200   1.355400
N    -1.251400  -0.790800  -1.330200
N    -1.259200   1.531500  -0.031300
C    -2.290000   0.272300   1.735600
C    -1.844300   1.643900   1.321200
C    -2.295900   1.367800  -1.091000
C    -1.844100   0.335700  -2.083300
C    -1.820700  -1.949800   0.757800
C    -2.280000  -1.621800  -0.635600
H    -2.502000   0.223400   2.816300
H    -1.078900   0.729200  -2.775200
H    -2.684200  -0.004100  -2.716400
H    -0.757000  -1.391500  -2.006500
H    -1.074500   2.052700   1.999100
H    -3.227900  -0.005700   1.227800
H    -2.497200  -2.537400  -1.210100
H    -2.514800   2.329600  -1.583400
H    -0.740800  -1.003500   2.209500
H    -3.219800  -1.046500  -0.611900
H    -2.684600   2.361600   1.341200
H    -0.750100   2.408000  -0.220500
H    -2.656100  -2.335200   1.370600
H    -3.233600   1.056800  -0.602300
H    -1.047100  -2.737900   0.767400
N     1.259200  -1.531500  -0.031300
N     1.244300   0.722200   1.355400
N     1.251400   0.790800  -1.330200
C     2.295900  -1.367800  -1.091000
C     1.844300  -1.643900   1.321200
H     0.750100  -2.408000  -0.220500
C     1.820700   1.949800   0.757800
C     2.290000  -0.272300   1.735600
H     0.740800   1.003500   2.209500
C     1.844100  -0.335700  -2.083300
C     2.280000   1.621800  -0.635600
H     0.757000   1.391500  -2.006500
H     2.514800  -2.329600  -1.583400
H     3.233600  -1.056800  -0.602300
H     2.684600  -2.361600   1.341200
H     1.074500  -2.052700   1.999100
H     1.047100   2.737900   0.767400
H     2.656100   2.335200   1.370600
H     2.502000  -0.223400   2.816300
H     3.227900   0.005700   1.227800
H     1.078900  -0.729200  -2.775200
H     2.684200   0.004100  -2.716400
H     2.497200   2.537400  -1.210100
H     3.219800   1.046500  -0.611900

 49
Fe^3+ ^6A_1 D_3 OPBE
Fe    0.000000   0.000000   0.000000
N    -0.670256  -1.462411  -1.543335
N    -0.931357   1.311664  -1.543335
N     1.601613   0.150747  -1.543335
C     0.389708  -1.737301  -2.559195
C     1.735286  -1.219835  -2.093012
C     1.309693   1.206148  -2.559195
C     0.188765   2.112720  -2.093012
C    -1.924052  -0.892884  -2.093012
C    -1.699401   0.531153  -2.559195
H     0.458430  -2.814292  -2.751951
H     0.535787   2.786770  -1.299606
H    -0.146492   2.753833  -2.920240
H    -1.584707   1.966675  -1.117825
H     2.145520  -1.857390  -1.299606
H     0.098395  -1.279640  -3.508281
H    -2.666463   1.010134  -2.751951
H     2.208033   1.804158  -2.751951
H    -0.910837  -2.355734  -1.117825
H    -1.157398   0.554607  -3.508281
H     2.458135  -1.250051  -2.920240
H     2.495544   0.389059  -1.117825
H    -2.311644  -1.503782  -2.920240
H     1.059003   0.725033  -3.508281
H    -2.681307  -0.929380  -1.299606
N    -0.670256   1.462411   1.543335
N    -0.931357  -1.311664   1.543335
N     1.601613  -0.150747   1.543335
C     0.389708   1.737301   2.559195
C    -1.924052   0.892884   2.093012
H    -0.910837   2.355734   1.117825
C     0.188765  -2.112720   2.093012
C    -1.699401  -0.531153   2.559195
H    -1.584707  -1.966675   1.117825
C     1.735286   1.219835   2.093012
C     1.309693  -1.206148   2.559195
H     2.495544  -0.389059   1.117825
H     0.458430   2.814292   2.751951
H     0.098395   1.279640   3.508281
H    -2.311644   1.503782   2.920240
H    -2.681307   0.929380   1.299606
H     0.535787  -2.786770   1.299606
H    -0.146492  -2.753833   2.920240
H    -2.666463  -1.010134   2.751951
H    -1.157398  -0.554607   3.508281
H     2.145520   1.857390   1.299606
H     2.458135   1.250051   2.920240
H     2.208033  -1.804158   2.751951
H     1.059003  -0.725033   3.508281

 49
Fe^3+ ^2E D_3 OPBE
Fe    0.000000   0.000000   0.000000
N     1.316100  -0.749600  -1.353900
C     1.914400  -1.975400  -0.758100
C     2.349800   0.263100  -1.762000
H     0.835900  -1.041900  -2.203600
H     1.163000  -2.771800  -0.786200
H     2.760500  -2.333400  -1.360200
H     2.510400   0.224300  -2.845600
H     3.303100  -0.009900  -1.301500
N     1.316100  -0.797700   1.326100
N     1.316100   1.547300   0.027800
N    -1.316100   0.797700   1.326100
N    -1.316100  -1.547300   0.027800
N    -1.316100   0.749600  -1.353900
C     2.349800  -1.657500   0.653100
C     1.914400   1.644300  -1.331700
C     1.914400   0.331200   2.089800
H     0.835900  -1.387500   2.004200
C     2.349800   1.394300   1.108900
H     0.835900   2.429400   0.199500
C    -1.914400  -0.331200   2.089800
C    -2.349800   1.657500   0.653100
H    -0.835900   1.387500   2.004200
C    -1.914400  -1.644300  -1.331700
C    -2.349800  -1.394300   1.108900
H    -0.835900  -2.429400   0.199500
C    -1.914400   1.975400  -0.758100
C    -2.349800  -0.263100  -1.762000
H    -0.835900   1.041900  -2.203600
H     2.510400  -2.576600   1.228600
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H       3.303100   -1.122100    0.659400
H       1.163000    2.066800   -2.007300
H       2.760500    2.344700   -1.340700
H       1.163000    0.705000    2.793500
H       2.760500   -0.011300    2.700900
H       2.510400    2.352200    1.617100
H       3.303100    1.132100    0.642100
H      -1.163000   -0.705000    2.793500
H      -2.760500    0.011300    2.700900
H      -2.510400    2.576600    1.228600
H      -3.303100    1.122100    0.659400
H      -1.163000   -2.066800   -2.007300
H      -2.760500   -2.344700   -1.340700
H      -2.510400   -2.352200    1.617100
H      -3.303100   -1.132100    0.642100
H      -1.163000    2.771800   -0.786200
H      -2.760500    2.333400   -1.360200
H      -2.510400   -0.224300   -2.845600
H      -3.303100    0.009900   -1.301500

 49
Fe^3+ ^2A_ C_2 OPBE
Fe      0.000000    0.000000    0.003600
N      -1.303400    0.745200   -1.366400
N      -1.308600    0.808000    1.339200
N      -1.349100   -1.519700    0.027800
C      -2.358100   -0.245900   -1.771800
C      -1.947300   -1.629300   -1.328800
C      -2.380600   -1.361100    1.108300
C      -1.930200   -0.311100    2.095800
C      -1.875100    1.982800   -0.765100
C      -2.321500    1.679100    0.647700
H      -2.512700   -0.209600   -2.856300
H      -1.187800   -0.700800    2.800100
H      -2.772600    0.044200    2.704700
H      -0.828400    1.392600    2.021600
H      -1.200200   -2.068200   -1.998400
H      -3.307700    0.048700   -1.317000
H      -2.470600    2.606200    1.213300
H      -2.557500   -2.319500    1.610100
H      -0.819300    1.030200   -2.216100
H      -3.283900    1.160600    0.651900
H      -2.803700   -2.317000   -1.331800
H      -0.869000   -2.400600    0.207900
H      -2.712900    2.359600   -1.367400
H      -3.328900   -1.081200    0.641800
H      -1.107700    2.764000   -0.793400
N       1.349100    1.519700    0.027800
N       1.303400   -0.745200   -1.366400
N       1.308600   -0.808000    1.339200
C       2.380600    1.361100    1.108300
C       1.947300    1.629300   -1.328800
H       0.869000    2.400600    0.207900
C       1.875100   -1.982800   -0.765100
C       2.358100    0.245900   -1.771800
H       0.819300   -1.030200   -2.216100
C       1.930200    0.311100    2.095800
C       2.321500   -1.679100    0.647700
H       0.828400   -1.392600    2.021600
H       2.557500    2.319500    1.610100
H       3.328900    1.081200    0.641800
H       2.803700    2.317000   -1.331800
H       1.200200    2.068200   -1.998400
H       1.107700   -2.764000   -0.793400
H       2.712900   -2.359600   -1.367400
H       2.512700    0.209600   -2.856300
H       3.307700   -0.048700   -1.317000
H       1.187800    0.700800    2.800100
H       2.772600   -0.044200    2.704700
H       2.470600   -2.606200    1.213300
H       3.283900   -1.160600    0.651900

 49
Fe^3+ ^6A_1 D_3 SSB-D
Fe      0.000000000    0.000000000    0.000000000
N       1.582152584    0.299407432   -1.483673558
C       1.832148444   -1.049272873   -2.022479681
C       1.185309149    1.307892373   -2.494853986
H       2.440910344    0.618359034   -1.054562788
H       2.275728486   -1.642381648   -1.221021419
H       2.553076458   -1.024804250   -2.842016317
H       2.014173486    1.982515679   -2.704272222
H       0.956561933    0.799007819   -3.427864258
N      -0.531781850   -1.519888046   -1.483673558
N      -1.050370734    1.220480615   -1.483673558
N      -0.531781850    1.519888046    1.483673558
N      -1.050370734   -1.220480615    1.483673558
N       1.582152584   -0.299407432    1.483673558
C       0.540013446   -1.680454021   -2.494853986
C      -0.007377259    2.111323532   -2.022479681
C      -1.824771185   -1.062050659   -2.022479681
H      -0.684940540   -2.423069883   -1.054562788
C      -1.725322595    0.372561648   -2.494853986
H      -1.755969804    1.804710849   -1.054562788
C      -1.824771185    1.062050659    2.022479681
C       0.540013446    1.680454021    2.494853986
H      -0.684940540    2.423069883    1.054562788
C      -0.007377259   -2.111323532    2.022479681
C      -1.725322595   -0.372561648    2.494853986
H      -1.755969804   -1.804710849    1.054562788
C       1.832148444    1.049272873    2.022479681
C       1.185309149   -1.307892373    2.494853986
H       2.440910344   -0.618359034    1.054562788
H       0.709822199   -2.735583246   -2.704272222
H       0.213680103   -1.227910843   -3.427864258
H       0.284479987    2.792029505   -1.221021419
H      -0.389031715    2.723431195   -2.842016317
H      -2.560208473   -1.149647857   -1.221021419
H      -2.164044743   -1.698626945   -2.842016317
H      -2.723995685    0.753067567   -2.704272222
H      -1.170242035    0.428903025   -3.427864258
H      -2.560208473    1.149647857    1.221021419
H      -2.164044743    1.698626945    2.842016317
H       0.709822199    2.735583246    2.704272222
H       0.213680103    1.227910843    3.427864258
H       0.284479987   -2.792029505    1.221021419
H      -0.389031715   -2.723431195    2.842016317
H      -2.723995685   -0.753067567    2.704272222
H      -1.170242035   -0.428903025    3.427864258
H       2.275728486    1.642381648    1.221021419
H       2.553076458    1.024804250    2.842016317
H       2.014173486   -1.982515679    2.704272222
H       0.956561933   -0.799007819    3.427864258

 49
Fe^3+ ^2E D_3 SSB-D
Fe      0.000000    0.000000    0.000000
N      -1.367916   -0.747407    1.289136
C      -0.762585   -1.966890    1.863380
C      -1.746577    0.266165    2.313418
H      -2.215962   -1.033534    0.814988
H      -0.772457   -2.734468    1.090635
H      -1.355163   -2.346811    2.697588
H      -2.819549    0.237679    2.497677
H      -1.259741    0.007462    3.250302
N       1.331232   -0.810947    1.289136
N       0.036685    1.558354    1.289136
N       1.331232    0.810947   -1.289136
N       0.036685   -1.558354   -1.289136
N      -1.367916    0.747407   -1.289136
C       0.642783   -1.645662    2.313418
C      -1.322085    1.643863    1.863380
C       2.084669    0.323027    1.863380
H       2.003048   -1.402312    0.814988
C       1.103794    1.379497    2.313418
```

H	0.212914	2.435846	0.814988
C	2.084669	-0.323027	-1.863380
C	0.642783	1.645662	-2.313418
H	2.003048	1.402312	-0.814988
C	-1.322085	-1.643863	-1.863380
C	1.103794	-1.379497	-2.313418
H	0.212914	-2.435846	-0.814988
C	-0.762585	1.966890	-1.863380
C	-1.746577	-0.266165	-2.313418
H	-2.215962	1.033534	-0.814988
H	1.203938	-2.560640	2.497677
H	0.623408	-1.094698	3.250302
H	-1.981890	2.036201	1.090635
H	-1.354816	2.347011	2.697588
H	2.754347	0.698267	1.090635
H	2.709979	-0.000200	2.697588
H	1.615610	2.322961	2.497677
H	0.636333	1.087236	3.250302
H	2.754347	-0.698267	-1.090635
H	2.709979	0.000200	-2.697588
H	1.203938	2.560640	-2.497677
H	0.623408	1.094698	-3.250302
H	-1.981890	-2.036201	-1.090635
H	-1.354816	-2.347011	-2.697588
H	1.615610	-2.322961	-2.497677
H	0.636333	-1.087236	-3.250302
H	-0.772457	2.734468	-1.090635
H	-1.355163	2.346811	-2.697588
H	-2.819549	-0.237679	-2.497677
H	-1.259741	-0.007462	-3.250302

49
Fe^3+ ^2A_ C_2 SSB-D

Fe	0.000000000	0.000000000	-0.009100897
N	1.308631571	-0.749321593	-1.362074684
N	1.305060461	-0.807088222	1.315289495
N	1.275266891	1.574618548	0.047757602
C	2.316220392	0.282856493	-1.734769361
C	1.844373857	1.655916911	-1.314647775
C	2.302952826	1.395928224	1.111662106
C	1.862684225	0.326314235	2.082229408
C	1.900866114	-1.961645808	-0.763788833
C	2.345021892	-1.630367724	0.639475035
H	2.508935476	0.259052958	-2.806423416
H	1.083097837	0.688272743	2.751282771
H	2.698093643	0.007855803	2.708314644
H	0.828859922	-1.404590439	1.980152162
H	1.064920461	2.034593338	-1.974810038
H	3.254081975	0.039903924	-1.241708309
H	2.541706837	-2.538874913	1.206901123
H	2.476286030	2.337337307	1.631063465
H	0.840083842	-1.036244640	-2.213190739
H	3.273499671	-1.065074659	0.619015397
H	2.668226839	2.371004868	-1.352318783
H	0.796331831	2.449687070	0.222861524
H	2.738859030	-2.331146893	-1.357507847
H	3.242689681	1.118074287	0.641013057
H	1.136356968	-2.737565207	-0.771382252
N	-1.275266891	-1.574618548	0.047757602
N	-1.308631571	0.749321593	-1.362074684
N	-1.305060461	0.807088222	1.315289495
C	-2.302952826	-1.395928224	1.111662106
C	-1.844373857	-1.655916911	-1.314647775
H	-0.796331831	-2.449687070	0.222861524
C	-1.900866114	1.961645808	-0.763788833
C	-2.316220392	-0.282856493	-1.734769361
H	-0.840083842	1.036244640	-2.213190739
C	-1.862684225	-0.326314235	2.082229408
C	-2.345021892	1.630367724	0.639475035
H	-0.828859922	1.404590439	1.980152162
H	-2.476286030	-2.337337307	1.631063465
H	-3.242689681	-1.118074287	0.641013057
H	-2.668226839	-2.371004868	-1.352318783
H	-1.064920461	-2.034593338	-1.974810038
H	-1.136356968	2.737565207	-0.771382252
H	-2.738859030	2.331146893	-1.357507847
H	-2.508935476	-0.259052958	-2.806423416
H	-3.254081975	-0.039903924	-1.241708309
H	-1.083097837	-0.688272743	2.751282771
H	-2.698093643	-0.007855803	2.708314644
H	-2.541706837	2.538874913	1.206901123
H	-3.273499671	1.065074659	0.619015397

49
Fe^2+ ^5E D_3 LDA

Fe	0.000000	0.000000	0.000000
N	-1.374936	-0.875225	-1.434729
N	-0.070499	1.628342	-1.434729
N	1.445435	-0.753117	-1.434729
C	-0.615420	-1.636896	-2.439740
C	0.788618	-1.947969	-1.976937
C	1.725304	0.285478	-2.439740
C	1.292682	1.656948	-1.976937
C	-2.081300	0.291021	-1.976937
C	-1.109883	1.351418	-2.439740
H	-1.126311	-2.577502	-2.703635
H	1.960191	2.020080	-1.175221
H	1.390449	2.370418	-2.816721
H	-0.255921	2.541466	-1.005986
H	0.769345	-2.707614	-1.175221
H	-0.584234	-1.048273	-3.371788
H	-1.669027	2.264165	-2.703635
H	2.795338	0.313337	-2.703635
H	-2.073014	-1.492367	-1.005986
H	-0.615714	1.030099	-3.371788
H	1.357617	-2.389373	-2.816721
H	2.328934	-1.049099	-1.005986
H	-2.748067	0.018956	-2.816721
H	1.199949	0.018175	-3.371788
H	-2.729535	0.687535	-1.175221
N	-1.374936	0.875225	1.434729
N	-0.070499	-1.628342	1.434729
N	1.445435	0.753117	1.434729
C	-0.615420	1.636896	2.439740
C	-2.081300	-0.291021	1.976937
H	-2.073014	1.492367	1.005986
C	1.292682	-1.656948	1.976937
C	-1.109883	-1.351418	2.439740
H	-0.255921	-2.541466	1.005986
C	0.788618	1.947969	1.976937
C	1.725304	-0.285478	2.439740
H	2.328934	1.049099	1.005986
H	-1.126311	2.577502	2.703635
H	-0.584234	1.048273	3.371788
H	-2.748067	-0.018956	2.816721
H	-2.729535	-0.687535	1.175221
H	1.960191	-2.020080	1.175221
H	1.390449	-2.370418	2.816721
H	-1.669027	-2.264165	2.703635
H	-0.615714	-1.030099	3.371788
H	0.769345	2.707614	1.175221
H	1.357617	2.389373	2.816721
H	2.795338	-0.313337	2.703635
H	1.199949	-0.018175	3.371788

49
Fe^2+ ^1A_1 D_3 LDA

Fe	0.000000	0.000000	0.000000
N	-1.318417	-0.787508	-1.242263
N	-0.022794	1.535536	-1.242263
N	1.341210	-0.748029	-1.242263
C	-0.650794	-1.620623	-2.276747
C	0.744460	-1.958476	-1.829627
C	1.728898	0.246707	-2.276747
C	1.323860	1.623960	-1.829627
C	-2.068320	0.334516	-1.829627

	C	-1.078103	1.373916	-2.276747
	H	-1.228630	-2.532274	-2.499135
	H	2.007047	2.012047	-1.053695
	H	1.369662	2.337628	-2.673179
5	H	-0.200141	2.420750	-0.747002
	H	0.738961	-2.744177	-1.053695
	H	-0.621254	-1.044467	-3.216420
	H	-1.578699	2.330162	-2.499135
	H	2.807329	0.202112	-2.499135
10	H	-1.996360	-1.383702	-0.747002
	H	-0.593908	1.060255	-3.216420
	H	1.339615	-2.354976	-2.673179
	H	2.196502	-1.037048	-0.747002
	H	-2.709276	0.017347	-2.673179
15	H	1.215161	-0.015788	-3.216420
	H	-2.746007	0.732129	-1.053695
	N	-1.318417	0.787508	1.242263
	N	-0.022794	-1.535536	1.242263
	N	1.341210	0.748029	1.242263
20	C	-0.650794	1.620623	2.276747
	C	-2.068320	-0.334516	1.829627
	H	-1.996360	1.383702	0.747002
	C	1.323860	-1.623960	1.829627
	C	-1.078103	-1.373916	2.276747
25	H	-0.200141	-2.420750	0.747002
	C	0.744460	1.958476	1.829627
	C	1.728898	-0.246707	2.276747
	H	2.196502	1.037048	0.747002
	H	-1.228630	2.532274	2.499135
30	H	-0.621254	1.044467	3.216420
	H	-2.709276	-0.017347	2.673179
	H	-2.746007	-0.732129	1.053695
	H	2.007047	-2.012047	1.053695
	H	1.369662	-2.337628	2.673179
35	H	-1.578699	-2.330162	2.499135
	H	-0.593908	-1.060255	3.216420
	H	0.738961	2.744177	1.053695
	H	1.339615	2.354976	2.673179
	H	2.807329	-0.202112	2.499135
40	H	1.215161	0.015788	3.216420

49
Fe^2+ ^5B C_2 LDA

	Fe	0.000000	0.000000	0.027541
45	N	0.251077	-1.672332	1.414291
	N	-2.035673	-0.791569	0.047513
	N	0.196569	-1.661616	-1.377667
	C	0.623101	-2.898687	0.690159
	C	1.109229	-2.593200	-0.707473
50	C	-1.119522	-2.237711	-1.698889
	C	-2.245047	-1.310411	-1.306163
	C	-1.042949	-1.744744	2.099745
	C	-2.177404	-1.806806	1.104836
	H	1.393405	-3.471853	1.231406
55	H	-2.282271	-0.443959	-1.989292
	H	-3.209468	-1.842974	-1.413056
	H	-2.712877	-0.039743	0.211985
	H	2.103993	-2.114449	-0.670288
	H	-0.259872	-3.558065	0.647438
60	H	-3.137109	-1.708696	1.638348
	H	-1.203020	-2.486513	-2.769445
	H	0.974152	-1.459432	2.108974
	H	-2.207374	-2.801601	0.629479
	H	1.232917	-3.538378	-1.268830
65	H	0.644131	-1.335250	-2.240273
	H	-1.107768	-2.612336	2.783627
	H	-1.217805	-3.197631	-1.165013
	H	-1.134270	-0.840356	2.726848
	N	-0.251077	1.672332	1.414291
70	N	2.035673	0.791569	0.047513
	N	-0.196569	1.661616	-1.377667
	C	-0.623101	2.898687	0.690159
	C	1.042949	1.744744	2.099745
	H	-0.974152	1.459432	2.108974
75	C	2.245047	1.310411	-1.306163
	C	2.177404	1.806806	1.104836
	H	2.712877	0.039743	0.211985
	C	-1.109229	2.593200	-0.707473
	C	1.119522	2.237711	-1.698889
80	H	-0.644131	1.335250	-2.240273
	H	-1.393405	3.471853	1.231406
	H	0.259872	3.558065	0.647438
	H	1.107768	2.612336	2.783627
	H	1.134270	0.840356	2.726848
85	H	2.282271	0.443959	-1.989292
	H	3.209468	1.842974	-1.413056
	H	3.137109	1.708696	1.638348
	H	2.207374	2.801601	0.629479
	H	-2.103993	2.114449	-0.670288
90	H	-1.232917	3.538378	-1.268830
	H	1.203020	2.486513	-2.769445
	H	1.217805	3.197631	-1.165013

49
Fe^2+ ^5E D_3 OPBE

	Fe	0.000000	0.000000	0.000000
	N	-1.366360	-0.910271	-1.549677
	N	-0.105137	1.638438	-1.549677
	N	1.471497	-0.728167	-1.549677
100	C	-0.592573	-1.682467	-2.552706
	C	0.840954	-1.938690	-2.112080
	C	1.753346	0.328050	-2.552706
	C	1.258478	1.697632	-2.112080
	C	-2.099431	0.241058	-2.112080
105	C	-1.160773	1.354417	-2.552706
	H	-1.073058	-2.647372	-2.753973
	H	1.913451	2.104964	-1.332451
	H	1.321329	2.389759	-2.964812
	H	-0.294477	2.553744	-1.151476
110	H	0.866227	-2.709580	-1.332451
	H	-0.605971	-1.143844	-3.505304
	H	-1.756162	2.252982	-2.753973
	H	2.829220	0.394390	-2.753973
	H	-2.064369	-1.531897	-1.151476
115	H	-0.687612	1.096709	-3.505304
	H	1.408928	-2.339184	-2.964812
	H	2.358846	-1.021848	-1.151476
	H	-2.730256	-0.050575	-2.964812
	H	1.293584	0.047135	-3.505304
120	H	-2.779678	0.604615	-1.332451
	N	-1.366360	0.910271	1.549677
	N	-0.105137	-1.638438	1.549677
	N	1.471497	0.728167	1.549677
	C	-0.592573	1.682467	2.552706
125	C	-2.099431	-0.241058	2.112080
	H	-2.064369	1.531897	1.151476
	C	1.258478	-1.697632	2.112080
	C	-1.160773	-1.354417	2.552706
	H	-0.294477	-2.553744	1.151476
130	C	0.840954	1.938690	2.112080
	C	1.753346	-0.328050	2.552706
	H	2.358846	1.021848	1.151476
	H	-1.073058	2.647372	2.753973
	H	-0.605971	1.143844	3.505304
135	H	-2.730256	0.050575	2.964812
	H	-2.779678	-0.604615	1.332451
	H	1.913451	-2.104964	1.332451
	H	1.321329	-2.389759	2.964812
	H	-1.756162	-2.252982	2.753973
140	H	-0.687612	-1.096709	3.505304
	H	0.866227	2.709580	1.332451
	H	1.408928	2.339184	2.964812
	H	2.829220	-0.394390	2.753973
	H	1.293584	-0.047135	3.505304
145				

49
Fe^2+ ^1A_1 D_3 OPBE
Fe 0.000000 0.000000 0.000000
N -1.329702 -0.790700 -1.313255
N -0.019915 1.546906 -1.313255
N 1.349617 -0.756206 -1.313255
C -0.666308 -1.649739 -2.342765
C 0.750069 -1.968038 -1.916350
C 1.761870 0.247830 -2.342765
C 1.329336 1.633598 -1.916350
C -2.079405 0.334440 -1.916350
C -1.095562 1.401909 -2.342765
H -1.234505 -2.572450 -2.508428
H 2.007577 2.046522 -1.162076
H 1.358524 2.324947 -2.770732
H -0.182216 2.433497 -0.842366
H 0.768552 -2.761873 -1.162076
H -0.668315 -1.119456 -3.299588
H -1.610554 2.355338 -2.508428
H 2.845060 0.217111 -2.508428
H -2.016362 -1.374552 -0.842366
H -0.635320 1.138505 -3.299588
H 1.334201 -2.338989 -2.770732
H 2.198578 -1.058945 -0.842366
H -2.692725 0.014043 -2.770732
H 1.303635 -0.019050 -3.299588
H -2.776128 0.715351 -1.162076
N -1.329702 0.790700 1.313255
N -0.019915 -1.546906 1.313255
N 1.349617 0.756206 1.313255
C -0.666308 1.649739 2.342765
C -2.079405 -0.334440 1.916350
H -2.016362 1.374552 0.842366
C 1.329336 -1.633598 1.916350
C -1.095562 -1.401909 2.342765
H -0.182216 -2.433497 0.842366
C 0.750069 1.968038 1.916350
C 1.761870 -0.247830 2.342765
H 2.198578 1.058945 0.842366
H -1.234505 2.572450 2.508428
H -0.668315 1.119456 3.299588
H -2.692725 -0.014043 2.770732
H -2.776128 -0.715351 1.162076
H 2.007577 -2.046522 1.162076
H 1.358524 -2.324947 2.770732
H -1.610554 -2.355338 2.508428
H -0.635320 -1.138505 3.299588
H 0.768552 2.761873 1.162076
H 1.334201 2.338989 2.770732
H 2.845060 -0.217111 2.508428
H 1.303635 0.019050 3.299588

49
Fe^2+ ^5B C_2 OPBE
Fe 0.000000 0.000000 0.043749
N 0.249722 -1.812534 1.398767
N -2.088876 -0.898074 0.101423
N 0.124077 -1.750101 -1.414138
C 0.625302 -3.032946 0.643262
C 1.047942 -2.712001 -0.783152
C -1.211870 -2.310940 -1.732140
C -2.338713 -1.404350 -1.260860
C -1.033908 -1.914221 2.120149
C -2.215954 -1.927487 1.162161
H 1.441458 -3.567029 1.143981
H -2.423166 -0.531794 -1.919112
H -3.292133 -1.947972 -1.337879
H -2.783990 -0.179855 0.282611
H 2.045407 -2.256190 -0.789862
H -0.221207 -3.726128 0.641146
H -3.138484 -1.785960 1.737736
H -1.318447 -2.479522 -2.810360
H 0.969930 -1.645457 2.095501
H -2.312284 -2.911930 0.694366
H 1.129052 -3.648066 -1.354841
H 0.554370 -1.454555 -2.285472
H -1.079955 -2.806715 2.761351
H -1.302528 -3.299384 -1.271697
H -1.098225 -1.047356 2.788535
N -0.249722 1.812534 1.398767
N 2.088876 0.898074 0.101423
N -0.124077 1.750101 -1.414138
C -0.625302 3.032946 0.643262
C 1.033908 1.914221 2.120149
H -0.969930 1.645457 2.095501
C 2.338713 1.404350 -1.260860
C 2.215954 1.927487 1.162161
H 2.783990 0.179855 0.282611
C -1.047942 2.712001 -0.783152
C 1.211870 2.310940 -1.732140
H -0.554370 1.454555 -2.285472
H -1.441458 3.567029 1.143981
H 0.221207 3.726128 0.641146
H 1.079955 2.806715 2.761351
H 1.098225 1.047356 2.788535
H 2.423166 0.531794 -1.919112
H 3.292133 1.947972 -1.337879
H 3.138484 1.785960 1.737736
H 2.312284 2.911930 0.694366
H -2.045407 2.256190 -0.789862
H -1.129052 3.648066 -1.354841
H 1.318447 2.479522 -2.810360
H 1.302528 3.299384 -1.271697

49
Fe^2+ ^5E D_3 SSB-D
Fe 0.000000000 0.000000000 0.000000000
N 1.497829299 -0.672499091 -1.518182675
N -1.331315947 -0.960908678 -1.518182675
N -0.166513353 1.633407769 -1.518182675
C 1.722219400 0.386473464 -2.516745967
C 1.193480509 1.734562881 -2.059487189
C -1.195805538 1.298249019 -2.516745967
C -2.098915773 0.166302999 -2.059487189
C 0.905435265 -1.900865880 -2.059487189
C -0.526413862 -1.684722483 -2.516745967
H 2.782530585 0.491529101 -2.743100717
H -2.756887215 0.512358760 -1.261239103
H -2.734452894 -0.132441860 -2.896703097
H -1.999230461 -1.607026597 -1.126035165
H 1.822159310 2.131354984 -1.261239103
H 1.242063523 0.102695668 -3.450852858
H -0.965588604 -2.655506724 -2.743100717
H -1.816941981 2.163977623 -2.743100717
H 2.391341088 -0.927871069 -1.126035165
H -0.532094704 -1.127006398 -3.450852858
H 1.252528432 2.434326602 -2.896703097
H -0.392110627 2.534897666 -1.126035165
H 1.481924463 -2.301884742 -2.896703097
H -0.709968819 1.024310730 -3.450852858
H 0.934727905 -2.643713744 -1.261239103
N -0.166513353 -1.633407769 1.518182675
N 1.497829299 0.672499091 1.518182675
N -1.331315947 0.960908678 1.518182675
C -1.195805538 -1.298249019 2.516745967
C 1.193480509 -1.734562881 2.059487189
H -0.392110627 -2.534897666 1.126035165
C 0.905435265 1.900865880 2.059487189
C 1.722219400 -0.386473464 2.516745967
H 2.391341088 0.927871069 1.126035165
C -2.098915773 -0.166302999 2.059487189
C -0.526413862 1.684722483 2.516745967
H -1.999230461 1.607026597 1.126035165
H -1.816941981 -2.163977623 2.743100717
H -0.709968819 -1.024310730 3.450852858
H 1.252528432 -2.434326602 2.896703097

H 1.822159310 -2.131354984 1.261239103
H 0.934727905 2.643713744 1.261239103
H 1.481924463 2.301884742 2.896703097
H 2.782530585 -0.491529101 2.743100717
H 1.242063523 -0.102695668 3.450852858
H -2.756887215 -0.512358760 1.261239103
H -2.734452894 0.132441860 2.896703097
H -0.965588604 2.655506724 2.743100717
H -0.532094704 1.127006398 3.450852858

49
Fe^2+ ^1A_1 D_3 SSB-D
Fe 0.000000000 0.000000000 0.000000000
N -0.016345400 -1.561806640 1.306357864
N 1.360736926 0.766747788 1.306357864
N -1.344391526 0.795058852 1.306357864
C -1.078102262 -1.393781027 2.328673094
C -2.072230642 -0.345375937 1.882925116
C -0.667998646 1.630554460 2.328673094
C 0.737010986 1.967292347 1.882925116
C 1.335219656 -1.621916410 1.882925116
C 1.746100907 -0.236773433 2.328673094
H -1.588360364 -2.335803231 2.524223394
H 0.724771638 2.728163342 1.103502082
H 1.308740805 2.370565558 2.722061403
H 2.209949591 1.071130409 0.849947145
H -2.725044579 -0.736411020 1.103502082
H -0.617783043 -1.091065219 3.266572420
H 2.817045118 -0.207658810 2.524223394
H -1.228684755 2.543462041 2.524223394
H -0.177348650 -2.449437692 0.849947145
H 1.253781719 0.010516800 3.266572420
H -2.707340397 -0.051879995 2.722061403
H -2.032600941 1.378307282 0.849947145
H 1.398599592 -2.318685563 2.722061403
H -0.635998675 1.080548419 3.266572420
H 2.000272941 -1.991752322 1.103502082
N 1.360736926 -0.766747788 -1.306357864
N -1.344391526 -0.795058852 -1.306357864
N -0.016345400 1.561806640 -1.306357864
C 1.746100907 0.236773433 -2.328673094
C 0.737010986 -1.967292347 -1.882925116
H 2.209949591 -1.071130409 -0.849947145
C -2.072230642 0.345375937 -1.882925116
C -0.667998646 -1.630554460 -2.328673094
H -2.032600941 -1.378307282 -0.849947145
C 1.335219656 1.621916410 -1.882925116
C -1.078102262 1.393781027 -2.328673094
H -0.177348650 2.449437692 -0.849947145
H 2.817045118 0.207658810 -2.524223394
H 1.253781719 -0.010516800 -3.266572420
H 1.308740805 -2.370565558 -2.722061403
H 0.724771638 -2.728163342 -1.103502082
H -2.725044579 0.736411020 -1.103502082
H -2.707340397 0.051879995 -2.722061403
H -1.228684755 -2.543462041 -2.524223394
H -0.635998675 -1.080548419 -3.266572420
H 2.000272941 1.991752322 -1.103502082
H 1.398599592 2.318685563 -2.722061403
H -1.588360364 2.335803231 -2.524223394
H -0.617783043 1.091065219 -3.266572420

49
Fe^2+ ^5B C_2 SSB-D
Fe 0.000000000 0.000000000 0.103686655
N 1.600591416 0.916369765 1.375427934
N 1.554872471 -1.632610027 0.145351116
N 1.491644163 0.710110379 -1.427616568
C 2.572205790 1.670403277 0.564694405
C 2.057302770 1.927870354 -0.839837941
C 2.481152086 -0.334995255 -1.737966594
C 2.049246520 -1.699893302 -1.232912402
C 2.167001028 -0.228599301 2.097346123
C 2.591411239 -1.334196927 1.148162153
H 2.814272711 2.624760950 1.030380894
H 1.229690277 -2.081626553 -1.842342774
H 2.887426928 -2.393056918 -1.343297886
H 1.158579744 -2.534043951 0.363027896
H 1.256286082 2.667966272 -0.813602078
H 3.504075784 1.111083937 0.516717431
H 2.837221915 -2.218138695 1.735335523
H 2.659412268 -0.400656980 -2.810611241
H 1.215519447 1.542598079 2.066175407
H 3.508967974 -1.047381999 0.638550432
H 2.867409661 2.345887555 -1.442500507
H 1.032859619 0.977990746 -2.284620784
H 3.023570540 0.054878744 2.714132856
H 3.435706692 -0.065131189 -1.291285977
H 1.388948385 -0.592726466 2.769350262
N -1.600591416 -0.916369765 1.375427934
N -1.554872471 1.632610027 0.145351116
N -1.491644163 -0.710110379 -1.427616568
C -2.572205790 -1.670403277 0.564694405
C -2.167001028 0.228599301 2.097346123
H -1.215519447 -1.542598079 2.066175407
C -2.049246520 1.699893302 -1.232912402
C -2.591411239 1.334196927 1.148162153
H -1.158579744 2.534043951 0.363027896
C -2.057302770 -1.927870354 -0.839837941
C -2.481152086 0.334995255 -1.737966594
H -1.032859619 -0.977990746 -2.284620784
H -2.814272711 -2.624760950 1.030380894
H -3.504075784 -1.111083937 0.516717431
H -3.023570540 -0.054878744 2.714132856
H -1.388948385 0.592726466 2.769350262
H -1.229690277 2.081626553 -1.842342774
H -2.887426928 2.393056918 -1.343297886
H -2.837221915 2.218138695 1.735335523
H -3.508967974 1.047381999 0.638550432
H -1.256286082 -2.667966272 -0.813602078
H -2.867409661 -2.345887555 -1.442500507
H -2.659412268 0.400656980 -2.810611241
H -3.435706692 0.065131189 -1.291285977

49
Co^3+ ^5A_1 D_3 LDA
Co 0.000000 0.000000 0.000000
N 1.006887 -1.237375 -1.408508
N -1.575041 -0.253302 -1.408508
N 0.568155 1.490677 -1.408508
C 1.694033 -0.410822 -2.425500
C 1.849461 1.004717 -1.938993
C -0.491234 1.672487 -2.425500
C -1.794840 1.099322 -1.938993
C -0.054620 -2.104038 -1.938993
C -1.202799 -1.261665 -2.425500
H 2.681410 -0.836865 -2.671111
H -2.218929 1.722600 -1.130235
H -2.543105 1.097383 -2.754528
H -2.436234 -0.569123 -0.942523
H 2.601280 1.060349 -1.130235
H 1.110363 -0.445922 -3.359501
H -2.065451 -1.903737 -2.671111
H -0.615959 2.740602 -2.671111
H 1.710992 -1.825279 -0.942523
H -0.941361 -0.738641 -3.359501
H 2.221914 1.653702 -2.754528
H 0.725242 2.394402 -0.942523
H 0.321191 -2.751085 -2.754528
H -0.169002 1.184564 -3.359501
H -0.382351 -2.782949 -1.130235
N -1.575041 0.253302 1.408508
N 0.568155 -1.490677 1.408508
N 1.006887 1.237375 1.408508
C -1.202799 1.261665 2.425500
C -1.794840 -1.099322 1.938993

H	-2.436234	0.569123	0.942523
C	1.849461	-1.004717	1.938993
C	-0.491234	-1.672487	2.425500
H	0.725242	-2.394402	0.942523
C	-0.054620	2.104038	1.938993
C	1.694033	0.410822	2.425500
H	1.710992	1.825279	0.942523
H	-2.065451	1.903737	2.671111
H	-0.941361	0.738641	3.359501
H	-2.543105	-1.097383	2.754528
H	-2.218929	-1.722600	1.130235
H	2.601280	-1.060349	1.130235
H	2.221914	-1.653702	2.754528
H	-0.615959	-2.740602	2.671111
H	-0.169002	-1.184564	3.359501
H	-0.382351	2.782949	1.130235
H	0.321191	2.751085	2.754528
H	2.681410	0.836865	2.671111
H	1.110363	0.445922	3.359501

49

Co^3+ ^1A_1 D_3 LDA

Co	0.000000	0.000000	0.000000
N	-1.329612	0.745889	-1.216816
N	1.310765	0.778533	-1.216816
N	0.018847	-1.524422	-1.216816
C	-1.731007	-0.250199	-2.254643
C	-1.331975	-1.626474	-1.807099
C	1.082182	-1.373996	-2.254643
C	2.074555	-0.340287	-1.807099
C	-0.742580	1.966761	-1.807099
C	0.648825	1.624195	-2.254643
H	-2.812080	-0.187059	-2.461493
H	2.772773	-0.729246	-1.045307
H	2.703735	0.002278	-2.648949
H	1.974328	1.370813	-0.696428
H	-2.017932	-2.036669	-1.045307
H	-1.223729	0.016903	-3.196043
H	1.244042	2.528862	-2.461493
H	1.568038	-2.341803	-2.461493
H	-2.174323	1.024412	-0.696428
H	0.626503	1.051329	-3.196043
H	-1.349895	-2.342642	-2.648949
H	0.199995	-2.395225	-0.696428
H	-1.353840	2.340364	-2.648949
H	0.597226	-1.068232	-3.196043
H	-0.754841	2.765915	-1.045307
N	0.018847	1.524422	1.216816
N	-1.329612	-0.745889	1.216816
N	1.310765	-0.778533	1.216816
C	1.082182	1.373996	2.254643
C	-1.331975	1.626474	1.807099
H	0.199995	2.395225	0.696428
C	-0.742580	-1.966761	1.807099
C	-1.731007	0.250199	2.254643
H	-2.174323	-1.024412	0.696428
C	2.074555	0.340287	1.807099
C	0.648825	-1.624195	2.254643
H	1.974328	-1.370813	0.696428
H	1.568038	2.341803	2.461493
H	0.597226	1.068232	3.196043
H	-1.349895	2.342642	2.648949
H	-2.017932	2.036669	1.045307
H	-0.754841	-2.765915	1.045307
H	-1.353840	-2.340364	2.648949
H	-2.812080	0.187059	2.461493
H	-1.223729	-0.016903	3.196043
H	2.772773	0.729246	1.045307
H	2.703735	-0.002278	2.648949
H	1.244042	-2.528862	2.461493
H	0.626503	-1.051329	3.196043

49

Co^3+ ^5A_1 D_3 SSB-D

Co	0.000000000	0.000000000	0.000000000
N	1.061824212	-1.211907054	-1.435615749
N	-1.580454402	-0.313613215	-1.435615749
N	0.518630189	1.525520269	-1.435615749
C	1.728161715	-0.356689598	-2.443307211
C	1.814690980	1.077238696	-1.966636129
C	-0.555178605	1.674976746	-2.443307211
C	-1.840261566	1.032949141	-1.966636129
C	0.025570586	-2.110187837	-1.966636129
C	-1.172983110	-1.318287149	-2.443307211
H	2.730989044	-0.728050201	-2.650708691
H	-2.285587095	1.620989546	-1.162586767
H	-2.565572489	1.005139206	-2.783123886
H	-2.430106483	-0.641092290	-0.995456731
H	2.546611674	1.168881714	-1.162586767
H	1.175114216	-0.415459535	-3.377362913
H	-1.996004491	-2.001080789	-2.650708691
H	-0.734984552	2.729130990	-2.650708691
H	1.770255451	-1.783987803	-0.995456731
H	-0.947355619	-0.809948996	-3.377362913
H	2.153262331	1.719281348	-2.783123886
H	0.659851032	2.425080093	-0.995456731
H	0.412310158	-2.724420554	-2.783123886
H	-0.227758597	1.225408531	-3.377362913
H	-0.261024579	-2.789871260	-1.162586767
N	-1.580454402	0.313613215	1.435615749
N	0.518630189	-1.525520269	1.435615749
N	1.061824212	1.211907054	1.435615749
C	-1.172983110	1.318287149	2.443307211
C	-1.840261566	-1.032949141	1.966636129
H	-2.430106483	0.641092290	0.995456731
C	1.814690980	-1.077238696	1.966636129
C	-0.555178605	-1.674976746	2.443307211
H	0.659851032	-2.425080093	0.995456731
C	0.025570586	2.110187837	1.966636129
C	1.728161715	0.356689598	2.443307211
H	1.770255451	1.783987803	0.995456731
H	-1.996004491	2.001080789	2.650708691
H	-0.947355619	0.809948996	3.377362913
H	-2.565572489	-1.005139206	2.783123886
H	-2.285587095	-1.620989546	1.162586767
H	2.546611674	-1.168881714	1.162586767
H	2.153262331	-1.719281348	2.783123886
H	-0.734984552	-2.729130990	2.650708691
H	-0.227758597	-1.225408531	3.377362913
H	-0.261024579	2.789871260	1.162586767
H	0.412310158	2.724420554	2.783123886
H	2.730989044	0.728050201	2.650708691
H	1.175114216	0.415459535	3.377362913

49

Co^3+ ^1A_1 D_3 SSB-D

Co	0.000000	0.000000	0.000000
N	-0.028666	1.544501	-1.259792
N	1.351910	-0.747425	-1.259792
N	-1.323244	-0.797076	-1.259792
C	-1.098445	1.381747	-2.284683
C	-2.081759	0.327456	-1.839705
C	-0.647405	-1.642155	-2.284683
C	0.757295	-1.966584	-1.839705
C	1.324465	1.639129	-1.839705
C	1.745850	0.260408	-2.284683
H	-1.601387	2.331272	-2.459705
H	0.774006	-2.741522	-1.075382
H	1.351628	-2.334969	-2.677380
H	2.191711	-1.027849	-0.769731
H	-2.761231	0.700453	-1.075382
H	-0.632844	1.092335	-3.223015
H	2.819634	0.221206	-2.459705
H	-1.218247	-2.552478	-2.459705
H	-0.205713	2.412002	-0.769731

```
H       1.262412    0.001891   -3.223015
H      -2.697957   -0.003059   -2.677380
H      -1.985999   -1.384153   -0.769731
H       1.346329    2.338029   -2.677380
H      -0.629568   -1.094226   -3.223015
H       1.987225    2.041070   -1.075382
N       1.351910    0.747425    1.259792
N      -1.323244    0.797076    1.259792
N      -0.028666   -1.544501    1.259792
C       1.745850   -0.260408    2.284683
C       0.757295    1.966584    1.839705
H       2.191711    1.027849    0.769731
C      -2.081759   -0.327456    1.839705
C      -0.647405    1.642155    2.284683
H      -1.985999    1.384153    0.769731
C       1.324465   -1.639129    1.839705
C      -1.098445   -1.381747    2.284683
H      -0.205713   -2.412002    0.769731
H       2.819634   -0.221206    2.459705
H       1.262412   -0.001891    3.223015
H       1.351628    2.334969    2.677380
H       0.774006    2.741522    1.075382
H      -2.761231   -0.700453    1.075382
H      -2.697957    0.003059    2.677380
H      -1.218247    2.552478    2.459705
H      -0.629568    1.094226    3.223015
H       1.987225   -2.041070    1.075382
H       1.346329   -2.338029    2.677380
H      -1.601387   -2.331272    2.459705
H      -0.632844   -1.092335    3.223015

 49
Co^3+ ^5A_1 D_3 OPBE
Co      0.000000000    0.000000000    0.000000000
N      -1.601456871   -0.161499500   -1.500663212
N       0.660865766    1.467652083   -1.500663212
N       0.940591105   -1.306152583   -1.500663212
C      -1.298567792   -1.213115869   -2.513993567
C      -0.174526065   -2.112455012   -2.043169358
C       1.699873057   -0.518034762   -2.513993567
C       1.916702738    0.905083500   -2.043169358
C      -1.742176672    1.207371512   -2.043169358
C      -0.401305264    1.731150631   -2.513993567
H      -2.193196832   -1.816826831   -2.708075987
H       2.672371791    0.944255259   -1.248784619
H       2.304193334    1.520698576   -2.868046983
H       0.890131227    2.359414332   -1.066978885
H      -0.518436853   -2.786469489   -1.248784619
H      -1.047755703   -0.731667049   -3.462830558
H      -0.476819773    2.807777588   -2.708075987
H       2.670016606   -0.990950757   -2.708075987
H      -2.488378363   -0.408830911   -1.066978885
H      -0.109764400    1.273216581   -3.462830558
H       0.164866931   -2.755839251   -2.868046983
H       1.598247136   -1.950583421   -1.066978885
H      -2.469060265    1.235140675   -2.868046983
H       1.157520103   -0.541549532   -3.462830558
H      -2.153934938    1.842214230   -1.248784619
N       0.940591105    1.306152583    1.500663212
N      -1.601456871    0.161499500    1.500663212
N       0.660865766   -1.467652083    1.500663212
C       1.699873057    0.518034762    2.513993567
C      -0.174526065    2.112455012    2.043169358
H       1.598247136    1.950583421    1.066978885
C      -1.742176672   -1.207371512    2.043169358
C      -1.298567792    1.213115869    2.513993567
H      -2.488378363    0.408830911    1.066978885
C       1.916702738   -0.905083500    2.043169358
C      -0.401305264   -1.731150631    2.513993567
H       0.890131227   -2.359414332    1.066978885
H       2.670016606    0.990950757    2.708075987
H       1.157520103    0.541549532    3.462830558
H       0.164866931    2.755839251    2.868046983
H      -0.518436853    2.786469489    1.248784619
H      -2.153934938   -1.842214230    1.248784619
H      -2.469060265   -1.235140675    2.868046983
H      -2.193196832    1.816826831    2.708075987
H      -1.047755703    0.731667049    3.462830558
H       2.672371791   -0.944255259    1.248784619
H       2.304193334   -1.520698576    2.868046983
H      -0.476819773   -2.807777588    2.708075987
H      -0.109764400   -1.273216581    3.462830558

 49
Co^3+ ^1A_1 D_3 OPBE
Co      0.000000000    0.000000000    0.000000000
N      -1.337278357    0.750626855   -1.279268494
N       1.318701104    0.782803601   -1.279268494
N       0.018577253   -1.533430457   -1.279268494
C      -1.762172022   -0.255302916   -2.313170244
C      -1.336475549   -1.638001019   -1.881125672
C       1.102184822   -1.398434279   -2.313170244
C       2.086788268   -0.338421267   -1.881125672
C      -0.750312719    1.976422286   -1.881125672
C       0.659987200    1.653737195   -2.313170244
H      -2.846602807   -0.205513427   -2.465665614
H       2.796327272   -0.711844529   -1.135360088
H       2.692790847    0.008225751   -2.729181428
H       1.987292786    1.366917155   -0.780446569
H      -2.014639082   -2.065768190   -1.135360088
H      -1.305200360    0.015856493   -3.268633278
H       1.245321555    2.567987058   -2.465665614
H       1.601281252   -2.362473632   -2.465665614
H      -2.177431374    1.037587460   -0.780446569
H       0.666332306    1.122408423   -3.268633278
H      -1.339271714   -2.336138156   -2.729181428
H       0.190138587   -2.404504615   -0.780446569
H      -1.353519133    2.327912405   -2.729181428
H       0.638868055   -1.138264915   -3.268633278
H      -0.781688190    2.777612719   -1.135360088
N       0.018577253    1.533430457    1.279268494
N      -1.337278357   -0.750626855    1.279268494
N       1.318701104   -0.782803601    1.279268494
C       1.102184822    1.398434279    2.313170244
C      -1.336475549    1.638001019    1.881125672
H       0.190138587    2.404504615    0.780446569
C      -0.750312719   -1.976422286    1.881125672
C      -1.762172022    0.255302916    2.313170244
H      -2.177431374   -1.037587460    0.780446569
C       2.086788268    0.338421267    1.881125672
C       0.659987200   -1.653737195    2.313170244
H       1.987292786   -1.366917155    0.780446569
H       1.601281252    2.362473632    2.465665614
H       0.638868055    1.138264915    3.268633278
H      -1.339271714    2.336138156    2.729181428
H      -2.014639082    2.065768190    1.135360088
H      -0.781688190   -2.777612719    1.135360088
H      -1.353519133   -2.327912405    2.729181428
H      -2.846602807    0.205513427    2.465665614
H      -1.305200360   -0.015856493    3.268633278
H       2.796327272    0.711844529    1.135360088
H       2.692790847   -0.008225751    2.729181428
H       1.245321555   -2.567987058    2.465665614
H       0.666332306   -1.122408423    3.268633278

 49
Co^2+ ^2E D_3 LDA
Co      0.000000    0.000000    0.000000
N       0.018700   -1.565100    1.296100
N      -1.364800    0.766300    1.296100
N       1.346000    0.798800    1.296100
C       1.072100   -1.380400    2.316400
C       2.068700   -0.344000    1.864800
C       0.659400    1.618700    2.316400
C      -0.736400    1.963500    1.864800
C      -1.332300   -1.619500    1.864800
```

C	-1.731500	-0.238200	2.316400
H	1.581800	-2.328900	2.551600
H	-0.718400	2.739600	1.079800
H	-1.316100	2.383900	2.708100
H	-2.216000	1.059000	0.801500
H	2.731800	-0.747600	1.079800
H	0.590700	-1.058600	3.254800
H	-2.807800	-0.205400	2.551600
H	1.226000	2.534400	2.551600
H	0.190900	-2.448600	0.801500
H	-1.212100	0.017700	3.254800
H	2.722500	-0.052200	2.708100
H	2.025100	1.389600	0.801500
H	-1.406500	-2.331700	2.708100
H	0.621400	1.040800	3.254800
H	-2.013300	-1.992000	1.079800
N	-1.364800	-0.766300	-1.296100
N	1.346000	-0.798800	-1.296100
N	0.018700	1.565100	-1.296100
C	-1.731500	0.238200	-2.316400
C	-0.736400	-1.963500	-1.864800
H	-2.216000	-1.059000	-0.801500
C	2.068700	0.344000	-1.864800
C	0.659400	-1.618700	-2.316400
H	2.025100	-1.389600	-0.801500
C	-1.332300	1.619500	-1.864800
C	1.072100	1.380400	-2.316400
H	0.190900	2.448600	-0.801500
H	-2.807800	0.205400	-2.551600
H	-1.212100	-0.017700	-3.254800
H	-1.316100	-2.383900	-2.708100
H	-0.718400	-2.739600	-1.079800
H	2.731800	0.747600	-1.079800
H	2.722500	0.052200	-2.708100
H	1.226000	-2.534400	-2.551600
H	0.621400	-1.040800	-3.254800
H	-2.013300	1.992000	-1.079800
H	-1.406500	2.331700	-2.708100
H	1.581800	2.328900	-2.551600
H	0.590700	1.058600	-3.254800

49

Co^2+ ^2A C_2 LDA

Co	0.000000	0.000000	-0.005100
N	-1.390800	1.710000	0.035800
N	-1.249400	-0.695800	-1.333800
N	-1.268100	-0.715200	1.313900
C	-2.390600	1.436800	1.073300
C	-1.879700	0.402600	2.048400
C	-2.278300	-1.580400	0.652700
C	-1.815500	-1.917800	-0.736700
C	-1.907700	1.690300	-1.327900
C	-2.295900	0.285900	-1.712300
H	-2.680500	2.348900	1.620700
H	-1.018800	-2.679500	-0.717500
H	-2.645500	-2.328400	-1.341200
H	-0.748000	-0.975500	-2.187500
H	-1.107000	0.835700	2.708100
H	-3.316700	1.078100	0.592700
H	-2.519700	0.230900	-2.790300
H	-2.476200	-2.491700	1.239500
H	-0.957800	2.622400	0.209800
H	-3.228000	0.001200	-1.197000
H	-2.696800	0.060000	2.709800
H	-0.747400	-1.288400	1.990100
H	-2.781700	2.355200	-1.472300
H	-3.231400	-1.027500	0.618100
H	-1.115000	2.076800	-1.994000
N	1.249400	0.695800	-1.333800
N	1.268100	0.715200	1.313900
N	1.390800	-1.710000	0.035800
C	2.295900	-0.285900	-1.712300
C	1.815500	1.917800	-0.736700
H	0.748000	0.975500	-2.187500
C	1.879700	-0.402600	2.048400
C	2.278300	1.580400	0.652700
H	0.747400	1.288400	1.990100
C	1.907700	-1.690300	-1.327900
C	2.390600	-1.436800	1.073300
H	0.957800	-2.622400	0.209800
H	2.519700	-0.230900	-2.790300
H	3.228000	-0.001200	-1.197000
H	2.645500	2.328400	-1.341200
H	1.018800	2.679500	-0.717500
H	1.107000	-0.835700	2.708100
H	2.696800	-0.060000	2.709800
H	2.476200	2.491700	1.239500
H	3.231400	1.027500	0.618100
H	1.115000	-2.076800	-1.994000
H	2.781700	-2.355200	-1.472300
H	2.680500	-2.348900	1.620700
H	3.316700	-1.078100	0.592700

49

Co^2+ ^4E D_3 LDA

Co	0.000000	0.000000	0.000000
N	0.040500	-1.606500	-1.392000
N	-1.411500	0.768200	-1.392000
N	1.371000	0.838300	-1.392000
C	1.087000	-1.369500	-2.400500
C	2.075000	-0.324000	-1.941400
C	0.642600	1.626100	-2.400500
C	-0.756900	1.959000	-1.941400
C	-1.318100	-1.635000	-1.941400
C	-1.729500	-0.256600	-2.400500
H	1.622400	-2.298600	-2.655600
H	-0.731400	2.722500	-1.143900
H	-1.325500	2.399400	-2.782100
H	-2.277400	1.064300	-0.929000
H	2.723400	-0.727800	-1.143900
H	0.600300	-1.043100	-3.334800
H	-2.801900	-0.255800	-2.655600
H	1.179500	2.554400	-2.655600
H	0.217000	-2.504400	-0.929000
H	-1.203500	0.001700	-3.334800
H	2.740700	-0.051800	-2.782100
H	2.060400	1.440200	-0.929000
H	-1.415200	-2.347600	-2.782100
H	0.603200	1.041500	-3.334800
H	-1.992000	-1.994700	-1.143900
N	-1.411500	-0.768200	1.392000
N	1.371000	-0.838300	1.392000
N	0.040500	1.606500	1.392000
C	-1.729500	0.256600	2.400500
C	-0.756900	-1.959000	1.941400
H	-2.277400	-1.064300	0.929000
C	2.075000	0.324000	1.941400
C	0.642600	-1.626100	2.400500
H	2.060400	-1.440200	0.929000
C	-1.318100	1.635000	1.941400
C	1.087000	1.369500	2.400500
H	0.217000	2.504400	0.929000
H	-2.801900	0.255800	2.655600
H	-1.203500	-0.001700	3.334800
H	-1.325500	-2.399400	2.782100
H	-0.731400	-2.722500	1.143900
H	2.723400	0.727800	1.143900
H	2.740700	0.051800	2.782100
H	1.179500	-2.554400	2.655600
H	0.603200	-1.041500	3.334800
H	-1.992000	1.994700	1.143900
H	-1.415200	2.347600	2.782100
H	1.622400	2.298600	2.655600
H	0.600300	1.043100	3.334800

49
Co^2+ ^4B C_2 LDA
Co 0.000000 0.000000 0.025400
N -1.291400 1.691100 0.063700
N -1.432600 -0.638900 -1.416500
N -1.460900 -0.761200 1.373500
C -2.318300 1.512600 1.102700
C -1.934300 0.431100 2.083600
C -2.510700 -1.466200 0.618100
C -2.057600 -1.804800 -0.782900
C -1.831500 1.785900 -1.294000
C -2.375400 0.447300 -1.729400
H -2.517500 2.451000 1.646000
H -1.306800 -2.614900 -0.761100
H -2.916500 -2.187000 -1.365900
H -0.976900 -0.950900 -2.280500
H -1.113800 0.774900 2.737700
H -3.268700 1.251500 0.608000
H -2.621400 0.474700 -2.803500
H -2.832900 -2.385200 1.134500
H -0.763400 2.548600 0.258900
H -3.327900 0.240800 -1.213400
H -2.794400 0.210100 2.743500
H -1.053400 -1.402600 2.062200
H -2.623000 2.554000 -1.381800
H -3.403400 -0.820000 0.579600
H -1.007800 2.102500 -1.957700
N 1.432600 0.638900 -1.416500
N 1.460900 0.761200 1.373500
N 1.291400 -1.691100 0.063700
C 2.375400 -0.447300 -1.729400
C 2.057600 1.804800 -0.782900
H 0.976900 0.950900 -2.280500
C 1.934300 -0.431100 2.083600
C 2.510700 1.466200 0.618100
H 1.053400 1.402600 2.062200
C 1.831500 -1.785900 -1.294000
C 2.318300 -1.512600 1.102700
H 0.763400 -2.548600 0.258900
H 2.621400 -0.474700 -2.803500
H 3.327900 -0.240800 -1.213400
H 2.916500 2.187000 -1.365900
H 1.306800 2.614900 -0.761100
H 1.113800 -0.774900 2.737700
H 2.794400 -0.210100 2.743500
H 2.832900 2.385200 1.134500
H 3.403400 0.820000 0.579600
H 1.007800 -2.102500 -1.957700
H 2.623000 -2.554000 -1.381800
H 2.517500 -2.451000 1.646000
H 3.268700 -1.251500 0.608000

49
Co^2+ ^2E D_3 OPBE
Co 0.000000 0.000000 0.000000
N 0.018758 -1.578657 1.388903
N -1.376536 0.773083 1.388903
N 1.357778 0.805573 1.388903
C 1.092422 -1.406735 2.405174
C 2.080731 -0.340159 1.973602
C 0.672057 1.649433 2.405174
C -0.745780 1.972045 1.973602
C -1.334952 -1.631886 1.973602
C -1.764479 -0.242698 2.405174
H 1.619479 -2.351799 2.581870
H -0.750927 2.755969 1.208698
H -1.316234 2.367019 2.826968
H -2.225989 1.080732 0.924791
H 2.762203 -0.727663 1.208698
H 0.634292 -1.137580 3.361557
H -2.846457 -0.226610 2.581870
H 1.226978 2.578409 2.581870
H 0.177053 -2.468129 0.924791
H -1.302319 0.019477 3.361557
H 2.708016 -0.043617 2.826968
H 2.048936 1.387397 0.924791
H -1.391782 -2.323402 2.826968
H 0.668027 1.118103 3.361557
H -2.011276 -2.028307 1.208698
N -1.376536 -0.773083 -1.388903
N 1.357778 -0.805573 -1.388903
N 0.018758 1.578657 -1.388903
C -1.764479 0.242698 -2.405174
C -0.745780 -1.972045 -1.973602
H -2.225989 -1.080732 -0.924791
C 2.080731 0.340159 -1.973602
C 0.672057 -1.649433 -2.405174
H 2.048936 -1.387397 -0.924791
C -1.334952 1.631886 -1.973602
C 1.092422 1.406735 -2.405174
H 0.177053 2.468129 -0.924791
H -2.846457 0.226610 -2.581870
H -1.302319 -0.019477 -3.361557
H -1.316234 -2.367019 -2.826968
H -0.750927 -2.755969 -1.208698
H 2.762203 0.727663 -1.208698
H 2.708016 0.043617 -2.826968
H 1.226978 -2.578409 -2.581870
H 0.668027 -1.118103 -3.361557
H -2.011276 2.028307 -1.208698
H -1.391782 2.323402 -2.826968
H 1.619479 2.351799 -2.581870
H 0.634292 1.137580 -3.361557

49
Co^2+ ^2A C_2 OPBE
Co 0.000000 0.000000 0.000298
N -1.319349 1.477478 0.006634
N -1.447313 -0.837760 -1.399352
N -1.419293 -0.887299 1.375756
C -2.346257 1.352740 1.090476
C -1.959616 0.283141 2.089007
C -2.451357 -1.691455 0.678270
C -2.040781 -2.016224 -0.750599
C -1.930920 1.571212 -1.341857
C -2.434669 0.206705 -1.767011
H -2.485647 2.314793 1.597178
H -1.290637 -2.815605 -0.765044
H -2.911885 -2.405005 -1.298232
H -0.996787 -1.154455 -2.251906
H -1.181503 0.646243 2.768314
H -3.307842 1.113965 0.627754
H -2.636907 0.205850 -2.844782
H -2.651765 -2.625226 1.217004
H -0.827903 2.353755 0.162880
H -3.391880 -0.017527 -1.286749
H -2.828523 0.032821 2.716169
H -0.980271 -1.483745 2.070420
H -2.743433 2.311192 -1.362370
H -3.397062 -1.140877 0.682368
H -1.159876 1.932760 -2.029130
N 1.447313 0.837760 -1.399352
N 1.419293 0.887299 1.375756
N 1.319349 -1.477478 0.006634
C 2.434669 -0.206705 -1.767011
C 2.040781 2.016224 -0.750599
H 0.996787 1.154455 -2.251906
C 1.959616 -0.283141 2.089007
C 2.451357 1.691455 0.678270
H 0.980271 1.483745 2.070420
C 1.930920 -1.571212 -1.341857
C 2.346257 -1.352740 1.090476
H 0.827903 -2.353755 0.162880
H 2.636907 -0.205850 -2.844782
H 3.391880 0.017527 -1.286749
H 2.911885 2.405005 -1.298232

H 1.290637 2.815605 -0.765044
H 1.181503 -0.646243 2.768314
H 2.828523 -0.032821 2.716169
H 2.651765 2.625226 1.217004
H 3.397062 1.140877 0.682368
H 1.159876 -1.932760 -2.029130
H 2.743433 -2.311192 -1.362370
H 2.485647 -2.314793 1.597178
H 3.307842 -1.113965 0.627754

49
Co^2+ ^4E D_3 OPBE
Co 0.000000 0.000000 0.000000
N 0.069100 -1.617900 -1.505400
N -1.435700 0.749100 -1.505400
N 1.366600 0.868800 -1.505400
C 1.132000 -1.376300 -2.512100
C 2.093100 -0.283300 -2.072100
C 0.625800 1.668500 -2.512100
C -0.801200 1.954300 -2.072100
C -1.291900 -1.671000 -2.072100
C -1.757900 -0.292300 -2.512100
H 1.699600 -2.293500 -2.709200
H -0.813700 2.726100 -1.294000
H -1.368700 2.360000 -2.922400
H -2.306600 1.046400 -1.075900
H 2.767700 -0.658400 -1.294000
H 0.665500 -1.109600 -3.465100
H -2.836000 -0.325200 -2.709200
H 1.136400 2.618600 -2.709200
H 0.247100 -2.520800 -1.075900
H -1.293700 -0.021600 -3.465100
H 2.728200 0.005300 -2.922400
H 2.059500 1.474400 -1.075900
H -1.359500 -2.365300 -2.922400
H 0.628200 1.131200 -3.465100
H -1.954000 -2.067700 -1.294000
N -1.435700 -0.749100 1.505400
N 1.366600 -0.868800 1.505400
N 0.069100 1.617900 1.505400
C -1.757900 0.292300 2.512100
C -0.801200 -1.954300 2.072100
H -2.306600 -1.046400 1.075900
C 2.093100 0.283300 2.072100
C 0.625800 -1.668500 2.512100
H 2.059500 -1.474400 1.075900
C -1.291900 1.671000 2.072100
C 1.132000 1.376300 2.512100
H 0.247100 2.520800 1.075900
H -2.836000 0.325200 2.709200
H -1.293700 0.021600 3.465100
H -1.368700 -2.360000 2.922400
H -0.813700 -2.726100 1.294000
H 2.767700 0.658400 1.294000
H 2.728200 -0.005300 2.922400
H 1.136400 -2.618600 2.709200
H 0.628200 -1.131200 3.465100
H -1.954000 2.067700 1.294000
H -1.359500 2.365300 2.922400
H 1.699600 2.293500 2.709200
H 0.665500 1.109600 3.465100

49
Co^2+ ^4B C_2 OPBE
Co 0.000000 0.000000 0.011521
N -1.527828 1.601632 0.068773
N -1.499302 -0.739612 -1.444719
N -1.511724 -0.882017 1.372871
C -2.535448 1.355492 1.129402
C -2.093497 0.266288 2.093178
C -2.504574 -1.683676 0.613899
C -2.054018 -1.953115 -0.813956
C -2.094632 1.667752 -1.290297
C -2.517158 0.289327 -1.770142
H -2.738947 2.271875 1.696317
H -1.267311 -2.716874 -0.827139
H -2.897587 -2.366346 -1.386317
H -1.062051 -1.031950 -2.313369
H -1.323757 0.647247 2.774269
H -3.485137 1.082962 0.659033
H -2.702132 0.326435 -2.850257
H -2.692007 -2.642258 1.112261
H -1.096496 2.502522 0.254095
H -3.471465 0.003864 -1.316835
H -2.947634 -0.029761 2.720024
H -1.092002 -1.486928 2.072579
H -2.952453 2.353769 -1.349721
H -3.464022 -1.157393 0.616334
H -1.319690 2.078672 -1.947460
N 1.499302 0.739612 -1.444719
N 1.511724 0.882017 1.372871
N 1.527828 -1.601632 0.068773
C 2.517158 -0.289327 -1.770142
C 2.054018 1.953115 -0.813956
H 1.062051 1.031950 -2.313369
C 2.093497 -0.266288 2.093178
C 2.504574 1.683676 0.613899
H 1.092002 1.486928 2.072579
C 2.094632 -1.667752 -1.290297
C 2.535448 -1.355492 1.129402
H 1.096496 -2.502522 0.254095
H 2.702132 -0.326435 -2.850257
H 3.471465 -0.003864 -1.316835
H 2.897587 2.366346 -1.386317
H 1.267311 2.716874 -0.827139
H 1.323757 -0.647247 2.774269
H 2.947634 0.029761 2.720024
H 2.692007 2.642258 1.112261
H 3.464022 1.157393 0.616334
H 1.319690 -2.078672 -1.947460
H 2.952453 -2.353769 -1.349721
H 2.738947 -2.271875 1.696317
H 3.485137 -1.082962 0.659033

49
Co^2+ ^2E D_3 SSB-D
Co 0.000000 0.000000 0.000000
N -0.017800 -1.589700 -1.375200
N 1.385600 0.779500 -1.375200
N -1.367900 0.810300 -1.375200
C -1.076800 -1.395300 -2.386000
C -2.073400 -0.347200 -1.935200
C -0.670000 1.630200 -2.386000
C 0.736000 1.969300 -1.935200
C 1.337400 -1.622000 -1.935200
C 1.746800 -0.234900 -2.386000
H -1.599100 -2.328500 -2.593100
H 0.713000 2.721400 -1.147400
H 1.295400 2.392700 -2.773100
H 2.235100 1.086300 -0.924700
H -2.713300 -0.743200 -1.147400
H -0.617500 -1.087000 -3.322700
H 2.816100 -0.220600 -2.593100
H -1.217000 2.549100 -2.593100
H -0.176700 -2.478800 -0.924700
H 1.250100 0.008700 -3.322700
H -2.719800 -0.074500 -2.773100
H -2.058400 1.392500 -0.924700
H 1.424400 -2.318200 -2.773100
H -0.632600 1.078300 -3.322700
H 2.000300 -1.978100 -1.147400
N 1.385600 -0.779500 1.375200
N -1.367900 -0.810300 1.375200
N -0.017800 1.589700 1.375200
C 1.746800 0.234900 2.386000
C 0.736000 -1.969300 1.935200

H	2.235100	-1.086300	0.924700
C	-2.073400	0.347200	1.935200
C	-0.670000	-1.630200	2.386000
H	-2.058400	-1.392500	0.924700
C	1.337400	1.622000	1.935200
C	-1.076800	1.395300	2.386000
H	-0.176700	2.478800	0.924700
H	2.816100	0.220600	2.593100
H	1.250100	-0.008700	3.322700
H	1.295400	-2.392700	2.773100
H	0.713000	-2.721400	1.147400
H	-2.713300	0.743200	1.147400
H	-2.719800	0.074500	2.773100
H	-1.217000	-2.549100	2.593100
H	-0.632600	-1.078300	3.322700
H	2.000300	1.978100	1.147400
H	1.424400	2.318200	2.773100
H	-1.599100	2.328500	2.593100
H	-0.617500	1.087000	3.322700

49

Co^2+ ^4E D_3 SSB-D

Co	0.000000000	0.000000000	0.000000000
N	0.087799750	1.620143467	1.471648780
N	-1.446985275	-0.734034919	1.471648780
N	1.359185525	-0.886108547	1.471648780
C	1.133880452	1.351722102	2.473763736
C	2.087971873	0.263245748	2.017697365
C	0.603685453	-1.657830328	2.473763736
C	-0.816008431	-1.939859559	2.017697365
C	-1.271963442	1.676613810	2.017697365
C	-1.737565905	0.306108226	2.473763736
H	1.706710991	2.251658121	2.693783267
H	-0.813247596	-2.683893072	1.220594642
H	-1.380303009	-2.360380811	2.853664649
H	-2.318469723	-1.018738660	1.051061420
H	2.730943380	0.637653458	1.220594642
H	0.662342741	1.057460556	3.408928435
H	-2.803348629	0.352226014	2.693783267
H	1.096637638	-2.603884136	2.693783267
H	0.276981302	2.517223008	1.051061420
H	-1.246959076	0.044875362	3.408928435
H	2.734301249	-0.015187066	2.853664649
H	2.041488421	-1.498484348	1.051061420
H	-1.353998240	2.375567876	2.853664649
H	0.584616335	-1.102335918	3.408928435
H	-1.917695784	2.046239614	1.220594642
N	-1.446985275	0.734034919	-1.471648780
N	1.359185525	0.886108547	-1.471648780
N	0.087799750	-1.620143467	-1.471648780
C	-1.737565905	-0.306108226	-2.473763736
C	-0.816008431	1.939859559	-2.017697365
H	-2.318469723	1.018738660	-1.051061420
C	2.087971873	-0.263245748	-2.017697365
C	0.603685453	1.657830328	-2.473763736
H	2.041488421	1.498484348	-1.051061420
C	-1.271963442	-1.676613810	-2.017697365
C	1.133880452	-1.351722102	-2.473763736
H	0.276981302	-2.517223008	-1.051061420
H	-2.803348629	-0.352226014	-2.693783267
H	-1.246959076	-0.044875362	-3.408928435
H	-1.380303009	2.360380811	-2.853664649
H	-0.813247596	2.683893072	-1.220594642
H	2.730943380	-0.637653458	-1.220594642
H	2.734301249	0.015187066	-2.853664649
H	1.096637638	2.603884136	-2.693783267
H	0.584616335	1.102335918	-3.408928435
H	-1.917695784	-2.046239614	-1.220594642
H	-1.353998240	-2.375567876	-2.853664649
H	1.706710991	-2.251658121	-2.693783267
H	0.662342741	-1.057460556	-3.408928435

49

Co^2+ ^4B C_2 SSB-D

Co	0.000000000	0.000000000	0.035740276
N	1.494280156	-1.607654543	0.106978474
N	1.451636427	0.710390915	-1.450099312
N	1.489832817	0.908163008	1.364179698
C	2.507103468	-1.324537271	1.137527451
C	2.055925704	-0.233368680	2.090543670
C	2.471099148	1.675596880	0.576315264
C	1.988043889	1.931630363	-0.840112320
C	2.025663589	-1.686308850	-1.256402426
C	2.462293220	-0.318702379	-1.746508322
H	2.743438053	-2.218043506	1.714068751
H	1.178787590	2.663121374	-0.833293760
H	2.807681448	2.360115944	-1.421951851
H	1.010577616	0.979684390	-2.316110638
H	1.271445602	-0.609162313	2.748070913
H	3.432948074	-1.025866647	0.650687930
H	2.665325566	-0.373357163	-2.815225111
H	2.690230180	2.631862357	1.049430088
H	1.073997544	-2.500729888	0.315580628
H	3.402148226	-0.041741434	-1.273844733
H	2.899743411	0.056176320	2.721578892
H	1.084726850	1.525497111	2.051366448
H	2.866397316	-2.379704647	-1.336935016
H	3.411072793	1.128687910	0.549182385
H	1.223792536	-2.072021709	-1.886401899
N	-1.451636427	-0.710390915	-1.450099312
N	-1.489832817	-0.908163008	1.364179698
N	-1.494280156	1.607654543	0.106978474
C	-2.462293220	0.318702379	-1.746508322
C	-1.988043889	-1.931630363	-0.840112320
H	-1.010577616	-0.979684390	-2.316110638
C	-2.055925704	0.233368680	2.090543670
C	-2.471099148	-1.675596880	0.576315264
H	-1.084726850	-1.525497111	2.051366448
C	-2.025663589	1.686308850	-1.256402426
C	-2.507103468	1.324537271	1.137527451
H	-1.073997544	2.500729888	0.315580628
H	-2.665325566	0.373357163	-2.815225111
H	-3.402148226	0.041741434	-1.273844733
H	-2.807681448	-2.360115944	-1.421951851
H	-1.178787590	-2.663121374	-0.833293760
H	-1.271445602	0.609162313	2.748070913
H	-2.899743411	-0.056176320	2.721578892
H	-2.690230180	-2.631862357	1.049430088
H	-3.411072793	-1.128687910	0.549182385
H	-1.223792536	2.072021709	-1.886401899
H	-2.866397316	2.379704647	-1.336935016
H	-2.743438053	2.218043506	1.714068751
H	-3.432948074	1.025866647	0.650687930

49

Co^2+ ^2A C_2 SSB-D

Co	0.000000000	0.000000000	0.002497274
N	-1.667101149	-1.549625582	-0.028025618
N	-1.226324448	0.855573273	1.352759885
N	-1.247700575	0.864880976	-1.341715295
C	-2.617669361	-1.162348402	-1.074813499
C	-1.983247962	-0.190924719	-2.053366004
C	-2.132845644	1.847654944	-0.671171788
C	-1.630123387	2.125250981	0.726694276
C	-2.171226783	-1.448591411	1.337442707
C	-2.374787149	-0.000422872	1.734490739
H	-2.979435444	-2.027566848	-1.629516381
H	-0.745670696	2.758524899	0.696082334
H	-2.394811890	2.643768083	1.309556124
H	-0.729727342	1.093718527	2.200274917
H	-1.263614875	-0.709456896	-2.686382467
H	-3.497090402	-0.708399001	-0.621815401
H	-2.555110342	0.059160457	2.806999692
H	-2.191201246	2.773892451	-1.240598058
H	-1.388571772	-2.505667604	-0.182137606

	H	-3.268695811	0.386768832	1.251444797
	H	-2.749451291	0.226074985	-2.710666845
	H	-0.706924486	1.364695779	-2.033685929
	H	-3.115204105	-1.980166313	1.490133944
5	H	-3.140785380	1.441530362	-0.633875459
	H	-1.432547445	-1.920387888	1.986437238
	N	1.226324448	-0.855573273	1.352759885
	N	1.247700575	-0.864880976	-1.341715295
	N	1.667101149	1.549625582	-0.028025618
10	C	2.374787149	0.000422872	1.734490739
	C	1.630123387	-2.125250981	0.726694276
	H	0.729727342	-1.093718527	2.200274917
	C	1.983247962	0.190924719	-2.053366004
	C	2.132845644	-1.847654944	-0.671171788
15	H	0.706924486	-1.364695779	-2.033685929
	C	2.171226783	1.448591411	1.337442707
	C	2.617669361	1.162348402	-1.074813499
	H	1.388571772	2.505667604	-0.182137606
	H	2.555110342	-0.059160457	2.806999692
20	H	3.268695811	-0.386768832	1.251444797
	H	2.394811890	-2.643768083	1.309556124
	H	0.745670696	-2.758524899	0.696082334
	H	1.263614875	0.709456896	-2.686382467
	H	2.749451291	-0.226074985	-2.710666845
25	H	2.191201246	-2.773892451	-1.240598058
	H	3.140785380	-1.441530362	-0.633875459
	H	1.432547445	1.920387888	1.986437238
	H	3.115204105	1.980166313	1.490133944
	H	2.979435444	2.027566848	-1.629516381
30	H	3.497090402	0.708399001	-0.621815401

49

Ni^3+ ^2E D_3 LDA

	Ni	0.000000	0.000000	0.000000
35	N	0.019800	-1.556700	1.276700
	N	-1.358100	0.761200	1.276700
	N	1.338200	0.795500	1.276700
	C	1.080800	-1.376000	2.301100
	C	2.076100	-0.344600	1.845900
40	C	0.651300	1.624000	2.301100
	C	-0.739600	1.970300	1.845900
	C	-1.336500	-1.625600	1.845900
	C	-1.732100	-0.247900	2.301100
	H	1.579300	-2.334600	2.522500
45	H	-0.738100	2.757500	1.071900
	H	-1.337700	2.371200	2.685700
	H	-2.203000	1.041400	0.760000
	H	2.757100	-0.739600	1.071900
	H	0.597500	-1.062000	3.240700
50	H	-2.811500	-0.200500	2.522500
	H	1.232100	2.535000	2.522500
	H	0.199700	-2.428600	0.760000
	H	-1.218500	0.013600	3.240700
	H	2.722300	-0.027100	2.685700
55	H	2.003400	1.387200	0.760000
	H	-1.384700	-2.344000	2.685700
	H	0.621000	1.048400	3.240700
	H	-2.019000	-2.018000	1.071900
	N	-1.358100	-0.761200	-1.276700
60	N	1.338200	-0.795500	-1.276700
	N	0.019800	1.556700	-1.276700
	C	-1.732100	0.247900	-2.301100
	C	-0.739600	-1.970300	-1.845900
	H	-2.203000	-1.041400	-0.760000
65	C	2.076100	0.344600	-1.845900
	C	0.651300	-1.624000	-2.301100
	H	2.003400	-1.387200	-0.760000
	C	-1.336500	1.625600	-1.845900
	C	1.080800	1.376000	-2.301100
70	H	0.199700	2.428600	-0.760000
	H	-2.811500	0.200500	-2.522500
	H	-1.218500	-0.013600	-3.240700
	H	-1.337700	-2.371200	-2.685700
	H	-0.738100	-2.757500	-1.071900
75	H	2.757100	0.739600	-1.071900
	H	2.722300	0.027100	-2.685700
	H	1.232100	-2.535000	-2.522500
	H	0.621000	-1.048400	-3.240700
	H	-2.019000	2.018000	-1.071900
80	H	-1.384700	2.344000	-2.685700
	H	1.579300	2.334600	-2.522500
	H	0.597500	1.062000	-3.240700

49

85 Ni^3+ ^2A C_2 LDA

	Ni	0.000000	0.000000	-0.004400
	N	-1.236700	-0.705500	-1.332800
	N	-1.252800	-0.725600	1.311100
	N	-1.348100	1.671800	0.033400
90	C	-2.281100	0.285600	-1.717000
	C	-1.880800	1.684200	-1.331900
	C	-2.357700	1.425800	1.080800
	C	-1.855600	0.393400	2.058000
	C	-1.802900	-1.935400	-0.736800
95	C	-2.270400	-1.591700	0.645200
	H	-2.489000	0.219600	-2.798200
	H	-1.092600	0.809700	2.739600
	H	-2.675200	0.033300	2.707400
	H	-0.710100	-1.302200	1.970300
100	H	-1.104000	2.091100	-2.004200
	H	-3.216000	-0.000600	-1.208600
	H	-2.466000	-2.495400	1.246100
	H	-2.621100	2.355000	1.613300
	H	-0.714400	-0.977100	-2.178600
105	H	-3.219100	-1.031700	0.614000
	H	-2.750500	2.360600	-1.436200
	H	-0.882200	2.569700	0.214100
	H	-2.627200	-2.331700	-1.358600
	H	-3.290500	1.085400	0.601200
110	H	-1.016800	-2.708400	-0.729400
	N	1.348100	-1.671800	0.033400
	N	1.236700	0.705500	-1.332800
	N	1.252800	0.725600	1.311100
	C	2.357700	-1.425800	1.080800
115	C	1.880800	-1.684200	-1.331900
	H	0.882200	-2.569700	0.214100
	C	1.802900	1.935400	-0.736800
	C	2.281100	-0.285600	-1.717000
	H	0.714400	0.977100	-2.178600
120	C	1.855600	-0.393400	2.058000
	C	2.270400	1.591700	0.645200
	H	0.710100	1.302200	1.970300
	H	2.621100	-2.355000	1.613300
	H	3.290500	-1.085400	0.601200
125	H	2.750500	-2.360600	-1.436200
	H	1.104000	-2.091100	-2.004200
	H	1.016800	2.708400	-0.729400
	H	2.627200	2.331700	-1.358600
	H	2.489000	-0.219600	-2.798200
130	H	3.216000	0.000600	-1.208600
	H	1.092600	-0.809700	2.739600
	H	2.675200	-0.033300	2.707400
	H	2.466000	2.495400	1.246100
	H	3.219100	1.031700	0.614000
135				

49

Ni^3+ ^2E D_3 OPBE

	Ni	0.000000	0.000000	0.000000
	N	-1.371300	-0.763100	-1.362800
140	N	1.346500	-0.806000	-1.362800
	N	0.024700	1.569100	-1.362800
	C	-1.763700	0.258600	-2.382700
	C	-1.335900	1.642100	-1.943400
	C	1.105800	1.398100	-2.382700
145	C	2.090000	0.335900	-1.943400
	C	-0.754100	-1.977900	-1.943400

C	0.657900	-1.656700	-2.382700
H	-2.847200	0.229500	-2.548700
H	2.784100	0.713300	-1.185300
H	2.712100	0.012900	-2.790300
H	2.018800	-1.391900	-0.872000
H	-2.009800	2.054500	-1.185300
H	-1.302500	-0.008300	-3.337300
H	1.224800	-2.580500	-2.548700
H	1.622400	2.351000	-2.548700
H	-2.214900	-1.052400	-0.872000
H	0.658400	-1.123900	-3.337300
H	-1.367200	2.342200	-2.790300
H	0.196000	2.444300	-0.872000
H	-1.344800	-2.355200	-2.790300
H	0.644100	1.132100	-3.337300
H	-0.774300	-2.767800	-1.185300
N	0.024700	-1.569100	1.362800
N	-1.371300	0.763100	1.362800
N	1.346500	0.806000	1.362800
C	1.105800	-1.398100	2.382700
C	-1.335900	-1.642100	1.943400
H	0.196000	-2.444300	0.872000
C	-0.754100	1.977900	1.943400
C	-1.763700	-0.258600	2.382700
H	-2.214900	1.052400	0.872000
C	2.090000	-0.335900	1.943400
C	0.657900	1.656700	2.382700
H	2.018800	1.391900	0.872000
H	1.622400	-2.351000	2.548700
H	0.644100	-1.132100	3.337300
H	-1.367200	-2.342200	2.790300
H	-2.009800	-2.054500	1.185300
H	-0.774300	2.767800	1.185300
H	-1.344800	2.355200	2.790300
H	-2.847200	-0.229500	2.548700
H	-1.302500	0.008300	3.337300
H	2.784100	-0.713300	1.185300
H	2.712100	-0.012900	2.790300
H	1.224800	2.580500	2.548700
H	0.658400	1.123900	3.337300

49
Ni^3+ ^2A C_2 OPBE

Ni	0.000000	0.000000	-0.007100
N	-1.254400	-0.800500	-1.345600
N	-1.269700	-0.828000	1.318300
N	-1.581500	1.573600	0.036700
C	-2.379400	0.108600	-1.749000
C	-2.129900	1.543200	-1.330500
C	-2.560200	1.253200	1.106000
C	-1.975400	0.238400	2.070700
C	-1.721900	-2.081400	-0.749700
C	-2.202800	-1.799400	0.651000
H	-2.524600	0.048300	-2.834400
H	-1.260600	0.701000	2.759800
H	-2.763100	-0.197900	2.701200
H	-0.706900	-1.352900	1.985300
H	-1.416100	2.041100	-1.996400
H	-3.298700	-0.270800	-1.295400
H	-2.268100	-2.722200	1.239500
H	-2.847400	2.157000	1.656500
H	-0.733700	-1.035700	-2.189100
H	-3.205300	-1.364100	0.647100
H	-3.066500	2.113300	-1.414700
H	-1.219400	2.508600	0.206500
H	-2.515000	-2.528400	-1.365300
H	-3.481800	0.875400	0.654000
H	-0.886200	-2.786700	-0.760100
N	1.581500	-1.573600	0.036700
N	1.254400	0.800500	-1.345600
N	1.269700	0.828000	1.318300
C	2.560200	-1.253200	1.106000
C	2.129900	-1.543200	-1.330500
H	1.219400	-2.508600	0.206500
C	1.721900	2.081400	-0.749700
C	2.379400	-0.108600	-1.749000
H	0.733700	1.035700	-2.189100
C	1.975400	-0.238400	2.070700
C	2.202800	1.799400	0.651000
H	0.706900	1.352900	1.985300
H	2.847400	-2.157000	1.656500
H	3.481800	-0.875400	0.654000
H	3.066500	-2.113300	-1.414700
H	1.416100	-2.041100	-1.996400
H	0.886200	2.786700	-0.760100
H	2.515000	2.528400	-1.365300
H	2.524600	-0.048300	-2.834400
H	3.298700	0.270800	-1.295400
H	1.260600	-0.701000	2.759800
H	2.763100	0.197900	2.701200
H	2.268100	2.722200	1.239500
H	3.205300	1.364100	0.647100

49
Ni^3+ ^2E D_3 SSB-D

Ni	0.000000000	0.000000000	0.000000000
N	0.028123588	1.578213723	-1.328353014
N	-1.380834971	-0.764751120	-1.328353014
N	1.352711383	-0.813462604	-1.328353014
C	1.094817934	1.385538446	-2.341219217
C	2.083250454	0.335307445	-1.886950381
C	0.652502525	-1.640909367	-2.341219217
C	-0.751240462	-1.971801538	-1.886950381
C	-1.332009992	1.636494094	-1.886950381
C	-1.747320460	0.255370921	-2.341219217
H	1.610211823	2.326102674	-2.532632958
H	-0.750462035	-2.733276017	-1.108191382
H	-1.332208566	-2.371304479	-2.721208506
H	-2.222692264	-1.050916137	-0.845511189
H	2.742317484	0.716718822	-1.108191382
H	0.631164575	1.086100294	-3.277897615
H	-2.819569919	0.231433007	-2.532632958
H	1.209358096	-2.557535681	-2.532632958
H	0.201226061	2.450366034	-0.845511189
H	-1.256172733	0.003554409	-3.277897615
H	2.719714202	0.031925778	-2.721208506
H	2.021466204	-1.399449897	-0.845511189
H	-1.387505636	2.339378701	-2.721208506
H	0.625008158	-1.089654703	-3.277897615
H	-1.991855449	2.016557195	-1.108191382
N	-1.380834971	0.764751120	1.328353014
N	1.352711383	0.813462604	1.328353014
N	0.028123588	-1.578213723	1.328353014
C	-1.747320460	-0.255370921	2.341219217
C	-0.751240462	1.971801538	1.886950381
H	-2.222692264	1.050916137	0.845511189
C	2.083250454	-0.335307445	1.886950381
C	0.652502525	1.640909367	2.341219217
H	2.021466204	1.399449897	0.845511189
C	-1.332009992	-1.636494094	1.886950381
C	1.094817934	-1.385538446	2.341219217
H	0.201226061	-2.450366034	0.845511189
H	-2.819569919	-0.231433007	2.532632958
H	-1.256172733	-0.003554409	3.277897615
H	-1.332208566	2.371304479	2.721208506
H	-0.750462035	2.733276017	1.108191382
H	2.742317484	-0.716718822	1.108191382
H	2.719714202	-0.031925778	2.721208506
H	1.209358096	2.557535681	2.532632958
H	0.625008158	1.089654703	3.277897615
H	-1.991855449	-2.016557195	1.108191382
H	-1.387505636	-2.339378701	2.721208506
H	1.610211823	-2.326102674	2.532632958
H	0.631164575	-1.086100294	3.277897615

49
Ni^3+ ^2A C_2 OPBE

Ni	0.000000000	0.000000000	0.000035566
N	1.575299182	-1.496298281	0.043563766
N	1.184349265	0.860429612	-1.354976989
N	1.206918518	0.896896958	1.331678305
C	2.544729841	-1.138559548	1.096308026
C	1.929054255	-0.153242409	2.069774631
C	2.101638023	1.871494794	0.646201276
C	1.592071357	2.143243953	-0.745701850
C	2.098437916	-1.450863353	-1.325231038
C	2.324295302	-0.013398023	-1.741043956
H	2.876184729	-2.022572756	1.639588237
H	0.718699383	2.791710108	-0.732893743
H	2.353883580	2.635222919	-1.354229792
H	0.656710012	1.077048967	-2.192048314
H	1.214802145	-0.640822126	2.732465419
H	3.432621120	-0.710307717	0.636976624
H	2.482297328	0.044180429	-2.817530570
H	2.164605950	2.794084618	1.221945467
H	1.247246899	-2.435772162	0.216881395
H	3.223044045	0.374613719	-1.269052611
H	2.700689322	0.286073369	2.705622308
H	0.635734240	1.405680820	1.995061111
H	3.034179568	-2.004403085	-1.431337328
H	3.102651386	1.449371964	0.613113014
H	1.369944528	-1.941037633	-1.971543570
N	-1.184349265	-0.860429612	-1.354976989
N	-1.206918518	-0.896896958	1.331678305
N	-1.575299182	1.496298281	0.043563766
C	-2.324295302	0.013398023	-1.741043956
C	-1.592071357	-2.143243953	-0.745701850
H	-0.656710012	-1.077048967	-2.192048314
C	-1.929054255	0.153242409	2.069774631
C	-2.101638023	-1.871494794	0.646201276
H	-0.635734240	-1.405680820	1.995061111
C	-2.098437916	1.450863353	-1.325231038
C	-2.544729841	1.138559548	1.096308026
H	-1.247246899	2.435772162	0.216881395
H	-2.482297328	-0.044180429	-2.817530570
H	-3.223044045	-0.374613719	-1.269052611
H	-2.353883580	-2.635222919	-1.354229792
H	-0.718699383	-2.791710108	-0.732893743
H	-1.214802145	0.640822126	2.732465419
H	-2.700689322	-0.286073369	2.705622308
H	-2.164605950	-2.794084618	1.221945467
H	-3.102651386	-1.449371964	0.613113014
H	-1.369944528	1.941037633	-1.971543570
H	-3.034179568	2.004403085	-1.431337328
H	-2.876184729	2.022572756	1.639588237
H	-3.432621120	0.710307717	0.636976624

49

Ni^3+ ^4E D_3 LDA

Ni	0.000000	0.000000	0.000000
N	0.227500	-1.577900	-1.380300
N	-1.480300	0.592000	-1.380300
N	1.252800	0.986000	-1.380300
C	1.244700	-1.228400	-2.393100
C	2.102200	-0.089400	-1.910400
C	0.441400	1.692100	-2.393100
C	-0.973700	1.865300	-1.910400
C	-1.128500	-1.775900	-1.910400
C	-1.686200	-0.463800	-2.393100
H	1.874100	-2.100700	-2.637500
H	-1.034100	2.618200	-1.103900
H	-1.616600	2.241700	-2.730500
H	-2.367300	0.776500	-0.894200
H	2.784500	-0.413600	-1.103900
H	0.727200	-0.959700	-3.328400
H	-2.756300	-0.572600	-2.637500
H	0.882200	2.673400	-2.637500
H	0.511200	-2.438400	-0.894200
H	-1.194700	-0.149900	-3.328400
H	2.749700	0.279200	-2.730500
H	1.856100	1.661900	-0.894200
H	-1.133100	-2.520900	-2.730500
H	0.467500	1.109600	-3.328400
H	-1.750400	-2.204700	-1.103900
N	-1.480300	-0.592000	1.380300
N	1.252800	-0.986000	1.380300
N	0.227500	1.577900	1.380300
C	-1.686200	0.463800	2.393100
C	-0.973700	-1.865300	1.910400
H	-2.367300	-0.776500	0.894200
C	2.102200	0.089400	1.910400
C	0.441400	-1.692100	2.393100
H	1.856100	-1.661900	0.894200
C	-1.128500	1.775900	1.910400
C	1.244700	1.228400	2.393100
H	0.511200	2.438400	0.894200
H	-2.756300	0.572600	2.637500
H	-1.194700	0.149900	3.328400
H	-1.616600	-2.241700	2.730500
H	-1.034100	-2.618200	1.103900
H	2.784500	0.413600	1.103900
H	2.749700	-0.279200	2.730500
H	0.882200	-2.673400	2.637500
H	0.467500	-1.109600	3.328400
H	-1.750400	2.204700	1.103900
H	-1.133100	2.520900	2.730500
H	1.874100	2.100700	2.637500
H	0.727200	0.959700	3.328400

49

Ni^3+ ^4B C_2 LDA

Ni	0.000000	0.000000	0.228400
N	1.360900	-1.578300	0.280000
N	1.291400	0.622600	-1.381000
N	1.488100	1.013600	1.294500
C	2.433400	-1.238500	1.242000
C	2.014400	-0.081600	2.114000
C	2.470000	1.700300	0.433000
C	1.883400	1.891200	-0.934700
C	1.830100	-1.763900	-1.101500
C	2.271200	-0.441600	-1.671600
H	2.692200	-2.104700	1.873200
H	1.087000	2.656300	-0.922800
H	2.647500	2.247800	-1.652600
H	0.720300	0.811000	-2.214400
H	1.226000	-0.381900	2.830300
H	3.350200	-0.994500	0.680400
H	2.440300	-0.532600	-2.758700
H	2.769000	2.668000	0.870300
H	0.917700	-2.456400	0.578300
H	3.241100	-0.141700	-1.243100
H	2.867900	0.259000	2.736600
H	1.028300	1.700300	1.908100
H	2.661400	-2.491300	-1.156600
H	3.385800	1.088500	0.393100
H	1.000900	-2.202100	-1.684700
N	-1.291400	-0.622600	-1.381000
N	-1.488100	-1.013600	1.294500
N	-1.360900	1.578300	0.280000
C	-2.271200	0.441600	-1.671600
C	-1.883400	-1.891200	-0.934700
H	-0.720300	-0.811000	-2.214400
C	-2.014400	0.081600	2.114000
C	-2.470000	-1.700300	0.433000
H	-1.028300	-1.700300	1.908100
C	-1.830100	1.763900	-1.101500
C	-2.433400	1.238500	1.242000
H	-0.917700	2.456400	0.578300
H	-2.440300	0.532600	-2.758700
H	-3.241100	0.141700	-1.243100
H	-2.647500	-2.247800	-1.652600
H	-1.087000	-2.656300	-0.922800
H	-1.226000	0.381900	2.830300

H -2.867900 -0.259000 2.736600
H -2.769000 -2.668000 0.870300
H -3.385800 -1.088500 0.393100
H -1.000900 2.202100 -1.684700
H -2.661400 2.491300 -1.156600
H -2.692200 2.104700 1.873200
H -3.350200 0.994500 0.680400

49
Ni^3+ ^4E D_3 OPBE
Ni 0.000000 0.000000 0.000000
N 0.276500 -1.583600 -1.488400
N -1.509700 0.552300 -1.488400
N 1.233200 1.031300 -1.488400
C 1.306000 -1.213100 -2.497300
C 2.117300 -0.020300 -2.033900
C 0.397600 1.737500 -2.497300
C -1.041100 1.843800 -2.033900
C -1.076200 -1.823500 -2.033900
C -1.703500 -0.524500 -2.497300
H 1.975500 -2.061100 -2.685200
H -1.149300 2.599400 -1.247700
H -1.681900 2.175300 -2.865300
H -2.400500 0.723700 -1.026600
H 2.825700 -0.304400 -1.247700
H 0.809500 -1.004100 -3.448600
H -2.772800 -0.680300 -2.685200
H 0.797200 2.741400 -2.685200
H 0.573500 -2.440700 -1.026600
H -1.274300 -0.199000 -3.448600
H 2.724800 0.369000 -2.865300
H 1.827000 1.717100 -1.026600
H -1.042900 -2.544200 -2.865300
H 0.464800 1.203100 -3.448600
H -1.676500 -2.295000 -1.247700
N -1.509700 -0.552300 1.488400
N 1.233200 -1.031300 1.488400
N 0.276500 1.583600 1.488400
C -1.703500 0.524500 2.497300
C -1.041100 -1.843800 2.033900
H -2.400500 -0.723700 1.026600
C 2.117300 0.020300 2.033900
C 0.397600 -1.737500 2.497300
H 1.827000 -1.717100 1.026600
C -1.076200 1.823500 2.033900
C 1.306000 1.213100 2.497300
H 0.573500 2.440700 1.026600
H -2.772800 0.680300 2.685200
H -1.274300 0.199000 3.448600
H -1.681900 -2.175300 2.865300
H -1.149300 -2.599400 1.247700
H 2.825700 0.304400 1.247700
H 2.724800 -0.369000 2.865300
H 0.797200 -2.741400 2.685200
H 0.464800 -1.203100 3.448600
H -1.676500 2.295000 1.247700
H -1.042900 2.544200 2.865300
H 1.975500 2.061100 2.685200
H 0.809500 1.004100 3.448600

49
Ni^3+ ^4B C_2 OPBE
Ni 0.000000 0.000000 0.175100
N 1.473600 -1.565300 0.287100
N 1.415100 0.598400 -1.460100
N 1.565500 1.068200 1.239700
C 2.524300 -1.206200 1.282600
C 2.111300 0.003500 2.102800
C 2.547300 1.766700 0.367600
C 1.995900 1.890200 -1.033100
C 1.988800 -1.789700 -1.083000
C 2.409000 -0.477500 -1.714700
H 2.717400 -2.048100 1.957700
H 1.207100 2.648300 -1.079500
H 2.778600 2.215600 -1.735000
H 0.890900 0.768400 -2.315000
H 1.341500 -0.257400 2.840100
H 3.466400 -1.019800 0.759800
H 2.544700 -0.616300 -2.794600
H 2.774400 2.760200 0.773100
H 1.053800 -2.442800 0.586200
H 3.379200 -0.154700 -1.328400
H 2.970400 0.372500 2.685700
H 1.113900 1.757900 1.838900
H 2.837700 -2.487800 -1.082500
H 3.488300 1.210400 0.379900
H 1.195400 -2.273000 -1.662500
N -1.415100 -0.598400 -1.460100
N -1.565500 -1.068200 1.239700
N -1.473600 1.565300 0.287100
C -2.409000 0.477500 -1.714700
C -1.995900 -1.890200 -1.033100
H -0.890900 -0.768400 -2.315000
C -2.111300 -0.003500 2.102800
C -2.547300 -1.766700 0.367600
H -1.113900 -1.757900 1.838900
C -1.988800 1.789700 -1.083000
C -2.524300 1.206200 1.282600
H -1.053800 2.442800 0.586200
H -2.544700 0.616300 -2.794600
H -3.379200 0.154700 -1.328400
H -2.778600 -2.215600 -1.735000
H -1.207100 -2.648300 -1.079500
H -1.341500 0.257400 2.840100
H -2.970400 -0.372500 2.685700
H -2.774400 -2.760200 0.773100
H -3.488300 -1.210400 0.379900
H -1.195400 2.273000 -1.662500
H -2.837700 2.487800 -1.082500
H -2.717400 2.048100 1.957700
H -3.466400 1.019800 0.759800

49
Ni^3+ ^4E D_3 SSB-D
Ni 0.000000000 0.000000000 0.000000000
N 0.269737470 1.583567582 1.428537335
N -1.506278489 -0.558184289 1.428537335
N 1.236541019 -1.025383292 1.428537335
C 1.285619166 1.208886715 2.433569427
C 2.109063723 0.033766508 1.953753675
C 0.404117022 -1.717822215 2.433569427
C -1.025289208 -1.843386017 1.953753675
C -1.083774516 1.809619508 1.953753675
C -1.689736189 0.508935500 2.433569427
H 1.943730612 2.051490676 2.643296663
H -1.103307450 -2.572242684 1.146112480
H -1.661494752 -2.200298657 2.768401847
H -2.392253032 -0.728139992 0.971950773
H 2.779281234 0.330629062 1.146112480
H 0.784372012 0.965058473 3.367033869
H -2.748508347 0.657574750 2.643296663
H 0.804777735 -2.709065426 2.643296663
H 0.565538786 2.435821894 0.971950773
H -1.227951160 0.196756852 3.367033869
H 2.736261909 -0.338747335 2.768401847
H 1.826714246 -1.707681902 0.971950773
H -1.074767157 2.539045992 2.768401847
H 0.443579148 -1.161815325 3.367033869
H -1.675973784 2.241613622 1.146112480
N -1.506278489 0.558184289 -1.428537335
N 1.236541019 1.025383292 -1.428537335
N 0.269737470 -1.583567582 -1.428537335
C -1.689736189 -0.508935500 -2.433569427
C -1.025289208 1.843386017 -1.953753675
H -2.392253032 0.728139992 -0.971950773
C 2.109063723 -0.033766508 -1.953753675

C	0.404117022	1.717822215	-2.433569427
H	1.826714246	1.707681902	-0.971950773
C	-1.083774516	-1.809619508	-1.953753675
C	1.285619166	-1.208886715	-2.433569427
H	0.565538786	-2.435821894	-0.971950773
H	-2.748508347	-0.657574750	-2.643296663
H	-1.227951160	-0.196756852	-3.367033869
H	-1.661494752	2.200298657	-2.768401847
H	-1.103307450	2.572242684	-1.146112480
H	2.779281234	-0.330629062	-1.146112480
H	2.736261909	0.338747335	-2.768401847
H	0.804777735	2.709065426	-2.643296663
H	0.443579148	1.161815325	-3.367033869
H	-1.675973784	-2.241613622	-1.146112480
H	-1.074767157	-2.539045992	-2.768401847
H	1.943730612	-2.051490676	-2.643296663
H	0.784372012	-0.965058473	-3.367033869

49

Ni^3+ ^4B C_2 SSB-D

Ni	0.000000000	0.000000000	0.222851726
N	-1.424960256	1.576942170	0.284126089
N	-1.307937738	-0.617553329	-1.422543304
N	-1.531359160	-1.043025358	1.271098749
C	-2.501796155	1.215147231	1.232753627
C	-2.087870981	0.038167924	2.093476624
C	-2.490367025	-1.735229701	0.386902470
C	-1.894210955	-1.893774991	-0.988833272
C	-1.869645197	1.770974943	-1.104352507
C	-2.281796866	0.450826925	-1.720099479
H	-2.747030161	2.057752668	1.877630723
H	-1.096117003	-2.635322449	-0.981849746
H	-2.648755011	-2.238442107	-1.700922777
H	-0.759330408	-0.803625005	-2.250070947
H	-1.318506996	0.329184947	2.811751427
H	-3.405483322	0.979168913	0.676039174
H	-2.392299682	0.572206383	-2.797811041
H	-2.750896213	-2.710593497	0.796634292
H	-1.021779219	2.452645021	0.588269301
H	-3.255017557	0.149049168	-1.341897053
H	-2.943685179	-0.313997428	2.677782054
H	-1.107709673	-1.723961942	1.889203913
H	-2.702927109	2.473852632	-1.166653458
H	-3.409261774	-1.155945468	0.345404327
H	-1.037857388	2.215030360	-1.649959272
N	1.307937738	0.617553329	-1.422543304
N	1.531359160	1.043025358	1.271098749
N	1.424960256	-1.576942170	0.284126089
C	2.281796866	-0.450826925	-1.720099479
C	1.894210955	1.893774991	-0.988833272
H	0.759330408	0.803625005	-2.250070947
C	2.087870981	-0.038167924	2.093476624
C	2.490367025	1.735229701	0.386902470
H	1.107709673	1.723961942	1.889203913
C	1.869645197	-1.770974943	-1.104352507
C	2.501796155	-1.215147231	1.232753627
H	1.021779219	-2.452645021	0.588269301
H	2.392299682	-0.572206383	-2.797811041
H	3.255017557	-0.149049168	-1.341897053
H	2.648755011	2.238442107	-1.700922777
H	1.096117003	2.635322449	-0.981849746
H	1.318506996	-0.329184947	2.811751427
H	2.943685179	0.313997428	2.677782054
H	2.750896213	2.710593497	0.796634292
H	3.409261774	1.155945468	0.345404327
H	1.037857388	-2.215030360	-1.649959272
H	2.702927109	-2.473852632	-1.166653458
H	2.747030161	-2.057752668	1.877630723
H	3.405483322	-0.979168913	0.676039174