

Supplementary data for the article:

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Supplementary Information for

**Resolving origin of the multimode Jahn-Teller effect in
metallophthalocyanines**

Ljubica Andjelković^a, Stepan Stepanović^a, Filip Vlahović^b, Matija Zlataar^a, Maja Gruden^{c,*}

^a*Department of Chemistry, IChTM, University of Belgrade, Studentski Trg 12-16, 11001 Belgrade, Republic of Serbia*

^b*Innovation center of the Faculty of Chemistry, University of Belgrade, Studentski Trg 12-16, 11001 Belgrade, Republic of Serbia*

^c*Center for Computational Chemistry and Bioinformatics, Faculty of Chemistry, University of Belgrade, Studentski Trg 12-16, 11001 Belgrade, Republic of Serbia*

Table S1. EDA analysis for MnPc in HS and LS point groups using different density functional approximations; energies are given in cm⁻¹.

p. S2

Table S2. EDA analysis for MgPc in HS and LS point groups using different density functional approximations; energies are given in cm⁻¹.

p. S3

Cartesian coordinates and electronic occupations for all spin states of MnPc obtained by all performed DFAs.

p. S3-S29

Cartesian coordinates for Pc³⁻, MgPc⁻ and MnPc in HS and LS minimum structures obtained by LDA.

p. S30-S35

Table S1 EDA analysis for MnPc in HS and LS point groups using different density functional approximations; energies are given in cm⁻¹.

	LDA		OPBE		OPBE/LDA*	
	<i>D</i> _{4h}	<i>D</i> _{2h}	<i>D</i> _{4h}	<i>D</i> _{2h}	<i>D</i> _{4h}	<i>D</i> _{2h}
E _{prep} (Mn ²⁺)	35369	35369	38820	38820	38820	38820
E _{prep} (Pc ²⁻)	3830	4005	3846	3950	5043	5224
E _{int}	-286926	-287239	-263128	-263410	-264268	-264618
E _{Pauli}	91115	91270	89844	89883	97513	97657
E _{elstat}	-218983	-219139	-203610	-203670	-207748	-207892
Total steric	-127869	-127870	-113765	-113787	-110234	-110234
<i>A</i> _g	-74362	-74493	-71795	-71994	-73470	-73632
<i>B</i> _{1g}	-11498	-11554	-9726	-9758	-10423	-10470
<i>B</i> _{2g}	-6249	-6361	-3752	-3975	-4463	-4599
<i>B</i> _{3g}	-18470	-18400	-16516	-16243	-17185	-17094
<i>A</i> _u	-4027	-4023	-3978	-3981	-4011	-4009
<i>B</i> _{1u}	-19911	-19956	-19165	-19190	-19778	-19828
<i>B</i> _{2u}	-12623	-12649	-12482	-12514	-12628	-12652
<i>B</i> _{3u}	-11915	-11931	-11948	-11968	-12075	-12099
ΔE _{orbint}	-159057	-159368	-149363	-149623	-154033	-154384

*OPBE single point on LDA geometries

Table S2 EDA analysis for MgPc in HS and LS point groups using different density functional approximations; energies are given in cm⁻¹.

	LDA		OPBE		OPBE/LDA*	
	<i>D</i> _{4h}	<i>D</i> _{2h}	<i>D</i> _{4h}	<i>D</i> _{2h}	<i>D</i> _{4h}	<i>D</i> _{2h}
E _{prep} (Pc ³⁻)	2408	2112	2251	1969	2307	2007
E _{int}	-278703	-278807	-268217	-268357	-268730	-268839
E _{Pauli}	36502	36576	35057	35049	37866	37945
E _{elstat}	-227656	-227839	-218998	-219163	-221235	-221425
Total steric	-191154	-191263	-183941	-184114	-183368	-183480
<i>A</i> _g	-19733	-19778	-19065	-19104	-19062	-19108
<i>B</i> _{1g}	-4751	-4765	-4706	-4718	-4830	-4845
<i>B</i> _{2g}	-11931	-11931	-11292	-11281	-11541	-11536
<i>B</i> _{3g}	-10135	-9952	-9787	-9607	-10042	-9861
<i>A</i> _u	-3738	-3751	-3714	-3723	-3726	-3738
<i>B</i> _{1u}	-15335	-15388	-14521	-14572	-14875	-14930
<i>B</i> _{2u}	-10897	-10914	-10522	-10530	-10568	-10580
<i>B</i> _{3u}	-11029	-11064	-10670	-10708	-10718	-10759
ΔE _{orbint}	-87549	-87544	-84277	-84243	-85363	-85358

*OPBE single point on LDA geometries

Cartesian coordinates and electronic occupations for all spin states of MnPc obtained by all performed DFAs.

level of theory bp86
spin state HS

Occup.	alpha	beta	
A _{1g}	21.0 //	20.0	
A _{2g}	11.0 //	11.0	
B _{1g}	16.0 //	15.0	
B _{2g}	14.0 //	13.0	
E _{1g}	12.0 //	10.0	
A _{1u}	2.0 //	2.0	
A _{2u}	6.0 //	6.0	
B _{1u}	2.0 //	2.0	
B _{2u}	3.0 //	3.0	
E _{1u}	60.0 //	60.0	
Mn	0.00000000	0.00000000	0.00000000
N	2.40279915	2.40279915	0.00000000
N	-2.40279915	2.40279915	0.00000000
N	-2.40279915	-2.40279915	0.00000000
N	2.40279915	-2.40279915	0.00000000
N	0.00000000	2.02952598	0.00000000
C	1.13176726	2.81196693	0.00000000
C	0.70834608	4.21068983	0.00000000
C	-0.70834608	4.21068983	0.00000000
C	-1.13176726	2.81196693	0.00000000
N	-2.02952598	0.00000000	0.00000000
C	-2.81196693	1.13176726	0.00000000
C	-4.21068983	0.70834608	0.00000000
C	-4.21068983	-0.70834608	0.00000000
C	-2.81196693	-1.13176726	0.00000000
N	0.00000000	-2.02952598	0.00000000
C	-1.13176726	-2.81196693	0.00000000
C	-0.70834608	-4.21068983	0.00000000
C	0.70834608	-4.21068983	0.00000000
C	1.13176726	-2.81196693	0.00000000
N	2.02952598	0.00000000	0.00000000
C	2.81196693	-1.13176726	0.00000000
C	4.21068983	-0.70834608	0.00000000
C	4.21068983	0.70834608	0.00000000
C	2.81196693	1.13176726	0.00000000
C	-5.40686430	-1.42505052	0.00000000
C	-6.60197884	-0.70362423	0.00000000
C	-6.60197884	0.70362423	0.00000000
C	-5.40686430	1.42505052	0.00000000
C	-1.42505052	5.40686430	0.00000000
C	-0.70362423	6.60197884	0.00000000
C	0.70362423	6.60197884	0.00000000
C	1.42505052	5.40686430	0.00000000
C	5.40686430	1.42505052	0.00000000
C	6.60197884	0.70362423	0.00000000

C	6.60197884	-0.70362423	0.00000000
C	5.40686430	-1.42505052	0.00000000
C	1.42505052	-5.40686430	0.00000000
C	0.70362423	-6.60197884	0.00000000
C	-0.70362423	-6.60197884	0.00000000
C	-1.42505052	-5.40686430	0.00000000
H	-5.39810748	-2.51324161	0.00000000
H	-7.55227746	-1.23589823	0.00000000
H	-7.55227746	1.23589823	0.00000000
H	-5.39810748	2.51324161	0.00000000
H	-2.51324161	5.39810748	0.00000000
H	-1.23589823	7.55227746	0.00000000
H	1.23589823	7.55227746	0.00000000
H	2.51324161	5.39810748	0.00000000
H	5.39810748	2.51324161	0.00000000
H	7.55227746	1.23589823	0.00000000
H	7.55227746	-1.23589823	0.00000000
H	5.39810748	-2.51324161	0.00000000
H	2.51324161	-5.39810748	0.00000000
H	1.23589823	-7.55227746	0.00000000
H	-1.23589823	-7.55227746	0.00000000
H	-2.51324161	-5.39810748	0.00000000

level of theory bp86
spin state IS

Occup.	alpha	beta	
A _{1g}	21.0 //	20.0	
A _{2g}	11.0 //	11.0	
B _{1g}	15.0 //	15.0	
B _{2g}	14.0 //	13.0	
E _{1g}	12.0 //	11.0	
A _{1u}	2.0 //	2.0	
A _{2u}	6.0 //	6.0	
B _{1u}	2.0 //	2.0	
B _{2u}	3.0 //	3.0	
E _{1u}	60.0 //	60.0	
Mn	0.00000000	0.00000000	0.00000000
N	2.39266329	2.39266329	0.00000000
N	-2.39266329	2.39266329	0.00000000
N	-2.39266329	-2.39266329	0.00000000
N	2.39266329	-2.39266329	0.00000000
N	0.00000000	1.94821420	0.00000000
C	1.12597065	2.76852572	0.00000000
C	0.70440636	4.15443193	0.00000000
C	-0.70440636	4.15443193	0.00000000
C	-1.12597065	2.76852572	0.00000000
N	-1.94821420	0.00000000	0.00000000
C	-2.76852572	1.12597065	0.00000000
C	-4.15443193	0.70440636	0.00000000
C	-4.15443193	-0.70440636	0.00000000
C	-2.76852572	-1.12597065	0.00000000
N	0.00000000	-1.94821420	0.00000000

C	-1.12597065	-2.76852572	0.00000000	E _{1u}	60.0	//	60.0		
C	-0.70440636	-4.15443193	0.00000000						
C	0.70440636	-4.15443193	0.00000000						
C	1.12597065	-2.76852572	0.00000000	Mn	0.00000000	0.00000000	0.00000000		
N	1.94821420	0.00000000	0.00000000	N	2.39149539	2.39149539	0.00000000		
C	2.76852572	-1.12597065	0.00000000	N	-2.39149539	2.39149539	0.00000000		
C	4.15443193	-0.70440636	0.00000000	N	-2.39149539	-2.39149539	0.00000000		
C	4.15443193	0.70440636	0.00000000	N	2.39149539	-2.39149539	0.00000000		
C	2.76852572	1.12597065	0.00000000	N	0.00000000	1.95674982	0.00000000		
C	-5.34993224	-1.42667297	0.00000000	C	1.12113079	2.76956290	0.00000000		
C	-6.54263637	-0.70500009	0.00000000	C	0.70486674	4.16135992	0.00000000		
C	-6.54263637	0.70500009	0.00000000	C	-0.70486674	4.16135992	0.00000000		
C	-5.34993224	1.42667297	0.00000000	C	-1.12113079	2.76956290	0.00000000		
C	-1.42667297	5.34993224	0.00000000	N	-1.95674982	0.00000000	0.00000000		
C	-0.70500009	6.54263637	0.00000000	C	-2.76956290	1.12113079	0.00000000		
C	0.70500009	6.54263637	0.00000000	C	-4.16135992	0.70486674	0.00000000		
C	1.42667297	5.34993224	0.00000000	C	-4.16135992	-0.70486674	0.00000000		
C	5.34993224	1.42667297	0.00000000	C	-2.76956290	-1.12113079	0.00000000		
C	6.54263637	0.70500009	0.00000000	N	0.00000000	-1.95674982	0.00000000		
C	6.54263637	-0.70500009	0.00000000	C	-1.12113079	-2.76956290	0.00000000		
C	5.34993224	-1.42667297	0.00000000	C	-0.70486674	-4.16135992	0.00000000		
C	1.42667297	-5.34993224	0.00000000	C	0.70486674	-4.16135992	0.00000000		
C	0.70500009	-6.54263637	0.00000000	C	1.12113079	-2.76956290	0.00000000		
C	-0.70500009	-6.54263637	0.00000000	N	1.95674982	0.00000000	0.00000000		
C	-1.42667297	-5.34993224	0.00000000	C	2.76956290	-1.12113079	0.00000000		
H	-5.33956777	-2.51464076	0.00000000	C	4.16135992	-0.70486674	0.00000000		
H	-7.49332023	-1.23638189	0.00000000	C	4.16135992	0.70486674	0.00000000		
H	-7.49332023	1.23638189	0.00000000	C	2.76956290	1.12113079	0.00000000		
H	-5.33956777	2.51464076	0.00000000	C	-5.35608075	-1.42638775	0.00000000		
H	-2.51464076	5.33956777	0.00000000	C	-6.54946964	-0.70452013	0.00000000		
H	-1.23638189	7.49332023	0.00000000	C	-6.54946964	0.70452013	0.00000000		
H	1.23638189	7.49332023	0.00000000	C	-5.35608075	1.42638775	0.00000000		
H	2.51464076	5.33956777	0.00000000	C	-1.42638775	5.35608075	0.00000000		
H	5.33956777	2.51464076	0.00000000	C	-0.70452013	6.54946964	0.00000000		
H	7.49332023	1.23638189	0.00000000	C	0.70452013	6.54946964	0.00000000		
H	7.49332023	-1.23638189	0.00000000	C	1.42638775	5.35608075	0.00000000		
H	5.33956777	-2.51464076	0.00000000	C	5.35608075	1.42638775	0.00000000		
H	2.51464076	-5.33956777	0.00000000	C	6.54946964	0.70452013	0.00000000		
H	1.23638189	-7.49332023	0.00000000	C	6.54946964	-0.70452013	0.00000000		
H	-1.23638189	-7.49332023	0.00000000	C	5.35608075	-1.42638775	0.00000000		
H	-2.51464076	-5.33956777	0.00000000	C	1.42638775	-5.35608075	0.00000000		
				C	0.70452013	-6.54946964	0.00000000		
				C	-0.70452013	-6.54946964	0.00000000		
				C	-1.42638775	-5.35608075	0.00000000		
				H	-5.34404567	-2.51443385	0.00000000		
				H	-7.50048318	-1.23539498	0.00000000		
				H	-7.50048318	1.23539498	0.00000000		
				H	-5.34404567	2.51443385	0.00000000		
				H	-2.51443385	5.34404567	0.00000000		
				H	-1.23539498	7.50048318	0.00000000		
				H	1.23539498	7.50048318	0.00000000		
				H	2.51443385	5.34404567	0.00000000		
				H	5.34404567	2.51443385	0.00000000		
				H	7.50048318	1.23539498	0.00000000		
				H	7.50048318	-1.23539498	0.00000000		

level of theory bp86
spin state IS2

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	14.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0

H	5.34404567	-2.51443385	0.00000000
H	2.51443385	-5.34404567	0.00000000
H	1.23539498	-7.50048318	0.00000000
H	-1.23539498	-7.50048318	0.00000000
H	-2.51443385	-5.34404567	0.00000000

level of theory bp86
spin state IS3

Occup.	alpha		beta
A _{1g}	21.0	//	21.0
A _{2g}	11.0	//	11.0
B _{1g}	15.0	//	15.0
B _{2g}	14.0	//	13.0
E _{1g}	12.0	//	10.0
A _{1u}	2.0	//	2.0
A _{2u}	6.0	//	6.0
B _{1u}	2.0	//	2.0
B _{2u}	3.0	//	3.0
E _{1u}	60.0	//	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.39077889	2.39077889	0.00000000
N	-2.39077889	2.39077889	0.00000000
N	-2.39077889	-2.39077889	0.00000000
N	2.39077889	-2.39077889	0.00000000
N	0.00000000	1.95515965	0.00000000
C	1.12185100	2.76711175	0.00000000
C	0.70414547	4.15823301	0.00000000
C	-0.70414547	4.15823301	0.00000000
C	-1.12185100	2.76711175	0.00000000
N	-1.95515965	0.00000000	0.00000000
C	-2.76711175	1.12185100	0.00000000
C	-4.15823301	0.70414547	0.00000000
C	-4.15823301	-0.70414547	0.00000000
C	-2.76711175	-1.12185100	0.00000000
N	0.00000000	-1.95515965	0.00000000
C	-1.12185100	-2.76711175	0.00000000
C	-0.70414547	-4.15823301	0.00000000
C	0.70414547	-4.15823301	0.00000000
C	1.12185100	-2.76711175	0.00000000
N	1.95515965	0.00000000	0.00000000
C	2.76711175	-1.12185100	0.00000000
C	4.15823301	-0.70414547	0.00000000
C	4.15823301	0.70414547	0.00000000
C	2.76711175	1.12185100	0.00000000
C	-5.35215108	-1.42662641	0.00000000
C	-6.54546165	-0.70448044	0.00000000
C	-6.54546165	0.70448044	0.00000000
C	-5.35215108	1.42662641	0.00000000
C	-1.42662641	5.35215108	0.00000000
C	-0.70448044	6.54546165	0.00000000
C	0.70448044	6.54546165	0.00000000
C	1.42662641	5.35215108	0.00000000

C	5.35215108	1.42662641	0.00000000
C	6.54546165	0.70448044	0.00000000
C	6.54546165	-0.70448044	0.00000000
C	5.35215108	-1.42662641	0.00000000
C	1.42662641	-5.35215108	0.00000000
C	0.70448044	-6.54546165	0.00000000
C	-0.70448044	-6.54546165	0.00000000
C	-1.42662641	-5.35215108	0.00000000
H	-5.34176703	-2.51455927	0.00000000
H	-7.49619737	-1.23577440	0.00000000
H	-7.49619737	1.23577440	0.00000000
H	-5.34176703	2.51455927	0.00000000
H	-2.51455927	5.34176703	0.00000000
H	-1.23577440	7.49619737	0.00000000
H	1.23577440	7.49619737	0.00000000
H	2.51455927	5.34176703	0.00000000
H	5.34176703	2.51455927	0.00000000
H	7.49619737	1.23577440	0.00000000
H	7.49619737	-1.23577440	0.00000000
H	5.34176703	-2.51455927	0.00000000
H	2.51455927	-5.34176703	0.00000000
H	1.23577440	-7.49619737	0.00000000
H	-1.23577440	-7.49619737	0.00000000
H	-2.51455927	-5.34176703	0.00000000

level of theory bp86
spin state LS

Occup.	alpha		beta
A _{1g}	20.0	//	21.0
A _{2g}	11.0	//	11.0
B _{1g}	15.0	//	15.0
B _{2g}	14.0	//	13.0
E _{1g}	12.0	//	11.0
A _{1u}	2.0	//	2.0
A _{2u}	6.0	//	6.0
B _{1u}	2.0	//	2.0
B _{2u}	3.0	//	3.0
E _{1u}	60.0	//	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.38936387	2.38936387	0.00000000
N	-2.38936387	2.38936387	0.00000000
N	-2.38936387	-2.38936387	0.00000000
N	2.38936387	-2.38936387	0.00000000
N	0.00000000	1.94217046	0.00000000
C	1.12377721	2.76540780	0.00000000
C	0.70389623	4.15217975	0.00000000
C	-0.70389623	4.15217975	0.00000000
C	-1.12377721	2.76540780	0.00000000
N	-1.94217046	0.00000000	0.00000000
C	-2.76540780	1.12377721	0.00000000
C	-4.15217975	0.70389623	0.00000000
C	-4.15217975	-0.70389623	0.00000000

C	-2.76540780	-1.12377721	0.00000000
N	0.00000000	-1.94217046	0.00000000
C	-1.12377721	-2.76540780	0.00000000
C	-0.70389623	-4.15217975	0.00000000
C	0.70389623	-4.15217975	0.00000000
C	1.12377721	-2.76540780	0.00000000
N	1.94217046	0.00000000	0.00000000
C	2.76540780	-1.12377721	0.00000000
C	4.15217975	-0.70389623	0.00000000
C	4.15217975	0.70389623	0.00000000
C	2.76540780	1.12377721	0.00000000
C	-5.34702335	-1.42637558	0.00000000
C	-6.54012860	-0.70467571	0.00000000
C	-6.54012860	0.70467571	0.00000000
C	-5.34702335	1.42637558	0.00000000
C	-1.42637558	5.34702335	0.00000000
C	-0.70467571	6.54012860	0.00000000
C	0.70467571	6.54012860	0.00000000
C	1.42637558	5.34702335	0.00000000
C	5.34702335	1.42637558	0.00000000
C	6.54012860	0.70467571	0.00000000
C	6.54012860	-0.70467571	0.00000000
C	5.34702335	-1.42637558	0.00000000
C	1.42637558	-5.34702335	0.00000000
C	0.70467571	-6.54012860	0.00000000
C	-0.70467571	-6.54012860	0.00000000
C	-1.42637558	-5.34702335	0.00000000
H	-5.33566033	-2.51431584	0.00000000
H	-7.49068334	-1.23627130	0.00000000
H	-7.49068334	1.23627130	0.00000000
H	-5.33566033	2.51431584	0.00000000
H	-2.51431584	5.33566033	0.00000000
H	-1.23627130	7.49068334	0.00000000
H	1.23627130	7.49068334	0.00000000
H	2.51431584	5.33566033	0.00000000
H	5.33566033	2.51431584	0.00000000
H	7.49068334	1.23627130	0.00000000
H	7.49068334	-1.23627130	0.00000000
H	5.33566033	-2.51431584	0.00000000
H	2.51431584	-5.33566033	0.00000000
H	1.23627130	-7.49068334	0.00000000
H	-1.23627130	-7.49068334	0.00000000
H	-2.51431584	-5.33566033	0.00000000

level of theory opbe
spin state HS

Occup.	alpha	beta
A _{1g}	21.0 // 20.0	
A _{2g}	11.0 // 11.0	
B _{1g}	16.0 // 15.0	
B _{2g}	14.0 // 13.0	
E _{1g}	12.0 // 10.0	
A _{1u}	2.0 // 2.0	
A _{2u}	6.0 // 6.0	

B _{1u}	2.0 // 2.0
B _{2u}	3.0 // 3.0
E _{1u}	60.0 // 60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.38860000	2.38860000	0.00000000
N	-2.38860000	2.38860000	0.00000000
N	-2.38860000	-2.38860000	0.00000000
N	2.38860000	-2.38860000	0.00000000
N	0.00000000	2.02570000	0.00000000
C	1.12340000	2.79840000	0.00000000
C	0.70480000	4.19490000	0.00000000
C	-0.70480000	4.19490000	0.00000000
C	-1.12340000	2.79840000	0.00000000
N	-2.02570000	0.00000000	0.00000000
C	-2.79840000	1.12340000	0.00000000
C	-4.19490000	0.70480000	0.00000000
C	-4.19490000	-0.70480000	0.00000000
C	-2.79840000	-1.12340000	0.00000000
N	0.00000000	-2.02570000	0.00000000
C	-1.12340000	-2.79840000	0.00000000
C	-0.70480000	-4.19490000	0.00000000
C	0.70480000	-4.19490000	0.00000000
C	1.12340000	-2.79840000	0.00000000
N	2.02570000	0.00000000	0.00000000
C	2.79840000	-1.12340000	0.00000000
C	4.19490000	-0.70480000	0.00000000
C	4.19490000	0.70480000	0.00000000
C	2.79840000	1.12340000	0.00000000
C	-5.38930000	-1.41840000	0.00000000
C	-6.57910000	-0.70030000	0.00000000
C	-6.57910000	0.70030000	0.00000000
C	-5.38930000	1.41840000	0.00000000
C	-1.41840000	5.38930000	0.00000000
C	-0.70030000	6.57910000	0.00000000
C	0.70030000	6.57910000	0.00000000
C	1.41840000	5.38930000	0.00000000
C	5.38930000	1.41840000	0.00000000
C	6.57910000	0.70030000	0.00000000
C	6.57910000	-0.70030000	0.00000000
C	5.38930000	-1.41840000	0.00000000
C	1.41840000	-5.38930000	0.00000000
C	0.70030000	-6.57910000	0.00000000
C	-0.70030000	-6.57910000	0.00000000
C	-1.41840000	-5.38930000	0.00000000
H	-5.38570000	-2.50540000	0.00000000
H	-7.52870000	-1.23230000	0.00000000
H	-7.52870000	1.23230000	0.00000000
H	-5.38570000	2.50540000	0.00000000
H	-2.50540000	5.38570000	0.00000000
H	-1.23230000	7.52870000	0.00000000
H	1.23230000	7.52870000	0.00000000
H	2.50540000	5.38570000	0.00000000
H	5.38570000	2.50540000	0.00000000

H	7.52870000	1.23230000	0.00000000
H	7.52870000	-1.23230000	0.00000000
H	5.38570000	-2.50540000	0.00000000
H	2.50540000	-5.38570000	0.00000000
H	1.23230000	-7.52870000	0.00000000
H	-1.23230000	-7.52870000	0.00000000
H	-2.50540000	-5.38570000	0.00000000

level of theory opbe
spin state IS

Occup.	alpha		beta
A _{1g}	21.0	//	20.0
A _{2g}	11.0	//	11.0
B _{1g}	15.0	//	15.0
B _{2g}	14.0	//	13.0
E _{1g}	12.0	//	11.0
A _{1u}	2.0	//	2.0
A _{2u}	6.0	//	6.0
B _{1u}	2.0	//	2.0
B _{2u}	3.0	//	3.0
E _{1u}	60.0	//	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.37830000	2.37830000	0.00000000
N	-2.37830000	2.37830000	0.00000000
N	-2.37830000	-2.37830000	0.00000000
N	2.37830000	-2.37830000	0.00000000
N	0.00000000	1.94090000	0.00000000
C	1.11700000	2.75220000	0.00000000
C	0.70080000	4.13490000	0.00000000
C	-0.70080000	4.13490000	0.00000000
C	-1.11700000	2.75220000	0.00000000
N	-1.94090000	0.00000000	0.00000000
C	-2.75220000	1.11700000	0.00000000
C	-4.13490000	0.70080000	0.00000000
C	-4.13490000	-0.70080000	0.00000000
C	-2.75220000	-1.11700000	0.00000000
N	0.00000000	-1.94090000	0.00000000
C	-1.11700000	-2.75220000	0.00000000
C	-0.70080000	-4.13490000	0.00000000
C	0.70080000	-4.13490000	0.00000000
C	1.11700000	-2.75220000	0.00000000
N	1.94090000	0.00000000	0.00000000
C	2.75220000	-1.11700000	0.00000000
C	4.13490000	-0.70080000	0.00000000
C	4.13490000	0.70080000	0.00000000
C	2.75220000	1.11700000	0.00000000
C	-5.32850000	-1.42040000	0.00000000
C	-6.51550000	-0.70180000	0.00000000
C	-6.51550000	0.70180000	0.00000000
C	-5.32850000	1.42040000	0.00000000
C	-1.42040000	5.32850000	0.00000000
C	-0.70180000	6.51550000	0.00000000

C	0.70180000	6.51550000	0.00000000
C	1.42040000	5.32850000	0.00000000
C	5.32850000	1.42040000	0.00000000
C	6.51550000	0.70180000	0.00000000
C	6.51550000	-0.70180000	0.00000000
C	5.32850000	-1.42040000	0.00000000
C	1.42040000	-5.32850000	0.00000000
C	0.70180000	-6.51550000	0.00000000
C	-0.70180000	-6.51550000	0.00000000
C	-1.42040000	-5.32850000	0.00000000
H	-5.32390000	-2.50700000	0.00000000
H	-7.46550000	-1.23290000	0.00000000
H	-7.46550000	1.23290000	0.00000000
H	-5.32390000	2.50700000	0.00000000
H	-2.50700000	5.32390000	0.00000000
H	-1.23290000	7.46550000	0.00000000
H	1.23290000	7.46550000	0.00000000
H	2.50700000	5.32390000	0.00000000
H	5.32390000	2.50700000	0.00000000
H	7.46550000	1.23290000	0.00000000
H	7.46550000	-1.23290000	0.00000000
H	5.32390000	-2.50700000	0.00000000
H	2.50700000	-5.32390000	0.00000000
H	1.23290000	-7.46550000	0.00000000
H	-1.23290000	-7.46550000	0.00000000
H	-2.50700000	-5.32390000	0.00000000

level of theory opbe
spin state IS2

Occup.	alpha		beta
A _{1g}	21.0	//	20.0
A _{2g}	11.0	//	11.0
B _{1g}	15.0	//	15.0
B _{2g}	14.0	//	14.0
E _{1g}	12.0	//	10.0
A _{1u}	2.0	//	2.0
A _{2u}	6.0	//	6.0
B _{1u}	2.0	//	2.0
B _{2u}	3.0	//	3.0
E _{1u}	60.0	//	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.37671336	2.37671336	0.00000000
N	-2.37671336	2.37671336	0.00000000
N	-2.37671336	-2.37671336	0.00000000
N	2.37671336	-2.37671336	0.00000000
N	0.00000000	1.94787870	0.00000000
C	1.11119285	2.75231913	0.00000000
C	0.70116250	4.14226932	0.00000000
C	-0.70116250	4.14226932	0.00000000
C	-1.11119285	2.75231913	0.00000000
N	-1.94787870	0.00000000	0.00000000
C	-2.75231913	1.11119285	0.00000000

C	-4.14226932	0.70116250	0.00000000
C	-4.14226932	-0.70116250	0.00000000
C	-2.75231913	-1.11119285	0.00000000
N	0.00000000	-1.94787870	0.00000000
C	-1.11119285	-2.75231913	0.00000000
C	-0.70116250	-4.14226932	0.00000000
C	0.70116250	-4.14226932	0.00000000
C	1.11119285	-2.75231913	0.00000000
N	1.94787870	0.00000000	0.00000000
C	2.75231913	-1.11119285	0.00000000
C	4.14226932	-0.70116250	0.00000000
C	4.14226932	0.70116250	0.00000000
C	2.75231913	1.11119285	0.00000000
C	-5.33486762	-1.42002915	0.00000000
C	-6.52279117	-0.70125405	0.00000000
C	-6.52279117	0.70125405	0.00000000
C	-5.33486762	1.42002915	0.00000000
C	-1.42002915	5.33486762	0.00000000
C	-0.70125405	6.52279117	0.00000000
C	0.70125405	6.52279117	0.00000000
C	1.42002915	5.33486762	0.00000000
C	5.33486762	1.42002915	0.00000000
C	6.52279117	0.70125405	0.00000000
C	6.52279117	-0.70125405	0.00000000
C	5.33486762	-1.42002915	0.00000000
C	1.42002915	-5.33486762	0.00000000
C	0.70125405	-6.52279117	0.00000000
C	-0.70125405	-6.52279117	0.00000000
C	-1.42002915	-5.33486762	0.00000000
H	-5.33037702	-2.50674861	0.00000000
H	-7.47304481	-1.23201036	0.00000000
H	-7.47304481	1.23201036	0.00000000
H	-5.33037702	2.50674861	0.00000000
H	-2.50674861	5.33037702	0.00000000
H	-1.23201036	7.47304481	0.00000000
H	1.23201036	7.47304481	0.00000000
H	2.50674861	5.33037702	0.00000000
H	5.33037702	2.50674861	0.00000000
H	7.47304481	1.23201036	0.00000000
H	7.47304481	-1.23201036	0.00000000
H	5.33037702	-2.50674861	0.00000000
H	2.50674861	-5.33037702	0.00000000
H	1.23201036	-7.47304481	0.00000000
H	-1.23201036	-7.47304481	0.00000000
H	-2.50674861	-5.33037702	0.00000000

level of theory opbe
spin state IS3

Occup.	alpha	beta
A _{1g}	21.0 // 21.0	
A _{2g}	11.0 // 11.0	
B _{1g}	15.0 // 15.0	
B _{2g}	14.0 // 13.0	
E _{1g}	12.0 // 10.0	

A _{1u}	2.0 // 2.0
A _{2u}	6.0 // 6.0
B _{1u}	2.0 // 2.0
B _{2u}	3.0 // 3.0
E _{1u}	60.0 // 60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.37615296	2.37615296	0.00000000
N	-2.37615296	2.37615296	0.00000000
N	-2.37615296	-2.37615296	0.00000000
N	2.37615296	-2.37615296	0.00000000
N	0.00000000	1.94998006	0.00000000
C	1.11249885	2.75195136	0.00000000
C	0.70057300	4.14115382	0.00000000
C	-0.70057300	4.14115382	0.00000000
C	-1.11249885	2.75195136	0.00000000
N	-1.94998006	0.00000000	0.00000000
C	-2.75195136	1.11249885	0.00000000
C	-4.14115382	0.70057300	0.00000000
C	-4.14115382	-0.70057300	0.00000000
C	-2.75195136	-1.11249885	0.00000000
N	0.00000000	-1.94998006	0.00000000
C	-1.11249885	-2.75195136	0.00000000
C	-0.70057300	-4.14115382	0.00000000
C	0.70057300	-4.14115382	0.00000000
C	1.11249885	-2.75195136	0.00000000
N	1.94998006	0.00000000	0.00000000
C	2.75195136	-1.11249885	0.00000000
C	4.14115382	-0.70057300	0.00000000
C	4.14115382	0.70057300	0.00000000
C	2.75195136	1.11249885	0.00000000
C	-5.33293983	-1.42022918	0.00000000
C	-6.52079987	-0.70114133	0.00000000
C	-6.52079987	0.70114133	0.00000000
C	-5.33293983	1.42022918	0.00000000
C	-1.42022918	5.33293983	0.00000000
C	-0.70114133	6.52079987	0.00000000
C	0.70114133	6.52079987	0.00000000
C	1.42022918	5.33293983	0.00000000
C	5.33293983	1.42022918	0.00000000
C	6.52079987	0.70114133	0.00000000
C	6.52079987	-0.70114133	0.00000000
C	5.33293983	-1.42022918	0.00000000
C	1.42022918	-5.33293983	0.00000000
C	0.70114133	-6.52079987	0.00000000
C	-0.70114133	-6.52079987	0.00000000
C	-1.42022918	-5.33293983	0.00000000
H	-5.32833281	-2.50690260	0.00000000
H	-7.47086618	-1.23209397	0.00000000
H	-7.47086618	1.23209397	0.00000000
H	-5.32833281	2.50690260	0.00000000
H	-2.50690260	5.32833281	0.00000000
H	-1.23209397	7.47086618	0.00000000
H	1.23209397	7.47086618	0.00000000

H	2.50690260	5.32833281	0.00000000
H	5.32833281	2.50690260	0.00000000
H	7.47086618	1.23209397	0.00000000
H	7.47086618	-1.23209397	0.00000000
H	5.32833281	-2.50690260	0.00000000
H	2.50690260	-5.32833281	0.00000000
H	1.23209397	-7.47086618	0.00000000
H	-1.23209397	-7.47086618	0.00000000
H	-2.50690260	-5.32833281	0.00000000

level of theory opbe
spin state LS

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	12.0
A _{1u}	1.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.38120000	2.38120000	0.00000000
N	-2.38120000	2.38120000	0.00000000
N	-2.38120000	-2.38120000	0.00000000
N	2.38120000	-2.38120000	0.00000000
N	0.00000000	1.93180000	0.00000000
C	1.11680000	2.74840000	0.00000000
C	0.69960000	4.13590000	0.00000000
C	-0.69960000	4.13590000	0.00000000
C	-1.11680000	2.74840000	0.00000000
N	-1.93180000	0.00000000	0.00000000
C	-2.74840000	1.11680000	0.00000000
C	-4.13590000	0.69960000	0.00000000
C	-4.13590000	-0.69960000	0.00000000
C	-2.74840000	-1.11680000	0.00000000
N	0.00000000	-1.93180000	0.00000000
C	-1.11680000	-2.74840000	0.00000000
C	-0.69960000	-4.13590000	0.00000000
C	0.69960000	-4.13590000	0.00000000
C	1.11680000	-2.74840000	0.00000000
N	1.93180000	0.00000000	0.00000000
C	2.74840000	-1.11680000	0.00000000
C	4.13590000	-0.69960000	0.00000000
C	4.13590000	0.69960000	0.00000000
C	2.74840000	1.11680000	0.00000000
C	-5.32580000	-1.41830000	0.00000000
C	-6.51860000	-0.69940000	0.00000000
C	-6.51860000	0.69940000	0.00000000
C	-5.32580000	1.41830000	0.00000000

C	-1.41830000	5.32580000	0.00000000
C	-0.69940000	6.51860000	0.00000000
C	0.69940000	6.51860000	0.00000000
C	1.41830000	5.32580000	0.00000000
C	5.32580000	1.41830000	0.00000000
C	6.51860000	0.69940000	0.00000000
C	6.51860000	-0.69940000	0.00000000
C	5.32580000	-1.41830000	0.00000000
C	1.41830000	-5.32580000	0.00000000
C	0.69940000	-6.51860000	0.00000000
C	-0.69940000	-6.51860000	0.00000000
C	-1.41830000	-5.32580000	0.00000000
H	-5.32100000	-2.50500000	0.00000000
H	-7.46730000	-1.23270000	0.00000000
H	-7.46730000	1.23270000	0.00000000
H	-5.32100000	2.50500000	0.00000000
H	-2.50500000	5.32100000	0.00000000
H	-1.23270000	7.46730000	0.00000000
H	1.23270000	7.46730000	0.00000000
H	2.50500000	5.32100000	0.00000000
H	5.32100000	2.50500000	0.00000000
H	7.46730000	1.23270000	0.00000000
H	7.46730000	-1.23270000	0.00000000
H	5.32100000	-2.50500000	0.00000000
H	2.50500000	-5.32100000	0.00000000
H	1.23270000	-7.46730000	0.00000000
H	-1.23270000	-7.46730000	0.00000000
H	-2.50500000	-5.32100000	0.00000000

level of theory s12g
spin state HS

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	16.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.40525665	2.40525665	0.00000000
N	-2.40525665	2.40525665	0.00000000
N	-2.40525665	-2.40525665	0.00000000
N	2.40525665	-2.40525665	0.00000000
N	0.00000000	2.02877984	0.00000000
C	1.13026386	2.80832619	0.00000000
C	0.70576105	4.20483448	0.00000000
C	-0.70576105	4.20483448	0.00000000
C	-1.13026386	2.80832619	0.00000000

N	-2.02877984	0.00000000	0.00000000
C	-2.80832619	1.13026386	0.00000000
C	-4.20483448	0.70576105	0.00000000
C	-4.20483448	-0.70576105	0.00000000
C	-2.80832619	-1.13026386	0.00000000
N	0.00000000	-2.02877984	0.00000000
C	-1.13026386	-2.80832619	0.00000000
C	-0.70576105	-4.20483448	0.00000000
C	0.70576105	-4.20483448	0.00000000
C	1.13026386	-2.80832619	0.00000000
N	2.02877984	0.00000000	0.00000000
C	2.80832619	-1.13026386	0.00000000
C	4.20483448	-0.70576105	0.00000000
C	4.20483448	0.70576105	0.00000000
C	2.80832619	1.13026386	0.00000000
C	-5.39926056	-1.41957089	0.00000000
C	-6.59083542	-0.70135406	0.00000000
C	-6.59083542	0.70135406	0.00000000
C	-5.39926056	1.41957089	0.00000000
C	-1.41957089	5.39926056	0.00000000
C	-0.70135406	6.59083542	0.00000000
C	0.70135406	6.59083542	0.00000000
C	1.41957089	5.39926056	0.00000000
C	5.39926056	1.41957089	0.00000000
C	6.59083542	0.70135406	0.00000000
C	6.59083542	-0.70135406	0.00000000
C	5.39926056	-1.41957089	0.00000000
C	1.41957089	-5.39926056	0.00000000
C	0.70135406	-6.59083542	0.00000000
C	-0.70135406	-6.59083542	0.00000000
C	-1.41957089	-5.39926056	0.00000000
H	-5.39190711	-2.50781649	0.00000000
H	-7.54107742	-1.23396832	0.00000000
H	-7.54107742	1.23396832	0.00000000
H	-5.39190711	2.50781649	0.00000000
H	-2.50781649	5.39190711	0.00000000
H	-1.23396832	7.54107742	0.00000000
H	1.23396832	7.54107742	0.00000000
H	2.50781649	5.39190711	0.00000000
H	5.39190711	2.50781649	0.00000000
H	7.54107742	1.23396832	0.00000000
H	7.54107742	-1.23396832	0.00000000
H	5.39190711	-2.50781649	0.00000000
H	2.50781649	-5.39190711	0.00000000
H	1.23396832	-7.54107742	0.00000000
H	-1.23396832	-7.54107742	0.00000000
H	-2.50781649	-5.39190711	0.00000000

level of theory s12g
spin state IS

Occup.	alpha	beta
A _{1g}	21.0 // 20.0	
A _{2g}	11.0 // 11.0	
B _{1g}	15.0 // 15.0	

B _{2g}	14.0 // 13.0
E _{1g}	12.0 // 11.0
A _{1u}	2.0 // 2.0
A _{2u}	6.0 // 6.0
B _{1u}	2.0 // 2.0
B _{2u}	3.0 // 3.0
E _{1u}	60.0 // 60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.39712954	2.39712954	0.00000000
N	-2.39712954	2.39712954	0.00000000
N	-2.39712954	-2.39712954	0.00000000
N	2.39712954	-2.39712954	0.00000000
N	0.00000000	1.95179990	0.00000000
C	1.12694063	2.76777164	0.00000000
C	0.70206263	4.15002547	0.00000000
C	-0.70206263	4.15002547	0.00000000
C	-1.12694063	2.76777164	0.00000000
N	-1.95179990	0.00000000	0.00000000
C	-2.76777164	1.12694063	0.00000000
C	-4.15002547	0.70206263	0.00000000
C	-4.15002547	-0.70206263	0.00000000
C	-2.76777164	-1.12694063	0.00000000
N	0.00000000	-1.95179990	0.00000000
C	-1.12694063	-2.76777164	0.00000000
C	-0.70206263	-4.15002547	0.00000000
C	0.70206263	-4.15002547	0.00000000
C	1.12694063	-2.76777164	0.00000000
N	1.95179990	0.00000000	0.00000000
C	2.76777164	-1.12694063	0.00000000
C	4.15002547	-0.70206263	0.00000000
C	4.15002547	0.70206263	0.00000000
C	2.76777164	1.12694063	0.00000000
C	-5.34442403	-1.42105629	0.00000000
C	-6.53332127	-0.70284264	0.00000000
C	-6.53332127	0.70284264	0.00000000
C	-5.34442403	1.42105629	0.00000000
C	-1.42105629	5.34442403	0.00000000
C	-0.70284264	6.53332127	0.00000000
C	0.70284264	6.53332127	0.00000000
C	1.42105629	5.34442403	0.00000000
C	5.34442403	1.42105629	0.00000000
C	6.53332127	0.70284264	0.00000000
C	6.53332127	-0.70284264	0.00000000
C	5.34442403	-1.42105629	0.00000000
C	1.42105629	-5.34442403	0.00000000
C	0.70284264	-6.53332127	0.00000000
C	-0.70284264	-6.53332127	0.00000000
C	-1.42105629	-5.34442403	0.00000000
H	-5.33454482	-2.50909075	0.00000000
H	-7.48398026	-1.23451284	0.00000000
H	-7.48398026	1.23451284	0.00000000
H	-5.33454482	2.50909075	0.00000000
H	-2.50909075	5.33454482	0.00000000

H	-1.23451284	7.48398026	0.00000000
H	1.23451284	7.48398026	0.00000000
H	2.50909075	5.33454482	0.00000000
H	5.33454482	2.50909075	0.00000000
H	7.48398026	1.23451284	0.00000000
H	7.48398026	-1.23451284	0.00000000
H	5.33454482	-2.50909075	0.00000000
H	2.50909075	-5.33454482	0.00000000
H	1.23451284	-7.48398026	0.00000000
H	-1.23451284	-7.48398026	0.00000000
H	-2.50909075	-5.33454482	0.00000000

level of theory s12g
spin state IS2

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	14.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.39453816	2.39453816	0.00000000
N	-2.39453816	2.39453816	0.00000000
N	-2.39453816	-2.39453816	0.00000000
N	2.39453816	-2.39453816	0.00000000
N	0.00000000	1.95774679	0.00000000
C	1.12011213	2.76632540	0.00000000
C	0.70235579	4.15610625	0.00000000
C	-0.70235579	4.15610625	0.00000000
C	-1.12011213	2.76632540	0.00000000
N	-1.95774679	0.00000000	0.00000000
C	-2.76632540	1.12011213	0.00000000
C	-4.15610625	0.70235579	0.00000000
C	-4.15610625	-0.70235579	0.00000000
C	-2.76632540	-1.12011213	0.00000000
N	0.00000000	-1.95774679	0.00000000
C	-1.12011213	-2.76632540	0.00000000
C	-0.70235579	-4.15610625	0.00000000
C	0.70235579	-4.15610625	0.00000000
C	1.12011213	-2.76632540	0.00000000
N	1.95774679	0.00000000	0.00000000
C	2.76632540	-1.12011213	0.00000000
C	4.15610625	-0.70235579	0.00000000
C	4.15610625	0.70235579	0.00000000
C	2.76632540	1.12011213	0.00000000
C	-5.34919986	-1.42093246	0.00000000
C	-6.53895065	-0.70233516	0.00000000

C	-6.53895065	0.70233516	0.00000000
C	-5.34919986	1.42093246	0.00000000
C	-1.42093246	5.34919986	0.00000000
C	-0.70233516	6.53895065	0.00000000
C	0.70233516	6.53895065	0.00000000
C	1.42093246	5.34919986	0.00000000
C	5.34919986	1.42093246	0.00000000
C	6.53895065	0.70233516	0.00000000
C	6.53895065	-0.70233516	0.00000000
C	5.34919986	-1.42093246	0.00000000
C	1.42093246	-5.34919986	0.00000000
C	0.70233516	-6.53895065	0.00000000
C	-0.70233516	-6.53895065	0.00000000
C	-1.42093246	-5.34919986	0.00000000
H	-5.33905236	-2.50904471	0.00000000
H	-7.48980491	-1.23373812	0.00000000
H	-7.48980491	1.23373812	0.00000000
H	-5.33905236	2.50904471	0.00000000
H	-2.50904471	5.33905236	0.00000000
H	-1.23373812	7.48980491	0.00000000
H	1.23373812	7.48980491	0.00000000
H	2.50904471	5.33905236	0.00000000
H	5.33905236	2.50904471	0.00000000
H	7.48980491	1.23373812	0.00000000
H	7.48980491	-1.23373812	0.00000000
H	5.33905236	-2.50904471	0.00000000
H	2.50904471	-5.33905236	0.00000000
H	1.23373812	-7.48980491	0.00000000
H	-1.23373812	-7.48980491	0.00000000
H	-2.50904471	-5.33905236	0.00000000

level of theory s12g
spin state IS3

Occup.	alpha	beta
A _{1g}	21.0 //	21.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.39383065	2.39383065	0.00000000
N	-2.39383065	2.39383065	0.00000000
N	-2.39383065	-2.39383065	0.00000000
N	2.39383065	-2.39383065	0.00000000
N	0.00000000	1.95651434	0.00000000
C	1.12116572	2.76441295	0.00000000
C	0.70165252	4.15329314	0.00000000

C	-0.70165252	4.15329314	0.00000000	A _{2g}	11.0	//	11.0
C	-1.12116572	2.76441295	0.00000000	B _{1g}	15.0	//	15.0
N	-1.95651434	0.00000000	0.00000000	B _{2g}	14.0	//	13.0
C	-2.76441295	1.12116572	0.00000000	E _{1g}	12.0	//	12.0
C	-4.15329314	0.70165252	0.00000000	A _{1u}	1.0	//	2.0
C	-4.15329314	-0.70165252	0.00000000	A _{2u}	6.0	//	6.0
C	-2.76441295	-1.12116572	0.00000000	B _{1u}	2.0	//	2.0
N	0.00000000	-1.95651434	0.00000000	B _{2u}	3.0	//	3.0
C	-1.12116572	-2.76441295	0.00000000	E _{1u}	60.0	//	60.0
C	-0.70165252	-4.15329314	0.00000000				
C	0.70165252	-4.15329314	0.00000000				
C	1.12116572	-2.76441295	0.00000000	Mn	0.00000000	0.00000000	0.00000000
N	1.95651434	0.00000000	0.00000000	N	2.39990084	2.39990084	0.00000000
C	2.76441295	-1.12116572	0.00000000	N	-2.39990084	2.39990084	0.00000000
C	4.15329314	-0.70165252	0.00000000	N	-2.39990084	-2.39990084	0.00000000
C	4.15329314	0.70165252	0.00000000	N	2.39990084	-2.39990084	0.00000000
C	2.76441295	1.12116572	0.00000000	N	0.00000000	1.94279225	0.00000000
C	-5.34555224	-1.42121028	0.00000000	C	1.12673796	2.76405470	0.00000000
C	-6.53523054	-0.70221345	0.00000000	C	0.70084288	4.15092560	0.00000000
C	-6.53523054	0.70221345	0.00000000	C	-0.70084288	4.15092560	0.00000000
C	-5.34555224	1.42121028	0.00000000	C	-1.12673796	2.76405470	0.00000000
C	-1.42121028	5.34555224	0.00000000	N	-1.94279225	0.00000000	0.00000000
C	-0.70221345	6.53523054	0.00000000	C	-2.76405470	1.12673796	0.00000000
C	0.70221345	6.53523054	0.00000000	C	-4.15092560	0.70084288	0.00000000
C	1.42121028	5.34555224	0.00000000	C	-4.15092560	-0.70084288	0.00000000
C	5.34555224	1.42121028	0.00000000	C	-2.76405470	-1.12673796	0.00000000
C	6.53523054	0.70221345	0.00000000	N	0.00000000	-1.94279225	0.00000000
C	6.53523054	-0.70221345	0.00000000	C	-1.12673796	-2.76405470	0.00000000
C	5.34555224	-1.42121028	0.00000000	C	-0.70084288	-4.15092560	0.00000000
C	1.42121028	-5.34555224	0.00000000	C	0.70084288	-4.15092560	0.00000000
C	0.70221345	-6.53523054	0.00000000	C	1.12673796	-2.76405470	0.00000000
C	-0.70221345	-6.53523054	0.00000000	N	1.94279225	0.00000000	0.00000000
C	-1.42121028	-5.34555224	0.00000000	C	2.76405470	-1.12673796	0.00000000
H	-5.33675837	-2.50920346	0.00000000	C	4.15092560	-0.70084288	0.00000000
H	-7.48588688	-1.23386566	0.00000000	C	4.15092560	0.70084288	0.00000000
H	-7.48588688	1.23386566	0.00000000	C	2.76405470	1.12673796	0.00000000
H	-5.33675837	2.50920346	0.00000000	C	-5.34136327	-1.41897080	0.00000000
H	-2.50920346	5.33675837	0.00000000	C	-6.53645347	-0.70023644	0.00000000
H	-1.23386566	7.48588688	0.00000000	C	-6.53645347	0.70023644	0.00000000
H	1.23386566	7.48588688	0.00000000	C	-5.34136327	1.41897080	0.00000000
H	2.50920346	5.33675837	0.00000000	C	-1.41897080	5.34136327	0.00000000
H	5.33675837	2.50920346	0.00000000	C	-0.70023644	6.53645347	0.00000000
H	7.48588688	1.23386566	0.00000000	C	0.70023644	6.53645347	0.00000000
H	7.48588688	-1.23386566	0.00000000	C	1.41897080	5.34136327	0.00000000
H	5.33675837	-2.50920346	0.00000000	C	5.34136327	1.41897080	0.00000000
H	2.50920346	-5.33675837	0.00000000	C	6.53645347	0.70023644	0.00000000
H	1.23386566	-7.48588688	0.00000000	C	6.53645347	-0.70023644	0.00000000
H	-1.23386566	-7.48588688	0.00000000	C	5.34136327	-1.41897080	0.00000000
H	-2.50920346	-5.33675837	0.00000000	C	1.41897080	-5.34136327	0.00000000
				C	0.70023644	-6.53645347	0.00000000
				C	-0.70023644	-6.53645347	0.00000000
				C	-1.41897080	-5.34136327	0.00000000
				H	-5.33125070	-2.50709310	0.00000000
				H	-7.48566039	-1.23432498	0.00000000
				H	-7.48566039	1.23432498	0.00000000

level of theory s12g
spin state LS

Occup.	alpha	beta
A _{1g}	21.0	// 20.0

H	-5.33125070	2.50709310	0.00000000
H	-2.50709310	5.33125070	0.00000000
H	-1.23432498	7.48566039	0.00000000
H	1.23432498	7.48566039	0.00000000
H	2.50709310	5.33125070	0.00000000
H	5.33125070	2.50709310	0.00000000
H	7.48566039	1.23432498	0.00000000
H	7.48566039	-1.23432498	0.00000000
H	5.33125070	-2.50709310	0.00000000
H	2.50709310	-5.33125070	0.00000000
H	1.23432498	-7.48566039	0.00000000
H	-1.23432498	-7.48566039	0.00000000
H	-2.50709310	-5.33125070	0.00000000

level of theory ssb-d
spin state HS

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	16.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.40640972	2.40640972	0.00000000
N	-2.40640972	2.40640972	0.00000000
N	-2.40640972	-2.40640972	0.00000000
N	2.40640972	-2.40640972	0.00000000
N	0.00000000	2.02121049	0.00000000
C	1.12800004	2.80138180	0.00000000
C	0.70471328	4.19439275	0.00000000
C	-0.70471328	4.19439275	0.00000000
C	-1.12800004	2.80138180	0.00000000
N	-2.02121049	0.00000000	0.00000000
C	-2.80138180	1.12800004	0.00000000
C	-4.19439275	0.70471328	0.00000000
C	-4.19439275	-0.70471328	0.00000000
C	-2.80138180	-1.12800004	0.00000000
N	0.00000000	-2.02121049	0.00000000
C	-1.12800004	-2.80138180	0.00000000
C	-0.70471328	-4.19439275	0.00000000
C	0.70471328	-4.19439275	0.00000000
C	1.12800004	-2.80138180	0.00000000
N	2.02121049	0.00000000	0.00000000
C	2.80138180	-1.12800004	0.00000000
C	4.19439275	-0.70471328	0.00000000
C	4.19439275	0.70471328	0.00000000
C	2.80138180	1.12800004	0.00000000

C	-5.38663333	-1.41929519	0.00000000
C	-6.57619785	-0.70085029	0.00000000
C	-6.57619785	0.70085029	0.00000000
C	-5.38663333	1.41929519	0.00000000
C	-1.41929519	5.38663333	0.00000000
C	-0.70085029	6.57619785	0.00000000
C	0.70085029	6.57619785	0.00000000
C	1.41929519	5.38663333	0.00000000
C	5.38663333	1.41929519	0.00000000
C	6.57619785	0.70085029	0.00000000
C	6.57619785	-0.70085029	0.00000000
C	5.38663333	-1.41929519	0.00000000
C	1.41929519	-5.38663333	0.00000000
C	0.70085029	-6.57619785	0.00000000
C	-0.70085029	-6.57619785	0.00000000
C	-1.41929519	-5.38663333	0.00000000
H	-5.37736690	-2.50103720	0.00000000
H	-7.52133911	-1.22916074	0.00000000
H	-7.52133911	1.22916074	0.00000000
H	-5.37736690	2.50103720	0.00000000
H	-2.50103720	5.37736690	0.00000000
H	-1.22916074	7.52133911	0.00000000
H	1.22916074	7.52133911	0.00000000
H	2.50103720	5.37736690	0.00000000
H	5.37736690	2.50103720	0.00000000
H	7.52133911	1.22916074	0.00000000
H	7.52133911	-1.22916074	0.00000000
H	5.37736690	-2.50103720	0.00000000
H	2.50103720	-5.37736690	0.00000000
H	1.22916074	-7.52133911	0.00000000
H	-1.22916074	-7.52133911	0.00000000
H	-2.50103720	-5.37736690	0.00000000

level of theory ssb-d
spin state IS

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	11.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.39971457	2.39971457	0.00000000
N	-2.39971457	2.39971457	0.00000000
N	-2.39971457	-2.39971457	0.00000000
N	2.39971457	-2.39971457	0.00000000
N	0.00000000	1.94728020	0.00000000

C	1.12653634	2.76272064	0.00000000
C	0.70117255	4.14097919	0.00000000
C	-0.70117255	4.14097919	0.00000000
C	-1.12653634	2.76272064	0.00000000
N	-1.94728020	0.00000000	0.00000000
C	-2.76272064	1.12653634	0.00000000
C	-4.14097919	0.70117255	0.00000000
C	-4.14097919	-0.70117255	0.00000000
C	-2.76272064	-1.12653634	0.00000000
N	0.00000000	-1.94728020	0.00000000
C	-1.12653634	-2.76272064	0.00000000
C	-0.70117255	-4.14097919	0.00000000
C	0.70117255	-4.14097919	0.00000000
C	1.12653634	-2.76272064	0.00000000
N	1.94728020	0.00000000	0.00000000
C	2.76272064	-1.12653634	0.00000000
C	4.14097919	-0.70117255	0.00000000
C	4.14097919	0.70117255	0.00000000
C	2.76272064	1.12653634	0.00000000
C	-5.33326580	-1.42083721	0.00000000
C	-6.52002251	-0.70239178	0.00000000
C	-6.52002251	0.70239178	0.00000000
C	-5.33326580	1.42083721	0.00000000
C	-1.42083721	5.33326580	0.00000000
C	-0.70239178	6.52002251	0.00000000
C	0.70239178	6.52002251	0.00000000
C	1.42083721	5.33326580	0.00000000
C	5.33326580	1.42083721	0.00000000
C	6.52002251	0.70239178	0.00000000
C	6.52002251	-0.70239178	0.00000000
C	5.33326580	-1.42083721	0.00000000
C	1.42083721	-5.33326580	0.00000000
C	0.70239178	-6.52002251	0.00000000
C	-0.70239178	-6.52002251	0.00000000
C	-1.42083721	-5.33326580	0.00000000
H	-5.32338765	-2.50236226	0.00000000
H	-7.46542624	-1.23018258	0.00000000
H	-7.46542624	1.23018258	0.00000000
H	-5.32338765	2.50236226	0.00000000
H	-2.50236226	5.32338765	0.00000000
H	-1.23018258	7.46542624	0.00000000
H	1.23018258	7.46542624	0.00000000
H	2.50236226	5.32338765	0.00000000
H	5.32338765	2.50236226	0.00000000
H	7.46542624	1.23018258	0.00000000
H	7.46542624	-1.23018258	0.00000000
H	5.32338765	-2.50236226	0.00000000
H	2.50236226	-5.32338765	0.00000000
H	1.23018258	-7.46542624	0.00000000
H	-1.23018258	-7.46542624	0.00000000
H	-2.50236226	-5.32338765	0.00000000

level of theory ssb-d
spin state IS2

Occup.	alpha	beta	
A _{1g}	21.0	//	20.0
A _{2g}	11.0	//	11.0
B _{1g}	15.0	//	15.0
B _{2g}	14.0	//	14.0
E _{1g}	12.0	//	10.0
A _{1u}	2.0	//	2.0
A _{2u}	6.0	//	6.0
B _{1u}	2.0	//	2.0
B _{2u}	3.0	//	3.0
E _{1u}	60.0	//	60.0
Mn	0.00000000	0.00000000	0.00000000
N	2.39606166	2.39606166	0.00000000
N	-2.39606166	2.39606166	0.00000000
N	-2.39606166	-2.39606166	0.00000000
N	2.39606166	-2.39606166	0.00000000
N	0.00000000	1.95261907	0.00000000
C	1.11848914	2.76064097	0.00000000
C	0.70123976	4.14738964	0.00000000
C	-0.70123976	4.14738964	0.00000000
C	-1.11848914	2.76064097	0.00000000
N	-1.95261907	0.00000000	0.00000000
C	-2.76064097	1.11848914	0.00000000
C	-4.14738964	0.70123976	0.00000000
C	-4.14738964	-0.70123976	0.00000000
C	-2.76064097	-1.11848914	0.00000000
N	0.00000000	-1.95261907	0.00000000
C	-1.11848914	-2.76064097	0.00000000
C	-0.70123976	-4.14738964	0.00000000
C	0.70123976	-4.14738964	0.00000000
C	1.11848914	-2.76064097	0.00000000
N	1.95261907	0.00000000	0.00000000
C	2.76064097	-1.11848914	0.00000000
C	4.14738964	-0.70123976	0.00000000
C	4.14738964	0.70123976	0.00000000
C	2.76064097	1.11848914	0.00000000
C	-5.33795749	-1.42052658	0.00000000
C	-6.52591173	-0.70173031	0.00000000
C	-6.52591173	0.70173031	0.00000000
C	-5.33795749	1.42052658	0.00000000
C	-1.42052658	5.33795749	0.00000000
C	-0.70173031	6.52591173	0.00000000
C	0.70173031	6.52591173	0.00000000
C	1.42052658	5.33795749	0.00000000
C	5.33795749	1.42052658	0.00000000
C	6.52591173	0.70173031	0.00000000
C	6.52591173	-0.70173031	0.00000000
C	5.33795749	-1.42052658	0.00000000
C	1.42052658	-5.33795749	0.00000000
C	0.70173031	-6.52591173	0.00000000
C	-0.70173031	-6.52591173	0.00000000
C	-1.42052658	-5.33795749	0.00000000
H	-5.32807828	-2.50215323	0.00000000

H	-7.47145780	-1.22934754	0.00000000
H	-7.47145780	1.22934754	0.00000000
H	-5.32807828	2.50215323	0.00000000
H	-2.50215323	5.32807828	0.00000000
H	-1.22934754	7.47145780	0.00000000
H	1.22934754	7.47145780	0.00000000
H	2.50215323	5.32807828	0.00000000
H	5.32807828	2.50215323	0.00000000
H	7.47145780	1.22934754	0.00000000
H	7.47145780	-1.22934754	0.00000000
H	5.32807828	-2.50215323	0.00000000
H	2.50215323	-5.32807828	0.00000000
H	1.22934754	-7.47145780	0.00000000
H	-1.22934754	-7.47145780	0.00000000
H	-2.50215323	-5.32807828	0.00000000

level of theory ssb-d
spin state IS3

Occup.	alpha	beta
A _{1g}	21.0 //	21.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.39553513	2.39553513	0.00000000
N	-2.39553513	2.39553513	0.00000000
N	-2.39553513	-2.39553513	0.00000000
N	2.39553513	-2.39553513	0.00000000
N	0.00000000	1.95287254	0.00000000
C	1.11984225	2.75940111	0.00000000
C	0.70056770	4.14521367	0.00000000
C	-0.70056770	4.14521367	0.00000000
C	-1.11984225	2.75940111	0.00000000
N	-1.95287254	0.00000000	0.00000000
C	-2.75940111	1.11984225	0.00000000
C	-4.14521367	0.70056770	0.00000000
C	-4.14521367	-0.70056770	0.00000000
C	-2.75940111	-1.11984225	0.00000000
N	0.00000000	-1.95287254	0.00000000
C	-1.11984225	-2.75940111	0.00000000
C	-0.70056770	-4.14521367	0.00000000
C	0.70056770	-4.14521367	0.00000000
C	1.11984225	-2.75940111	0.00000000
N	1.95287254	0.00000000	0.00000000
C	2.75940111	-1.11984225	0.00000000
C	4.14521367	-0.70056770	0.00000000

C	4.14521367	0.70056770	0.00000000
C	2.75940111	1.11984225	0.00000000
C	-5.33514703	-1.42070068	0.00000000
C	-6.52299702	-0.70162341	0.00000000
C	-6.52299702	0.70162341	0.00000000
C	-5.33514703	1.42070068	0.00000000
C	-1.42070068	5.33514703	0.00000000
C	-0.70162341	6.52299702	0.00000000
C	0.70162341	6.52299702	0.00000000
C	1.42070068	5.33514703	0.00000000
C	5.33514703	1.42070068	0.00000000
C	6.52299702	0.70162341	0.00000000
C	6.52299702	-0.70162341	0.00000000
C	5.33514703	-1.42070068	0.00000000
C	1.42070068	-5.33514703	0.00000000
C	0.70162341	-6.52299702	0.00000000
C	-0.70162341	-6.52299702	0.00000000
C	-1.42070068	-5.33514703	0.00000000
H	-5.32519585	-2.50224108	0.00000000
H	-7.46839546	-1.22937770	0.00000000
H	-7.46839546	1.22937770	0.00000000
H	-5.32519585	2.50224108	0.00000000
H	-2.50224108	5.32519585	0.00000000
H	-1.22937770	7.46839546	0.00000000
H	1.22937770	7.46839546	0.00000000
H	2.50224108	5.32519585	0.00000000
H	5.32519585	2.50224108	0.00000000
H	7.46839546	1.22937770	0.00000000
H	7.46839546	-1.22937770	0.00000000
H	5.32519585	-2.50224108	0.00000000
H	2.50224108	-5.32519585	0.00000000
H	1.22937770	-7.46839546	0.00000000
H	-1.22937770	-7.46839546	0.00000000
H	-2.50224108	-5.32519585	0.00000000

level of theory ssb-d
spin state LS

Occup.	alpha	beta
A _{1g}	20.0 //	21.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	11.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.39558752	2.39558752	0.00000000
N	-2.39558752	2.39558752	0.00000000
N	-2.39558752	-2.39558752	0.00000000

N	2.39558752	-2.39558752	0.00000000
N	0.00000000	1.93897529	0.00000000
C	1.12279982	2.75721667	0.00000000
C	0.70049732	4.13760568	0.00000000
C	-0.70049732	4.13760568	0.00000000
C	-1.12279982	2.75721667	0.00000000
N	-1.93897529	0.00000000	0.00000000
C	-2.75721667	1.12279982	0.00000000
C	-4.13760568	0.70049732	0.00000000
C	-4.13760568	-0.70049732	0.00000000
C	-2.75721667	-1.12279982	0.00000000
N	0.00000000	-1.93897529	0.00000000
C	-1.12279982	-2.75721667	0.00000000
C	-0.70049732	-4.13760568	0.00000000
C	0.70049732	-4.13760568	0.00000000
C	1.12279982	-2.75721667	0.00000000
N	1.93897529	0.00000000	0.00000000
C	2.75721667	-1.12279982	0.00000000
C	4.13760568	-0.70049732	0.00000000
C	4.13760568	0.70049732	0.00000000
C	2.75721667	1.12279982	0.00000000
C	-5.32894031	-1.42085308	0.00000000
C	-6.51610343	-0.70212825	0.00000000
C	-6.51610343	0.70212825	0.00000000
C	-5.32894031	1.42085308	0.00000000
C	-1.42085308	5.32894031	0.00000000
C	-0.70212825	6.51610343	0.00000000
C	0.70212825	6.51610343	0.00000000
C	1.42085308	5.32894031	0.00000000
C	5.32894031	1.42085308	0.00000000
C	6.51610343	0.70212825	0.00000000
C	6.51610343	-0.70212825	0.00000000
C	5.32894031	-1.42085308	0.00000000
C	1.42085308	-5.32894031	0.00000000
C	0.70212825	-6.51610343	0.00000000
C	-0.70212825	-6.51610343	0.00000000
C	-1.42085308	-5.32894031	0.00000000
H	-5.31818743	-2.50230511	0.00000000
H	-7.46135475	-1.23002595	0.00000000
H	-7.46135475	1.23002595	0.00000000
H	-5.31818743	2.50230511	0.00000000
H	-2.50230511	5.31818743	0.00000000
H	-1.23002595	7.46135475	0.00000000
H	1.23002595	7.46135475	0.00000000
H	2.50230511	5.31818743	0.00000000
H	5.31818743	2.50230511	0.00000000
H	7.46135475	1.23002595	0.00000000
H	7.46135475	-1.23002595	0.00000000
H	5.31818743	-2.50230511	0.00000000
H	2.50230511	-5.31818743	0.00000000
H	1.23002595	-7.46135475	0.00000000
H	-1.23002595	-7.46135475	0.00000000
H	-2.50230511	-5.31818743	0.00000000

level of theory m06l

spin state HS

Occup.	alpha		beta
A _{1g}	21.0	//	20.0
A _{2g}	11.0	//	11.0
B _{1g}	16.0	//	15.0
B _{2g}	14.0	//	13.0
E _{1g}	12.0	//	10.0
A _{1u}	2.0	//	2.0
A _{2u}	6.0	//	6.0
B _{1u}	2.0	//	2.0
B _{2u}	3.0	//	3.0
E _{1u}	60.0	//	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.38867488	2.38867488	0.00000000
N	-2.38867488	2.38867488	0.00000000
N	-2.38867488	-2.38867488	0.00000000
N	2.38867488	-2.38867488	0.00000000
N	0.00000000	2.02188784	0.00000000
C	1.12364968	2.79708330	0.00000000
C	0.70248333	4.18556290	0.00000000
C	-0.70248333	4.18556290	0.00000000
C	-1.12364968	2.79708330	0.00000000
N	-2.02188784	0.00000000	0.00000000
C	-2.79708330	1.12364968	0.00000000
C	-4.18556290	0.70248333	0.00000000
C	-4.18556290	-0.70248333	0.00000000
C	-2.79708330	-1.12364968	0.00000000
N	0.00000000	-2.02188784	0.00000000
C	-1.12364968	-2.79708330	0.00000000
C	-0.70248333	-4.18556290	0.00000000
C	0.70248333	-4.18556290	0.00000000
C	1.12364968	-2.79708330	0.00000000
N	2.02188784	0.00000000	0.00000000
C	2.79708330	-1.12364968	0.00000000
C	4.18556290	-0.70248333	0.00000000
C	4.18556290	0.70248333	0.00000000
C	2.79708330	1.12364968	0.00000000
C	-5.37475753	-1.41284716	0.00000000
C	-6.56093426	-0.69815730	0.00000000
C	-6.56093426	0.69815730	0.00000000
C	-5.37475753	1.41284716	0.00000000
C	-1.41284716	5.37475753	0.00000000
C	-0.69815730	6.56093426	0.00000000
C	0.69815730	6.56093426	0.00000000
C	1.41284716	5.37475753	0.00000000
C	5.37475753	1.41284716	0.00000000
C	6.56093426	0.69815730	0.00000000
C	6.56093426	-0.69815730	0.00000000
C	5.37475753	-1.41284716	0.00000000
C	1.41284716	-5.37475753	0.00000000
C	0.69815730	-6.56093426	0.00000000
C	-0.69815730	-6.56093426	0.00000000

C	-1.41284716	-5.37475753	0.00000000
H	-5.36786870	-2.49280056	0.00000000
H	-7.50360956	-1.22624233	0.00000000
H	-7.50360956	1.22624233	0.00000000
H	-5.36786870	2.49280056	0.00000000
H	-2.49280056	5.36786870	0.00000000
H	-1.22624233	7.50360956	0.00000000
H	1.22624233	7.50360956	0.00000000
H	2.49280056	5.36786870	0.00000000
H	5.36786870	2.49280056	0.00000000
H	7.50360956	1.22624233	0.00000000
H	7.50360956	-1.22624233	0.00000000
H	5.36786870	-2.49280056	0.00000000
H	2.49280056	-5.36786870	0.00000000
H	1.22624233	-7.50360956	0.00000000
H	-1.22624233	-7.50360956	0.00000000
H	-2.49280056	-5.36786870	0.00000000

level of theory m06l
spin state IS

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	11.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.38069806	2.38069806	0.00000000
N	-2.38069806	2.38069806	0.00000000
N	-2.38069806	-2.38069806	0.00000000
N	2.38069806	-2.38069806	0.00000000
N	0.00000000	1.94489572	0.00000000
C	1.12036772	2.75652398	0.00000000
C	0.69885899	4.13029245	0.00000000
C	-0.69885899	4.13029245	0.00000000
C	-1.12036772	2.75652398	0.00000000
N	-1.94489572	0.00000000	0.00000000
C	-2.75652398	1.12036772	0.00000000
C	-4.13029245	0.69885899	0.00000000
C	-4.13029245	-0.69885899	0.00000000
C	-2.75652398	-1.12036772	0.00000000
N	0.00000000	-1.94489572	0.00000000
C	-1.12036772	-2.75652398	0.00000000
C	-0.69885899	-4.13029245	0.00000000
C	0.69885899	-4.13029245	0.00000000
C	1.12036772	-2.75652398	0.00000000
N	1.94489572	0.00000000	0.00000000

C	2.75652398	-1.12036772	0.00000000
C	4.13029245	-0.69885899	0.00000000
C	4.13029245	0.69885899	0.00000000
C	2.75652398	1.12036772	0.00000000
C	-5.31942993	-1.41465113	0.00000000
C	-6.50254538	-0.69984379	0.00000000
C	-6.50254538	0.69984379	0.00000000
C	-5.31942993	1.41465113	0.00000000
C	-1.41465113	5.31942993	0.00000000
C	-0.69984379	6.50254538	0.00000000
C	0.69984379	6.50254538	0.00000000
C	1.41465113	5.31942993	0.00000000
C	5.31942993	1.41465113	0.00000000
C	6.50254538	0.69984379	0.00000000
C	6.50254538	-0.69984379	0.00000000
C	5.31942993	-1.41465113	0.00000000
C	1.41465113	-5.31942993	0.00000000
C	0.69984379	-6.50254538	0.00000000
C	-0.69984379	-6.50254538	0.00000000
C	-1.41465113	-5.31942993	0.00000000
H	-5.31041487	-2.49448863	0.00000000
H	-7.44587526	-1.22678844	0.00000000
H	-7.44587526	1.22678844	0.00000000
H	-5.31041487	2.49448863	0.00000000
H	-2.49448863	5.31041487	0.00000000
H	-1.22678844	7.44587526	0.00000000
H	1.22678844	7.44587526	0.00000000
H	2.49448863	5.31041487	0.00000000
H	5.31041487	2.49448863	0.00000000
H	7.44587526	1.22678844	0.00000000
H	7.44587526	-1.22678844	0.00000000
H	5.31041487	-2.49448863	0.00000000
H	2.49448863	-5.31041487	0.00000000
H	1.22678844	-7.44587526	0.00000000
H	-1.22678844	-7.44587526	0.00000000
H	-2.49448863	-5.31041487	0.00000000

level of theory m06l
spin state IS2

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	14.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.37822363	2.37822363	0.00000000

N	-2.37822363	2.37822363	0.00000000
N	-2.37822363	-2.37822363	0.00000000
N	2.37822363	-2.37822363	0.00000000
N	0.00000000	1.95639792	0.00000000
C	1.11385302	2.75792524	0.00000000
C	0.69922042	4.14048176	0.00000000
C	-0.69922042	4.14048176	0.00000000
C	-1.11385302	2.75792524	0.00000000
N	-1.95639792	0.00000000	0.00000000
C	-2.75792524	1.11385302	0.00000000
C	-4.14048176	0.69922042	0.00000000
C	-4.14048176	-0.69922042	0.00000000
C	-2.75792524	-1.11385302	0.00000000
N	0.00000000	-1.95639792	0.00000000
C	-1.11385302	-2.75792524	0.00000000
C	-0.69922042	-4.14048176	0.00000000
C	0.69922042	-4.14048176	0.00000000
C	1.11385302	-2.75792524	0.00000000
N	1.95639792	0.00000000	0.00000000
C	2.75792524	-1.11385302	0.00000000
C	4.14048176	-0.69922042	0.00000000
C	4.14048176	0.69922042	0.00000000
C	2.75792524	1.11385302	0.00000000
C	-5.32803171	-1.41423413	0.00000000
C	-6.51248227	-0.69904738	0.00000000
C	-6.51248227	0.69904738	0.00000000
C	-5.32803171	1.41423413	0.00000000
C	-1.41423413	5.32803171	0.00000000
C	-0.69904738	6.51248227	0.00000000
C	0.69904738	6.51248227	0.00000000
C	1.41423413	5.32803171	0.00000000
C	5.32803171	1.41423413	0.00000000
C	6.51248227	0.69904738	0.00000000
C	6.51248227	-0.69904738	0.00000000
C	5.32803171	-1.41423413	0.00000000
C	1.41423413	-5.32803171	0.00000000
C	0.69904738	-6.51248227	0.00000000
C	-0.69904738	-6.51248227	0.00000000
C	-1.41423413	-5.32803171	0.00000000
H	-5.31908226	-2.49418012	0.00000000
H	-7.45589311	-1.22597192	0.00000000
H	-7.45589311	1.22597192	0.00000000
H	-5.31908226	2.49418012	0.00000000
H	-2.49418012	5.31908226	0.00000000
H	-1.22597192	7.45589311	0.00000000
H	1.22597192	7.45589311	0.00000000
H	2.49418012	5.31908226	0.00000000
H	5.31908226	2.49418012	0.00000000
H	7.45589311	1.22597192	0.00000000
H	7.45589311	-1.22597192	0.00000000
H	5.31908226	-2.49418012	0.00000000
H	2.49418012	-5.31908226	0.00000000
H	1.22597192	-7.45589311	0.00000000
H	-1.22597192	-7.45589311	0.00000000
H	-2.49418012	-5.31908226	0.00000000

level of theory m06l
spin state IS3

Occup.	alpha	beta
A _{1g}	21.0 //	21.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.37738012	2.37738012	0.00000000
N	-2.37738012	2.37738012	0.00000000
N	-2.37738012	-2.37738012	0.00000000
N	2.37738012	-2.37738012	0.00000000
N	0.00000000	1.95346522	0.00000000
C	1.11414883	2.75453533	0.00000000
C	0.69827319	4.13628327	0.00000000
C	-0.69827319	4.13628327	0.00000000
C	-1.11414883	2.75453533	0.00000000
N	-1.95346522	0.00000000	0.00000000
C	-2.75453533	1.11414883	0.00000000
C	-4.13628327	0.69827319	0.00000000
C	-4.13628327	-0.69827319	0.00000000
C	-2.75453533	-1.11414883	0.00000000
N	0.00000000	-1.95346522	0.00000000
C	-1.11414883	-2.75453533	0.00000000
C	-0.69827319	-4.13628327	0.00000000
C	0.69827319	-4.13628327	0.00000000
C	1.11414883	-2.75453533	0.00000000
N	1.95346522	0.00000000	0.00000000
C	2.75453533	-1.11414883	0.00000000
C	4.13628327	-0.69827319	0.00000000
C	4.13628327	0.69827319	0.00000000
C	2.75453533	1.11414883	0.00000000
C	-5.32291668	-1.41441458	0.00000000
C	-6.50724976	-0.69891350	0.00000000
C	-6.50724976	0.69891350	0.00000000
C	-5.32291668	1.41441458	0.00000000
C	-1.41441458	5.32291668	0.00000000
C	-0.69891350	6.50724976	0.00000000
C	0.69891350	6.50724976	0.00000000
C	1.41441458	5.32291668	0.00000000
C	5.32291668	1.41441458	0.00000000
C	6.50724976	0.69891350	0.00000000
C	6.50724976	-0.69891350	0.00000000
C	5.32291668	-1.41441458	0.00000000
C	1.41441458	-5.32291668	0.00000000

C	0.69891350	-6.50724976	0.00000000
C	-0.69891350	-6.50724976	0.00000000
C	-1.41441458	-5.32291668	0.00000000
H	-5.31477529	-2.49417271	0.00000000
H	-7.45047328	-1.22598197	0.00000000
H	-7.45047328	1.22598197	0.00000000
H	-5.31477529	2.49417271	0.00000000
H	-2.49417271	5.31477529	0.00000000
H	-1.22598197	7.45047328	0.00000000
H	1.22598197	7.45047328	0.00000000
H	2.49417271	5.31477529	0.00000000
H	5.31477529	2.49417271	0.00000000
H	7.45047328	1.22598197	0.00000000
H	7.45047328	-1.22598197	0.00000000
H	5.31477529	-2.49417271	0.00000000
H	2.49417271	-5.31477529	0.00000000
H	1.22598197	-7.45047328	0.00000000
H	-1.22598197	-7.45047328	0.00000000
H	-2.49417271	-5.31477529	0.00000000

level of theory m06l
spin state LS

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	12.0
A _{1u}	1.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.38466636	2.38466636	0.00000000
N	-2.38466636	2.38466636	0.00000000
N	-2.38466636	-2.38466636	0.00000000
N	2.38466636	-2.38466636	0.00000000
N	0.00000000	1.93704697	0.00000000
C	1.12047567	2.75333939	0.00000000
C	0.69745350	4.13282774	0.00000000
C	-0.69745350	4.13282774	0.00000000
C	-1.12047567	2.75333939	0.00000000
N	-1.93704697	0.00000000	0.00000000
C	-2.75333939	1.12047567	0.00000000
C	-4.13282774	0.69745350	0.00000000
C	-4.13282774	-0.69745350	0.00000000
C	-2.75333939	-1.12047567	0.00000000
N	0.00000000	-1.93704697	0.00000000
C	-1.12047567	-2.75333939	0.00000000
C	-0.69745350	-4.13282774	0.00000000
C	0.69745350	-4.13282774	0.00000000

C	1.12047567	-2.75333939	0.00000000
N	1.93704697	0.00000000	0.00000000
C	2.75333939	-1.12047567	0.00000000
C	4.13282774	-0.69745350	0.00000000
C	4.13282774	0.69745350	0.00000000
C	2.75333939	1.12047567	0.00000000
C	-5.31741906	-1.41265454	0.00000000
C	-6.50648140	-0.69714552	0.00000000
C	-6.50648140	0.69714552	0.00000000
C	-5.31741906	1.41265454	0.00000000
C	-1.41265454	5.31741906	0.00000000
C	-0.69714552	6.50648140	0.00000000
C	0.69714552	6.50648140	0.00000000
C	1.41265454	5.31741906	0.00000000
C	5.31741906	1.41265454	0.00000000
C	6.50648140	0.69714552	0.00000000
C	6.50648140	-0.69714552	0.00000000
C	5.31741906	-1.41265454	0.00000000
C	1.41265454	-5.31741906	0.00000000
C	0.69714552	-6.50648140	0.00000000
C	-0.69714552	-6.50648140	0.00000000
C	-1.41265454	-5.31741906	0.00000000
H	-5.30891412	-2.49246241	0.00000000
H	-7.44833170	-1.22643125	0.00000000
H	-7.44833170	1.22643125	0.00000000
H	-5.30891412	2.49246241	0.00000000
H	-2.49246241	5.30891412	0.00000000
H	-1.22643125	7.44833170	0.00000000
H	1.22643125	7.44833170	0.00000000
H	2.49246241	5.30891412	0.00000000
H	5.30891412	2.49246241	0.00000000
H	7.44833170	1.22643125	0.00000000
H	7.44833170	-1.22643125	0.00000000
H	5.30891412	-2.49246241	0.00000000
H	2.49246241	-5.30891412	0.00000000
H	1.22643125	-7.44833170	0.00000000
H	-1.22643125	-7.44833170	0.00000000
H	-2.49246241	-5.30891412	0.00000000

level of theory pbe0
spin state HS

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	16.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.37466809	2.37466809	0.00000000
N	-2.37466809	2.37466809	0.00000000
N	-2.37466809	-2.37466809	0.00000000
N	2.37466809	-2.37466809	0.00000000
N	0.00000000	2.02204765	0.00000000
C	1.11811078	2.78764965	0.00000000
C	0.70146942	4.18087704	0.00000000
C	-0.70146942	4.18087704	0.00000000
C	-1.11811078	2.78764965	0.00000000
N	-2.02204765	0.00000000	0.00000000
C	-2.78764965	1.11811078	0.00000000
C	-4.18087704	0.70146942	0.00000000
C	-4.18087704	-0.70146942	0.00000000
C	-2.78764965	-1.11811078	0.00000000
N	0.00000000	-2.02204765	0.00000000
C	-1.11811078	-2.78764965	0.00000000
C	-0.70146942	-4.18087704	0.00000000
C	0.70146942	-4.18087704	0.00000000
C	1.11811078	-2.78764965	0.00000000
N	2.02204765	0.00000000	0.00000000
C	2.78764965	-1.11811078	0.00000000
C	4.18087704	-0.70146942	0.00000000
C	4.18087704	0.70146942	0.00000000
C	2.78764965	1.11811078	0.00000000
C	-5.36777557	-1.41318848	0.00000000
C	-6.55161016	-0.69790118	0.00000000
C	-6.55161016	0.69790118	0.00000000
C	-5.36777557	1.41318848	0.00000000
C	-1.41318848	5.36777557	0.00000000
C	-0.69790118	6.55161016	0.00000000
C	0.69790118	6.55161016	0.00000000
C	1.41318848	5.36777557	0.00000000
C	5.36777557	1.41318848	0.00000000
C	6.55161016	0.69790118	0.00000000
C	6.55161016	-0.69790118	0.00000000
C	5.36777557	-1.41318848	0.00000000
C	1.41318848	-5.36777557	0.00000000
C	0.69790118	-6.55161016	0.00000000
C	-0.69790118	-6.55161016	0.00000000
C	-1.41318848	-5.36777557	0.00000000
H	-5.36143549	-2.49372609	0.00000000
H	-7.49493369	-1.22666726	0.00000000
H	-7.49493369	1.22666726	0.00000000
H	-5.36143549	2.49372609	0.00000000
H	-2.49372609	5.36143549	0.00000000
H	-1.22666726	7.49493369	0.00000000
H	1.22666726	7.49493369	0.00000000
H	2.49372609	5.36143549	0.00000000
H	5.36143549	2.49372609	0.00000000
H	7.49493369	1.22666726	0.00000000
H	7.49493369	-1.22666726	0.00000000
H	5.36143549	-2.49372609	0.00000000
H	2.49372609	-5.36143549	0.00000000
H	1.22666726	-7.49493369	0.00000000

H	-1.22666726	-7.49493369	0.00000000
H	-2.49372609	-5.36143549	0.00000000

level of theory pbe0
spin state IS

Occup.	alpha		beta
A _{1g}	21.0	//	20.0
A _{2g}	11.0	//	11.0
B _{1g}	15.0	//	15.0
B _{2g}	14.0	//	13.0
E _{1g}	12.0	//	11.0
A _{1u}	2.0	//	2.0
A _{2u}	6.0	//	6.0
B _{1u}	2.0	//	2.0
B _{2u}	3.0	//	3.0
E _{1u}	60.0	//	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.36732416	2.36732416	0.00000000
N	-2.36732416	2.36732416	0.00000000
N	-2.36732416	-2.36732416	0.00000000
N	2.36732416	-2.36732416	0.00000000
N	0.00000000	1.93577377	0.00000000
C	1.11445628	2.74320511	0.00000000
C	0.69782339	4.11892149	0.00000000
C	-0.69782339	4.11892149	0.00000000
C	-1.11445628	2.74320511	0.00000000
N	-1.93577377	0.00000000	0.00000000
C	-2.74320511	1.11445628	0.00000000
C	-4.11892149	0.69782339	0.00000000
C	-4.11892149	-0.69782339	0.00000000
C	-2.74320511	-1.11445628	0.00000000
N	0.00000000	-1.93577377	0.00000000
C	-1.11445628	-2.74320511	0.00000000
C	-0.69782339	-4.11892149	0.00000000
C	0.69782339	-4.11892149	0.00000000
C	1.11445628	-2.74320511	0.00000000
N	1.93577377	0.00000000	0.00000000
C	2.74320511	-1.11445628	0.00000000
C	4.11892149	-0.69782339	0.00000000
C	4.11892149	0.69782339	0.00000000
C	2.74320511	1.11445628	0.00000000
C	-5.30693077	-1.41520041	0.00000000
C	-6.48707752	-0.70016341	0.00000000
C	-6.48707752	0.70016341	0.00000000
C	-5.30693077	1.41520041	0.00000000
C	-1.41520041	5.30693077	0.00000000
C	-0.70016341	6.48707752	0.00000000
C	0.70016341	6.48707752	0.00000000
C	1.41520041	5.30693077	0.00000000
C	5.30693077	1.41520041	0.00000000
C	6.48707752	0.70016341	0.00000000
C	6.48707752	-0.70016341	0.00000000

C	5.30693077	-1.41520041	0.00000000
C	1.41520041	-5.30693077	0.00000000
C	0.70016341	-6.48707752	0.00000000
C	-0.70016341	-6.48707752	0.00000000
C	-1.41520041	-5.30693077	0.00000000
H	-5.29872164	-2.49539776	0.00000000
H	-7.43102760	-1.22760972	0.00000000
H	-7.43102760	1.22760972	0.00000000
H	-5.29872164	2.49539776	0.00000000
H	-2.49539776	5.29872164	0.00000000
H	-1.22760972	7.43102760	0.00000000
H	1.22760972	7.43102760	0.00000000
H	2.49539776	5.29872164	0.00000000
H	5.29872164	2.49539776	0.00000000
H	7.43102760	1.22760972	0.00000000
H	7.43102760	-1.22760972	0.00000000
H	5.29872164	-2.49539776	0.00000000
H	2.49539776	-5.29872164	0.00000000
H	1.22760972	-7.43102760	0.00000000
H	-1.22760972	-7.43102760	0.00000000
H	-2.49539776	-5.29872164	0.00000000

level of theory pbe0
spin state IS2

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	14.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.36397077	2.36397077	0.00000000
N	-2.36397077	2.36397077	0.00000000
N	-2.36397077	-2.36397077	0.00000000
N	2.36397077	-2.36397077	0.00000000
N	0.00000000	1.95414892	0.00000000
C	1.10717004	2.74718188	0.00000000
C	0.69796098	4.13461689	0.00000000
C	-0.69796098	4.13461689	0.00000000
C	-1.10717004	2.74718188	0.00000000
N	-1.95414892	0.00000000	0.00000000
C	-2.74718188	1.10717004	0.00000000
C	-4.13461689	0.69796098	0.00000000
C	-4.13461689	-0.69796098	0.00000000
C	-2.74718188	-1.10717004	0.00000000
N	0.00000000	-1.95414892	0.00000000
C	-1.10717004	-2.74718188	0.00000000

C	-0.69796098	-4.13461689	0.00000000
C	0.69796098	-4.13461689	0.00000000
C	1.10717004	-2.74718188	0.00000000
N	1.95414892	0.00000000	0.00000000
C	2.74718188	-1.10717004	0.00000000
C	4.13461689	-0.69796098	0.00000000
C	4.13461689	0.69796098	0.00000000
C	2.74718188	1.10717004	0.00000000
C	-5.32013797	-1.41457863	0.00000000
C	-6.50204530	-0.69894154	0.00000000
C	-6.50204530	0.69894154	0.00000000
C	-5.32013797	1.41457863	0.00000000
C	-1.41457863	5.32013797	0.00000000
C	-0.69894154	6.50204530	0.00000000
C	0.69894154	6.50204530	0.00000000
C	1.41457863	5.32013797	0.00000000
C	5.32013797	1.41457863	0.00000000
C	6.50204530	0.69894154	0.00000000
C	6.50204530	-0.69894154	0.00000000
C	5.32013797	-1.41457863	0.00000000
C	1.41457863	-5.32013797	0.00000000
C	0.69894154	-6.50204530	0.00000000
C	-0.69894154	-6.50204530	0.00000000
C	-1.41457863	-5.32013797	0.00000000
H	-5.31162192	-2.49479026	0.00000000
H	-7.44599432	-1.22623333	0.00000000
H	-7.44599432	1.22623333	0.00000000
H	-5.31162192	2.49479026	0.00000000
H	-2.49479026	5.31162192	0.00000000
H	-1.22623333	7.44599432	0.00000000
H	1.22623333	7.44599432	0.00000000
H	2.49479026	5.31162192	0.00000000
H	5.31162192	2.49479026	0.00000000
H	7.44599432	1.22623333	0.00000000
H	7.44599432	-1.22623333	0.00000000
H	5.31162192	-2.49479026	0.00000000
H	2.49479026	-5.31162192	0.00000000
H	1.22623333	-7.44599432	0.00000000
H	-1.22623333	-7.44599432	0.00000000
H	-2.49479026	-5.31162192	0.00000000

level of theory pbe0
spin state IS3

Occup.	alpha	beta
A _{1g}	21.0 //	21.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.36321510	2.36321510	0.00000000
N	-2.36321510	2.36321510	0.00000000
N	-2.36321510	-2.36321510	0.00000000
N	2.36321510	-2.36321510	0.00000000
N	0.00000000	1.95165861	0.00000000
C	1.10757804	2.74428146	0.00000000
C	0.69738470	4.13101902	0.00000000
C	-0.69738470	4.13101902	0.00000000
C	-1.10757804	2.74428146	0.00000000
N	-1.95165861	0.00000000	0.00000000
C	-2.74428146	1.10757804	0.00000000
C	-4.13101902	0.69738470	0.00000000
C	-4.13101902	-0.69738470	0.00000000
C	-2.74428146	-1.10757804	0.00000000
N	0.00000000	-1.95165861	0.00000000
C	-1.10757804	-2.74428146	0.00000000
C	-0.69738470	-4.13101902	0.00000000
C	0.69738470	-4.13101902	0.00000000
C	1.10757804	-2.74428146	0.00000000
N	1.95165861	0.00000000	0.00000000
C	2.74428146	-1.10757804	0.00000000
C	4.13101902	-0.69738470	0.00000000
C	4.13101902	0.69738470	0.00000000
C	2.74428146	1.10757804	0.00000000
C	-5.31581195	-1.41484322	0.00000000
C	-6.49775738	-0.69889180	0.00000000
C	-6.49775738	0.69889180	0.00000000
C	-5.31581195	1.41484322	0.00000000
C	-1.41484322	5.31581195	0.00000000
C	-0.69889180	6.49775738	0.00000000
C	0.69889180	6.49775738	0.00000000
C	1.41484322	5.31581195	0.00000000
C	5.31581195	1.41484322	0.00000000
C	6.49775738	0.69889180	0.00000000
C	6.49775738	-0.69889180	0.00000000
C	5.31581195	-1.41484322	0.00000000
C	1.41484322	-5.31581195	0.00000000
C	0.69889180	-6.49775738	0.00000000
C	-0.69889180	-6.49775738	0.00000000
C	-1.41484322	-5.31581195	0.00000000
H	-5.30750228	-2.49506702	0.00000000
H	-7.44158998	-1.22649210	0.00000000
H	-7.44158998	1.22649210	0.00000000
H	-5.30750228	2.49506702	0.00000000
H	-2.49506702	5.30750228	0.00000000
H	-1.22649210	7.44158998	0.00000000
H	1.22649210	7.44158998	0.00000000
H	2.49506702	5.30750228	0.00000000
H	5.30750228	2.49506702	0.00000000
H	7.44158998	1.22649210	0.00000000
H	7.44158998	-1.22649210	0.00000000
H	5.30750228	-2.49506702	0.00000000

H	2.49506702	-5.30750228	0.00000000
H	1.22649210	-7.44158998	0.00000000
H	-1.22649210	-7.44158998	0.00000000
H	-2.49506702	-5.30750228	0.00000000

level of theory pbe0
spin state LS

Occup.	alpha	beta
A _{1g}	20.0 //	21.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	14.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.37045266	2.37045266	0.00000000
N	-2.37045266	2.37045266	0.00000000
N	-2.37045266	-2.37045266	0.00000000
N	2.37045266	-2.37045266	0.00000000
N	0.00000000	1.94749240	0.00000000
C	1.10976936	2.74366761	0.00000000
C	0.69715716	4.13279917	0.00000000
C	-0.69715716	4.13279917	0.00000000
C	-1.10976936	2.74366761	0.00000000
N	-1.94749240	0.00000000	0.00000000
C	-2.74366761	1.10976936	0.00000000
C	-4.13279917	0.69715716	0.00000000
C	-4.13279917	-0.69715716	0.00000000
C	-2.74366761	-1.10976936	0.00000000
N	0.00000000	-1.94749240	0.00000000
C	-1.10976936	-2.74366761	0.00000000
C	-0.69715716	-4.13279917	0.00000000
C	0.69715716	-4.13279917	0.00000000
C	1.10976936	-2.74366761	0.00000000
N	1.94749240	0.00000000	0.00000000
C	2.74366761	-1.10976936	0.00000000
C	4.13279917	-0.69715716	0.00000000
C	4.13279917	0.69715716	0.00000000
C	2.74366761	1.10976936	0.00000000
C	-5.31417944	-1.41360335	0.00000000
C	-6.50102346	-0.69700952	0.00000000
C	-6.50102346	0.69700952	0.00000000
C	-5.31417944	1.41360335	0.00000000
C	-1.41360335	5.31417944	0.00000000
C	-0.69700952	6.50102346	0.00000000
C	0.69700952	6.50102346	0.00000000
C	1.41360335	5.31417944	0.00000000
C	5.31417944	1.41360335	0.00000000

C	6.50102346	0.69700952	0.00000000
C	6.50102346	-0.69700952	0.00000000
C	5.31417944	-1.41360335	0.00000000
C	1.41360335	-5.31417944	0.00000000
C	0.69700952	-6.50102346	0.00000000
C	-0.69700952	-6.50102346	0.00000000
C	-1.41360335	-5.31417944	0.00000000
H	-5.30485586	-2.49379911	0.00000000
H	-7.44394323	-1.22589254	0.00000000
H	-7.44394323	1.22589254	0.00000000
H	-5.30485586	2.49379911	0.00000000
H	-2.49379911	5.30485586	0.00000000
H	-1.22589254	7.44394323	0.00000000
H	1.22589254	7.44394323	0.00000000
H	2.49379911	5.30485586	0.00000000
H	5.30485586	2.49379911	0.00000000
H	7.44394323	1.22589254	0.00000000
H	7.44394323	-1.22589254	0.00000000
H	5.30485586	-2.49379911	0.00000000
H	2.49379911	-5.30485586	0.00000000
H	1.22589254	-7.44394323	0.00000000
H	-1.22589254	-7.44394323	0.00000000
H	-2.49379911	-5.30485586	0.00000000

level of theory tpssh
spin state HS

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	16.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.39003275	2.39003275	0.00000000
N	-2.39003275	2.39003275	0.00000000
N	-2.39003275	-2.39003275	0.00000000
N	2.39003275	-2.39003275	0.00000000
N	0.00000000	2.02573390	0.00000000
C	1.12458473	2.80138127	0.00000000
C	0.70452860	4.19634224	0.00000000
C	-0.70452860	4.19634224	0.00000000
C	-1.12458473	2.80138127	0.00000000
N	-2.02573390	0.00000000	0.00000000
C	-2.80138127	1.12458473	0.00000000
C	-4.19634224	0.70452860	0.00000000
C	-4.19634224	-0.70452860	0.00000000
C	-2.80138127	-1.12458473	0.00000000

N	0.00000000	-2.02573390	0.00000000
C	-1.12458473	-2.80138127	0.00000000
C	-0.70452860	-4.19634224	0.00000000
C	0.70452860	-4.19634224	0.00000000
C	1.12458473	-2.80138127	0.00000000
N	2.02573390	0.00000000	0.00000000
C	2.80138127	-1.12458473	0.00000000
C	4.19634224	-0.70452860	0.00000000
C	4.19634224	0.70452860	0.00000000
C	2.80138127	1.12458473	0.00000000
C	-5.38855530	-1.41880358	0.00000000
C	-6.57754567	-0.70089685	0.00000000
C	-6.57754567	0.70089685	0.00000000
C	-5.38855530	1.41880358	0.00000000
C	-1.41880358	5.38855530	0.00000000
C	-0.70089685	6.57754567	0.00000000
C	0.70089685	6.57754567	0.00000000
C	1.41880358	5.38855530	0.00000000
C	5.38855530	1.41880358	0.00000000
C	6.57754567	0.70089685	0.00000000
C	6.57754567	-0.70089685	0.00000000
C	5.38855530	-1.41880358	0.00000000
C	1.41880358	-5.38855530	0.00000000
C	0.70089685	-6.57754567	0.00000000
C	-0.70089685	-6.57754567	0.00000000
C	-1.41880358	-5.38855530	0.00000000
H	-5.38277774	-2.50042653	0.00000000
H	-7.52233555	-1.23027572	0.00000000
H	-7.52233555	1.23027572	0.00000000
H	-5.38277774	2.50042653	0.00000000
H	-2.50042653	5.38277774	0.00000000
H	-1.23027572	7.52233555	0.00000000
H	1.23027572	7.52233555	0.00000000
H	2.50042653	5.38277774	0.00000000
H	5.38277774	2.50042653	0.00000000
H	7.52233555	1.23027572	0.00000000
H	7.52233555	-1.23027572	0.00000000
H	5.38277774	-2.50042653	0.00000000
H	2.50042653	-5.38277774	0.00000000
H	1.23027572	-7.52233555	0.00000000
H	-1.23027572	-7.52233555	0.00000000
H	-2.50042653	-5.38277774	0.00000000

level of theory tpssh
spin state IS

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	11.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0

B _{2u}	3.0	//	3.0
E _{1u}	60.0	//	60.0
Mn	0.00000000	0.00000000	0.00000000
N	2.38054301	2.38054301	0.00000000
N	-2.38054301	2.38054301	0.00000000
N	-2.38054301	-2.38054301	0.00000000
N	2.38054301	-2.38054301	0.00000000
N	0.00000000	1.94231916	0.00000000
C	1.11970466	2.75744421	0.00000000
C	0.70057035	4.13731675	0.00000000
C	-0.70057035	4.13731675	0.00000000
C	-1.11970466	2.75744421	0.00000000
N	-1.94231916	0.00000000	0.00000000
C	-2.75744421	1.11970466	0.00000000
C	-4.13731675	0.70057035	0.00000000
C	-4.13731675	-0.70057035	0.00000000
C	-2.75744421	-1.11970466	0.00000000
N	0.00000000	-1.94231916	0.00000000
C	-1.11970466	-2.75744421	0.00000000
C	-0.70057035	-4.13731675	0.00000000
C	0.70057035	-4.13731675	0.00000000
C	1.11970466	-2.75744421	0.00000000
N	1.94231916	0.00000000	0.00000000
C	2.75744421	-1.11970466	0.00000000
C	4.13731675	-0.70057035	0.00000000
C	4.13731675	0.70057035	0.00000000
C	2.75744421	1.11970466	0.00000000
C	-5.32958802	-1.42065517	0.00000000
C	-6.51541602	-0.70275585	0.00000000
C	-6.51541602	0.70275585	0.00000000
C	-5.32958802	1.42065517	0.00000000
C	-1.42065517	5.32958802	0.00000000
C	-0.70275585	6.51541602	0.00000000
C	0.70275585	6.51541602	0.00000000
C	1.42065517	5.32958802	0.00000000
C	5.32958802	1.42065517	0.00000000
C	6.51541602	0.70275585	0.00000000
C	6.51541602	-0.70275585	0.00000000
C	5.32958802	-1.42065517	0.00000000
C	1.42065517	-5.32958802	0.00000000
C	0.70275585	-6.51541602	0.00000000
C	-0.70275585	-6.51541602	0.00000000
C	-1.42065517	-5.32958802	0.00000000
H	-5.32152442	-2.50211990	0.00000000
H	-7.46101502	-1.23076362	0.00000000
H	-7.46101502	1.23076362	0.00000000
H	-5.32152442	2.50211990	0.00000000
H	-2.50211990	5.32152442	0.00000000
H	-1.23076362	7.46101502	0.00000000
H	1.23076362	7.46101502	0.00000000
H	2.50211990	5.32152442	0.00000000
H	5.32152442	2.50211990	0.00000000
H	7.46101502	1.23076362	0.00000000

H	7.46101502	-1.23076362	0.00000000
H	5.32152442	-2.50211990	0.00000000
H	2.50211990	-5.32152442	0.00000000
H	1.23076362	-7.46101502	0.00000000
H	-1.23076362	-7.46101502	0.00000000
H	-2.50211990	-5.32152442	0.00000000

level of theory tpssh
spin state IS2

Occup.	alpha		beta
A _{1g}	21.0	//	20.0
A _{2g}	11.0	//	11.0
B _{1g}	15.0	//	15.0
B _{2g}	14.0	//	14.0
E _{1g}	12.0	//	10.0
A _{1u}	2.0	//	2.0
A _{2u}	6.0	//	6.0
B _{1u}	2.0	//	2.0
B _{2u}	3.0	//	3.0
E _{1u}	60.0	//	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.37843530	2.37843530	0.00000000
N	-2.37843530	2.37843530	0.00000000
N	-2.37843530	-2.37843530	0.00000000
N	2.37843530	-2.37843530	0.00000000
N	0.00000000	1.95659583	0.00000000
C	1.11357732	2.76004036	0.00000000
C	0.70097517	4.14911635	0.00000000
C	-0.70097517	4.14911635	0.00000000
C	-1.11357732	2.76004036	0.00000000
N	-1.95659583	0.00000000	0.00000000
C	-2.76004036	1.11357732	0.00000000
C	-4.14911635	0.70097517	0.00000000
C	-4.14911635	-0.70097517	0.00000000
C	-2.76004036	-1.11357732	0.00000000
N	0.00000000	-1.95659583	0.00000000
C	-1.11357732	-2.76004036	0.00000000
C	-0.70097517	-4.14911635	0.00000000
C	0.70097517	-4.14911635	0.00000000
C	1.11357732	-2.76004036	0.00000000
N	1.95659583	0.00000000	0.00000000
C	2.76004036	-1.11357732	0.00000000
C	4.14911635	-0.70097517	0.00000000
C	4.14911635	0.70097517	0.00000000
C	2.76004036	1.11357732	0.00000000
C	-5.33975457	-1.42026040	0.00000000
C	-6.52690129	-0.70190652	0.00000000
C	-6.52690129	0.70190652	0.00000000
C	-5.33975457	1.42026040	0.00000000
C	-1.42026040	5.33975457	0.00000000
C	-0.70190652	6.52690129	0.00000000
C	0.70190652	6.52690129	0.00000000

C	1.42026040	5.33975457	0.00000000
C	5.33975457	1.42026040	0.00000000
C	6.52690129	0.70190652	0.00000000
C	6.52690129	-0.70190652	0.00000000
C	5.33975457	-1.42026040	0.00000000
C	1.42026040	-5.33975457	0.00000000
C	0.70190652	-6.52690129	0.00000000
C	-0.70190652	-6.52690129	0.00000000
C	-1.42026040	-5.33975457	0.00000000
H	-5.33184496	-2.50182038	0.00000000
H	-7.47257119	-1.22985661	0.00000000
H	-7.47257119	1.22985661	0.00000000
H	-5.33184496	2.50182038	0.00000000
H	-2.50182038	5.33184496	0.00000000
H	-1.22985661	7.47257119	0.00000000
H	1.22985661	7.47257119	0.00000000
H	2.50182038	5.33184496	0.00000000
H	5.33184496	2.50182038	0.00000000
H	7.47257119	1.22985661	0.00000000
H	7.47257119	-1.22985661	0.00000000
H	5.33184496	-2.50182038	0.00000000
H	2.50182038	-5.33184496	0.00000000
H	1.22985661	-7.47257119	0.00000000
H	-1.22985661	-7.47257119	0.00000000
H	-2.50182038	-5.33184496	0.00000000

level of theory tpssh
spin state IS3

Occup.	alpha	beta
A _{1g}	21.0 //	21.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.37768228	2.37768228	0.00000000
N	-2.37768228	2.37768228	0.00000000
N	-2.37768228	-2.37768228	0.00000000
N	2.37768228	-2.37768228	0.00000000
N	0.00000000	1.95333081	0.00000000
C	1.11412184	2.75695526	0.00000000
C	0.70029730	4.14489404	0.00000000
C	-0.70029730	4.14489404	0.00000000
C	-1.11412184	2.75695526	0.00000000
N	-1.95333081	0.00000000	0.00000000
C	-2.75695526	1.11412184	0.00000000
C	-4.14489404	0.70029730	0.00000000

C	-4.14489404	-0.70029730	0.00000000
C	-2.75695526	-1.11412184	0.00000000
N	0.00000000	-1.95333081	0.00000000
C	-1.11412184	-2.75695526	0.00000000
C	-0.70029730	-4.14489404	0.00000000
C	0.70029730	-4.14489404	0.00000000
C	1.11412184	-2.75695526	0.00000000
N	1.95333081	0.00000000	0.00000000
C	2.75695526	-1.11412184	0.00000000
C	4.14489404	-0.70029730	0.00000000
C	4.14489404	0.70029730	0.00000000
C	2.75695526	1.11412184	0.00000000
C	-5.33475967	-1.42048001	0.00000000
C	-6.52190427	-0.70184143	0.00000000
C	-6.52190427	0.70184143	0.00000000
C	-5.33475967	1.42048001	0.00000000
C	-1.42048001	5.33475967	0.00000000
C	-0.70184143	6.52190427	0.00000000
C	0.70184143	6.52190427	0.00000000
C	1.42048001	5.33475967	0.00000000
C	5.33475967	1.42048001	0.00000000
C	6.52190427	0.70184143	0.00000000
C	6.52190427	-0.70184143	0.00000000
C	5.33475967	-1.42048001	0.00000000
C	1.42048001	-5.33475967	0.00000000
C	0.70184143	-6.52190427	0.00000000
C	-0.70184143	-6.52190427	0.00000000
C	-1.42048001	-5.33475967	0.00000000
H	-5.32728345	-2.50184525	0.00000000
H	-7.46721962	-1.23012914	0.00000000
H	-7.46721962	1.23012914	0.00000000
H	-5.32728345	2.50184525	0.00000000
H	-2.50184525	5.32728345	0.00000000
H	-1.23012914	7.46721962	0.00000000
H	1.23012914	7.46721962	0.00000000
H	2.50184525	5.32728345	0.00000000
H	5.32728345	2.50184525	0.00000000
H	7.46721962	1.23012914	0.00000000
H	7.46721962	-1.23012914	0.00000000
H	5.32728345	-2.50184525	0.00000000
H	2.50184525	-5.32728345	0.00000000
H	1.23012914	-7.46721962	0.00000000
H	-1.23012914	-7.46721962	0.00000000
H	-2.50184525	-5.32728345	0.00000000

level of theory tpssh
spin state LS

Mn	0.00000000	0.00000000	0.00000000
N	2.38474097	2.38474097	0.00000000
N	-2.38474097	2.38474097	0.00000000
N	-2.38474097	-2.38474097	0.00000000
N	2.38474097	-2.38474097	0.00000000
N	0.00000000	1.96299147	0.00000000

C	1.11545537	2.77683962	0.00000000	Occup.	alpha	beta	
C	0.69907384	4.16643314	0.00000000	A _{1g}	21.0	//	20.0
C	-0.69907384	4.16643314	0.00000000	A _{2g}	11.0	//	11.0
C	-1.11545537	2.77683962	0.00000000	B _{1g}	16.0	//	15.0
N	-1.96299147	0.00000000	0.00000000	B _{2g}	14.0	//	13.0
C	-2.77683962	1.11545537	0.00000000	E _{1g}	12.0	//	10.0
C	-4.16643314	0.69907384	0.00000000	A _{1u}	2.0	//	2.0
C	-4.16643314	-0.69907384	0.00000000	A _{2u}	6.0	//	6.0
C	-2.77683962	-1.11545537	0.00000000	B _{1u}	2.0	//	2.0
N	0.00000000	-1.96299147	0.00000000	B _{2u}	3.0	//	3.0
C	-1.11545537	-2.77683962	0.00000000	E _{1u}	60.0	//	60.0
C	-0.69907384	-4.16643314	0.00000000				
C	0.69907384	-4.16643314	0.00000000				
C	1.11545537	-2.77683962	0.00000000	Mn	0.00000000	0.00000000	0.00000000
N	1.96299147	0.00000000	0.00000000	N	2.38643328	2.38643328	0.00000000
C	2.77683962	-1.11545537	0.00000000	N	-2.38643328	2.38643328	0.00000000
C	4.16643314	-0.69907384	0.00000000	N	-2.38643328	-2.38643328	0.00000000
C	4.16643314	0.69907384	0.00000000	N	2.38643328	-2.38643328	0.00000000
C	2.77683962	1.11545537	0.00000000	N	0.00000000	2.03183161	0.00000000
C	-5.35335443	-1.41213436	0.00000000	C	1.12523139	2.80363451	0.00000000
C	-6.52977842	-0.69729263	0.00000000	C	0.70503026	4.20146203	0.00000000
C	-6.52977842	0.69729263	0.00000000	C	-0.70503026	4.20146203	0.00000000
C	-5.35335443	1.41213436	0.00000000	C	-1.12523139	2.80363451	0.00000000
C	-1.41213436	5.35335443	0.00000000	N	-2.03183161	0.00000000	0.00000000
C	-0.69729263	6.52977842	0.00000000	C	-2.80363451	1.12523139	0.00000000
C	0.69729263	6.52977842	0.00000000	C	-4.20146203	0.70503026	0.00000000
C	1.41213436	5.35335443	0.00000000	C	-4.20146203	-0.70503026	0.00000000
C	5.35335443	1.41213436	0.00000000	C	-2.80363451	-1.12523139	0.00000000
C	6.52977842	0.69729263	0.00000000	N	0.00000000	-2.03183161	0.00000000
C	6.52977842	-0.69729263	0.00000000	C	-1.12523139	-2.80363451	0.00000000
C	5.35335443	-1.41213436	0.00000000	C	-0.70503026	-4.20146203	0.00000000
C	1.41213436	-5.35335443	0.00000000	C	0.70503026	-4.20146203	0.00000000
C	0.69729263	-6.52977842	0.00000000	C	1.12523139	-2.80363451	0.00000000
C	-0.69729263	-6.52977842	0.00000000	N	2.03183161	0.00000000	0.00000000
C	-1.41213436	-5.35335443	0.00000000	C	2.80363451	-1.12523139	0.00000000
H	-5.34962161	-2.44952232	0.00000000	C	4.20146203	-0.70503026	0.00000000
H	-7.44123543	-1.20541285	0.00000000	C	4.20146203	0.70503026	0.00000000
H	-7.44123543	1.20541285	0.00000000	C	2.80363451	1.12523139	0.00000000
H	-5.34962161	2.44952232	0.00000000	C	-5.39358460	-1.41703666	0.00000000
H	-2.44952232	5.34962161	0.00000000	C	-6.58290888	-0.70022744	0.00000000
H	-1.20541285	7.44123543	0.00000000	C	-6.58290888	0.70022744	0.00000000
H	1.20541285	7.44123543	0.00000000	C	-5.39358460	1.41703666	0.00000000
H	2.44952232	5.34962161	0.00000000	C	-1.41703666	5.39358460	0.00000000
H	5.34962161	2.44952232	0.00000000	C	-0.70022744	6.58290888	0.00000000
H	7.44123543	1.20541285	0.00000000	C	0.70022744	6.58290888	0.00000000
H	7.44123543	-1.20541285	0.00000000	C	1.41703666	5.39358460	0.00000000
H	5.34962161	-2.44952232	0.00000000	C	5.39358460	1.41703666	0.00000000
H	2.44952232	-5.34962161	0.00000000	C	6.58290888	0.70022744	0.00000000
H	1.20541285	-7.44123543	0.00000000	C	6.58290888	-0.70022744	0.00000000
H	-1.20541285	-7.44123543	0.00000000	C	5.39358460	-1.41703666	0.00000000
H	-2.44952232	-5.34962161	0.00000000	C	1.41703666	-5.39358460	0.00000000
				C	0.70022744	-6.58290888	0.00000000
				C	-0.70022744	-6.58290888	0.00000000
				C	-1.41703666	-5.39358460	0.00000000
				H	-5.38851984	-2.49811138	0.00000000

level of theory b3lyp*
spin state HS

H	-7.52624300	-1.22998414	0.00000000
H	-7.52624300	1.22998414	0.00000000
H	-5.38851984	2.49811138	0.00000000
H	-2.49811138	5.38851984	0.00000000
H	-1.22998414	7.52624300	0.00000000
H	1.22998414	7.52624300	0.00000000
H	2.49811138	5.38851984	0.00000000
H	5.38851984	2.49811138	0.00000000
H	7.52624300	1.22998414	0.00000000
H	7.52624300	-1.22998414	0.00000000
H	5.38851984	-2.49811138	0.00000000
H	2.49811138	-5.38851984	0.00000000
H	1.22998414	-7.52624300	0.00000000
H	-1.22998414	-7.52624300	0.00000000
H	-2.49811138	-5.38851984	0.00000000

level of theory b3lyp*
spin state IS

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	11.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.37773467	2.37773467	0.00000000
N	-2.37773467	2.37773467	0.00000000
N	-2.37773467	-2.37773467	0.00000000
N	2.37773467	-2.37773467	0.00000000
N	0.00000000	1.94906511	0.00000000
C	1.12071856	2.76053355	0.00000000
C	0.70122124	4.14288211	0.00000000
C	-0.70122124	4.14288211	0.00000000
C	-1.12071856	2.76053355	0.00000000
N	-1.94906511	0.00000000	0.00000000
C	-2.76053355	1.12071856	0.00000000
C	-4.14288211	0.70122124	0.00000000
C	-4.14288211	-0.70122124	0.00000000
C	-2.76053355	-1.12071856	0.00000000
N	0.00000000	-1.94906511	0.00000000
C	-1.12071856	-2.76053355	0.00000000
C	-0.70122124	-4.14288211	0.00000000
C	0.70122124	-4.14288211	0.00000000
C	1.12071856	-2.76053355	0.00000000
N	1.94906511	0.00000000	0.00000000
C	2.76053355	-1.12071856	0.00000000
C	4.14288211	-0.70122124	0.00000000

C	4.14288211	0.70122124	0.00000000
C	2.76053355	1.12071856	0.00000000
C	-5.33552010	-1.41849242	0.00000000
C	-6.52188575	-0.70203988	0.00000000
C	-6.52188575	0.70203988	0.00000000
C	-5.33552010	1.41849242	0.00000000
C	-1.41849242	5.33552010	0.00000000
C	-0.70203988	6.52188575	0.00000000
C	0.70203988	6.52188575	0.00000000
C	1.41849242	5.33552010	0.00000000
C	5.33552010	1.41849242	0.00000000
C	6.52188575	0.70203988	0.00000000
C	6.52188575	-0.70203988	0.00000000
C	5.33552010	-1.41849242	0.00000000
C	1.41849242	-5.33552010	0.00000000
C	0.70203988	-6.52188575	0.00000000
C	-0.70203988	-6.52188575	0.00000000
C	-1.41849242	-5.33552010	0.00000000
H	-5.32874028	-2.49935018	0.00000000
H	-7.46585593	-1.23072658	0.00000000
H	-7.46585593	1.23072658	0.00000000
H	-5.32874028	2.49935018	0.00000000
H	-2.49935018	5.32874028	0.00000000
H	-1.23072658	7.46585593	0.00000000
H	1.23072658	7.46585593	0.00000000
H	2.49935018	5.32874028	0.00000000
H	5.32874028	2.49935018	0.00000000
H	7.46585593	1.23072658	0.00000000
H	7.46585593	-1.23072658	0.00000000
H	5.32874028	-2.49935018	0.00000000
H	2.49935018	-5.32874028	0.00000000
H	1.23072658	-7.46585593	0.00000000
H	-1.23072658	-7.46585593	0.00000000
H	-2.49935018	-5.32874028	0.00000000

level of theory b3lyp*
spin state IS2

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	14.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.37580952	2.37580952	0.00000000
N	-2.37580952	2.37580952	0.00000000
N	-2.37580952	-2.37580952	0.00000000

N	2.37580952	-2.37580952	0.00000000
N	0.00000000	1.96485523	0.00000000
C	1.11472404	2.76371444	0.00000000
C	0.70155356	4.15561888	0.00000000
C	-0.70155356	4.15561888	0.00000000
C	-1.11472404	2.76371444	0.00000000
N	-1.96485523	0.00000000	0.00000000
C	-2.76371444	1.11472404	0.00000000
C	-4.15561888	0.70155356	0.00000000
C	-4.15561888	-0.70155356	0.00000000
C	-2.76371444	-1.11472404	0.00000000
N	0.00000000	-1.96485523	0.00000000
C	-1.11472404	-2.76371444	0.00000000
C	-0.70155356	-4.15561888	0.00000000
C	0.70155356	-4.15561888	0.00000000
C	1.11472404	-2.76371444	0.00000000
N	1.96485523	0.00000000	0.00000000
C	2.76371444	-1.11472404	0.00000000
C	4.15561888	-0.70155356	0.00000000
C	4.15561888	0.70155356	0.00000000
C	2.76371444	1.11472404	0.00000000
C	-5.34648200	-1.41809448	0.00000000
C	-6.53421134	-0.70113392	0.00000000
C	-6.53421134	0.70113392	0.00000000
C	-5.34648200	1.41809448	0.00000000
C	-1.41809448	5.34648200	0.00000000
C	-0.70113392	6.53421134	0.00000000
C	0.70113392	6.53421134	0.00000000
C	1.41809448	5.34648200	0.00000000
C	5.34648200	1.41809448	0.00000000
C	6.53421134	0.70113392	0.00000000
C	6.53421134	-0.70113392	0.00000000
C	5.34648200	-1.41809448	0.00000000
C	1.41809448	-5.34648200	0.00000000
C	0.70113392	-6.53421134	0.00000000
C	-0.70113392	-6.53421134	0.00000000
C	-1.41809448	-5.34648200	0.00000000
H	-5.33973552	-2.49915015	0.00000000
H	-7.47822334	-1.22995239	0.00000000
H	-7.47822334	1.22995239	0.00000000
H	-5.33973552	2.49915015	0.00000000
H	-2.49915015	5.33973552	0.00000000
H	-1.22995239	7.47822334	0.00000000
H	1.22995239	7.47822334	0.00000000
H	2.49915015	5.33973552	0.00000000
H	5.33973552	2.49915015	0.00000000
H	7.47822334	1.22995239	0.00000000
H	7.47822334	-1.22995239	0.00000000
H	5.33973552	-2.49915015	0.00000000
H	2.49915015	-5.33973552	0.00000000
H	1.22995239	-7.47822334	0.00000000
H	-1.22995239	-7.47822334	0.00000000
H	-2.49915015	-5.33973552	0.00000000

level of theory b3lyp*

spin state IS3

Occup.	alpha	beta
A _{1g}	21.0 //	21.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	10.0
A _{1u}	2.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.37466015	2.37466015	0.00000000
N	-2.37466015	2.37466015	0.00000000
N	-2.37466015	-2.37466015	0.00000000
N	2.37466015	-2.37466015	0.00000000
N	0.00000000	1.96180241	0.00000000
C	1.11512939	2.76066743	0.00000000
C	0.70085240	4.15151246	0.00000000
C	-0.70085240	4.15151246	0.00000000
C	-1.11512939	2.76066743	0.00000000
N	-1.96180241	0.00000000	0.00000000
C	-2.76066743	1.11512939	0.00000000
C	-4.15151246	0.70085240	0.00000000
C	-4.15151246	-0.70085240	0.00000000
C	-2.76066743	-1.11512939	0.00000000
N	0.00000000	-1.96180241	0.00000000
C	-1.11512939	-2.76066743	0.00000000
C	-0.70085240	-4.15151246	0.00000000
C	0.70085240	-4.15151246	0.00000000
C	1.11512939	-2.76066743	0.00000000
N	1.96180241	0.00000000	0.00000000
C	2.76066743	-1.11512939	0.00000000
C	4.15151246	-0.70085240	0.00000000
C	4.15151246	0.70085240	0.00000000
C	2.76066743	1.11512939	0.00000000
C	-5.34165114	-1.41830774	0.00000000
C	-6.52925877	-0.70112070	0.00000000
C	-6.52925877	0.70112070	0.00000000
C	-5.34165114	1.41830774	0.00000000
C	-1.41830774	5.34165114	0.00000000
C	-0.70112070	6.52925877	0.00000000
C	0.70112070	6.52925877	0.00000000
C	1.41830774	5.34165114	0.00000000
C	5.34165114	1.41830774	0.00000000
C	6.52925877	0.70112070	0.00000000
C	6.52925877	-0.70112070	0.00000000
C	5.34165114	-1.41830774	0.00000000
C	1.41830774	-5.34165114	0.00000000
C	0.70112070	-6.52925877	0.00000000
C	-0.70112070	-6.52925877	0.00000000

C	-1.41830774	-5.34165114	0.00000000
H	-5.33481629	-2.49916074	0.00000000
H	-7.47306809	-1.22993175	0.00000000
H	-7.47306809	1.22993175	0.00000000
H	-5.33481629	2.49916074	0.00000000
H	-2.49916074	5.33481629	0.00000000
H	-1.22993175	7.47306809	0.00000000
H	1.22993175	7.47306809	0.00000000
H	2.49916074	5.33481629	0.00000000
H	5.33481629	2.49916074	0.00000000
H	7.47306809	1.22993175	0.00000000
H	7.47306809	-1.22993175	0.00000000
H	5.33481629	-2.49916074	0.00000000
H	2.49916074	-5.33481629	0.00000000
H	1.22993175	-7.47306809	0.00000000
H	-1.22993175	-7.47306809	0.00000000
H	-2.49916074	-5.33481629	0.00000000

level of theory b3lyp*
spin state LS

Occup.	alpha	beta
A _{1g}	21.0 //	20.0
A _{2g}	11.0 //	11.0
B _{1g}	15.0 //	15.0
B _{2g}	14.0 //	13.0
E _{1g}	12.0 //	12.0
A _{1u}	1.0 //	2.0
A _{2u}	6.0 //	6.0
B _{1u}	2.0 //	2.0
B _{2u}	3.0 //	3.0
E _{1u}	60.0 //	60.0

Mn	0.00000000	0.00000000	0.00000000
N	2.38111558	2.38111558	0.00000000
N	-2.38111558	2.38111558	0.00000000
N	-2.38111558	-2.38111558	0.00000000
N	2.38111558	-2.38111558	0.00000000
N	0.00000000	1.94270652	0.00000000
C	1.12064818	2.75748020	0.00000000
C	0.69977129	4.14703404	0.00000000
C	-0.69977129	4.14703404	0.00000000
C	-1.12064818	2.75748020	0.00000000
N	-1.94270652	0.00000000	0.00000000
C	-2.75748020	1.12064818	0.00000000
C	-4.14703404	0.69977129	0.00000000
C	-4.14703404	-0.69977129	0.00000000
C	-2.75748020	-1.12064818	0.00000000
N	0.00000000	-1.94270652	0.00000000
C	-1.12064818	-2.75748020	0.00000000
C	-0.69977129	-4.14703404	0.00000000
C	0.69977129	-4.14703404	0.00000000
C	1.12064818	-2.75748020	0.00000000
N	1.94270652	0.00000000	0.00000000

C	2.75748020	-1.12064818	0.00000000
C	4.14703404	-0.69977129	0.00000000
C	4.14703404	0.69977129	0.00000000
C	2.75748020	1.12064818	0.00000000
C	-5.33448079	-1.41635402	0.00000000
C	-6.52735850	-0.69902568	0.00000000
C	-6.52735850	0.69902568	0.00000000
C	-5.33448079	1.41635402	0.00000000
C	-1.41635402	5.33448079	0.00000000
C	-0.69902568	6.52735850	0.00000000
C	0.69902568	6.52735850	0.00000000
C	1.41635402	5.33448079	0.00000000
C	5.33448079	1.41635402	0.00000000
C	6.52735850	0.69902568	0.00000000
C	6.52735850	-0.69902568	0.00000000
C	5.33448079	-1.41635402	0.00000000
C	1.41635402	-5.33448079	0.00000000
C	0.69902568	-6.52735850	0.00000000
C	-0.69902568	-6.52735850	0.00000000
C	-1.41635402	-5.33448079	0.00000000
H	-5.32736071	-2.49736048	0.00000000
H	-7.46990520	-1.23024556	0.00000000
H	-7.46990520	1.23024556	0.00000000
H	-5.32736071	2.49736048	0.00000000
H	-2.49736048	5.32736071	0.00000000
H	-1.23024556	7.46990520	0.00000000
H	1.23024556	7.46990520	0.00000000
H	2.49736048	5.32736071	0.00000000
H	5.32736071	2.49736048	0.00000000
H	7.46990520	1.23024556	0.00000000
H	7.46990520	-1.23024556	0.00000000
H	5.32736071	-2.49736048	0.00000000
H	2.49736048	-5.32736071	0.00000000
H	1.23024556	-7.46990520	0.00000000
H	-1.23024556	-7.46990520	0.00000000
H	-2.49736048	-5.32736071	0.00000000

**Cartesian coordinates for Pc^{3-} in HS and LS
minimum structures obtained by LDA.**

HS

N	2.377060	2.377060	0.000000
N	-2.377060	2.377060	0.000000
N	-2.377060	-2.377060	0.000000
N	2.377060	-2.377060	0.000000
N	0.000000	1.975477	0.000000
C	1.096449	2.752524	0.000000
C	0.707272	4.153510	0.000000
C	-0.707272	4.153510	0.000000
C	-1.096449	2.752524	0.000000
N	-1.975477	0.000000	0.000000
C	-2.752524	1.096449	0.000000
C	-4.153510	0.707272	0.000000
C	-4.153510	-0.707272	0.000000
C	-2.752524	-1.096449	0.000000
N	0.000000	-1.975477	0.000000
C	-1.096449	-2.752524	0.000000
C	-0.707272	-4.153510	0.000000
C	0.707272	-4.153510	0.000000
C	1.096449	-2.752524	0.000000
N	1.975477	0.000000	0.000000
C	2.752524	-1.096449	0.000000
C	4.153510	-0.707272	0.000000
C	4.153510	0.707272	0.000000
C	2.752524	1.096449	0.000000
C	-5.347039	-1.407140	0.000000
C	-6.543763	-0.701259	0.000000
C	-6.543763	0.701259	0.000000
C	-5.347039	1.407140	0.000000
C	-1.407140	5.347039	0.000000
C	-0.701259	6.543763	0.000000
C	0.701259	6.543763	0.000000
C	1.407140	5.347039	0.000000
C	5.347039	1.407140	0.000000
C	6.543763	0.701259	0.000000
C	6.543763	-0.701259	0.000000
C	5.347039	-1.407140	0.000000
C	1.407140	-5.347039	0.000000
C	0.701259	-6.543763	0.000000
C	-0.701259	-6.543763	0.000000
C	-1.407140	-5.347039	0.000000
H	-5.323716	-2.502401	0.000000
H	-7.499110	-1.239699	0.000000
H	-7.499110	1.239699	0.000000
H	-5.323716	2.502401	0.000000
H	-2.502401	5.323716	0.000000
H	-1.239699	7.499110	0.000000
H	1.239699	7.499110	0.000000

H	2.502401	5.323716	0.000000
H	5.323716	2.502401	0.000000
H	7.499110	1.239699	0.000000
H	7.499110	-1.239699	0.000000
H	5.323716	-2.502401	0.000000
H	2.502401	-5.323716	0.000000
H	1.239699	-7.499110	0.000000
H	-1.239699	-7.499110	0.000000
H	-2.502401	-5.323716	0.000000

LS min

N	0.000000	3.374861	0.000000
N	-3.348043	0.000000	0.000000
N	0.000000	-3.374861	0.000000
N	3.348043	0.000000	0.000000
N	-1.386818	1.404421	0.000000
C	-1.169459	2.721864	0.000000
C	-2.443845	3.433961	0.000000
C	-3.439556	2.430502	0.000000
C	-2.719108	1.172199	0.000000
N	-1.386818	-1.404421	0.000000
C	-2.719108	-1.172199	0.000000
C	-3.439556	-2.430502	0.000000
C	-2.443845	-3.433961	0.000000
C	-1.169459	-2.721864	0.000000
N	1.386818	-1.404421	0.000000
C	1.169459	-2.721864	0.000000
C	2.443845	-3.433961	0.000000
C	3.439556	-2.430502	0.000000
C	2.719108	-1.172199	0.000000
N	1.386818	1.404421	0.000000
C	2.719108	1.172199	0.000000
C	3.439556	2.430502	0.000000
C	2.443845	3.433961	0.000000
C	1.169459	2.721864	0.000000
C	-2.793803	-4.770772	0.000000
C	-4.140704	-5.117994	0.000000
C	-5.128537	-4.123079	0.000000
C	-4.780368	-2.778801	0.000000
C	-4.780368	2.778801	0.000000
C	-5.128537	4.123079	0.000000
C	-4.140704	5.117994	0.000000
C	-2.793803	4.770772	0.000000
C	2.793803	4.770772	0.000000
C	4.140704	5.117994	0.000000
C	5.128537	4.123079	0.000000
C	4.780368	2.778801	0.000000
C	4.780368	-2.778801	0.000000
C	5.128537	-4.123079	0.000000
C	4.140704	-5.117994	0.000000
C	2.793803	-4.770772	0.000000

H	-2.002491	-5.528628	0.000000
H	-4.437174	-6.173500	0.000000
H	-6.185788	-4.414408	0.000000
H	-5.538884	-1.988307	0.000000
H	-5.538884	1.988307	0.000000
H	-6.185788	4.414408	0.000000
H	-4.437174	6.173500	0.000000
H	-2.002491	5.528628	0.000000
H	2.002491	5.528628	0.000000
H	4.437174	6.173500	0.000000
H	6.185788	4.414408	0.000000
H	5.538884	1.988307	0.000000
H	5.538884	-1.988307	0.000000
H	6.185788	-4.414408	0.000000
H	4.437174	-6.173500	0.000000
H	2.002491	-5.528628	0.000000

LS TS

N	2.372782	2.381236	0.000000
N	-2.372782	2.381236	0.000000
N	-2.372782	-2.381236	0.000000
N	2.372782	-2.381236	0.000000
N	0.000000	1.954888	0.000000
C	1.096880	2.733517	0.000000
C	0.702649	4.143245	0.000000
C	-0.702649	4.143245	0.000000
C	-1.096880	2.733517	0.000000
N	-1.994017	0.000000	0.000000
C	-2.770691	1.094965	0.000000
C	-4.164122	0.711254	0.000000
C	-4.164122	-0.711254	0.000000
C	-2.770691	-1.094965	0.000000
N	0.000000	-1.954888	0.000000
C	-1.096880	-2.733517	0.000000
C	-0.702649	-4.143245	0.000000
C	0.702649	-4.143245	0.000000
C	1.096880	-2.733517	0.000000
N	1.994017	0.000000	0.000000
C	2.770691	-1.094965	0.000000
C	4.164122	-0.711254	0.000000
C	4.164122	0.711254	0.000000
C	2.770691	1.094965	0.000000
C	-5.361828	-1.407932	0.000000
C	-6.558096	-0.703207	0.000000
C	-6.558096	0.703207	0.000000
C	-5.361828	1.407932	0.000000
C	-1.406146	5.332906	0.000000
C	-0.698661	6.530228	0.000000
C	0.698661	6.530228	0.000000
C	1.406146	5.332906	0.000000
C	5.361828	1.407932	0.000000

C	6.558096	0.703207	0.000000
C	6.558096	-0.703207	0.000000
C	5.361828	-1.407932	0.000000
C	1.406146	-5.332906	0.000000
C	0.698661	-6.530228	0.000000
C	-0.698661	-6.530228	0.000000
C	-1.406146	-5.332906	0.000000
H	-5.342497	-2.503615	0.000000
H	-7.512995	-1.242482	0.000000
H	-7.512995	1.242482	0.000000
H	-5.342497	2.503615	0.000000
H	-2.501163	5.305584	0.000000
H	-1.236523	7.485775	0.000000
H	1.236523	7.485775	0.000000
H	2.501163	5.305584	0.000000
H	5.342497	2.503615	0.000000
H	7.512995	1.242482	0.000000
H	7.512995	-1.242482	0.000000
H	5.342497	-2.503615	0.000000
H	2.501163	-5.305584	0.000000
H	1.236523	-7.485775	0.000000
H	-1.236523	-7.485775	0.000000
H	-2.501163	-5.305584	0.000000

Cartesian coordinates for MgPc⁻ in HS and LS minimum structures obtained by LDA.

HS

Mg	0.000000	0.000000	0.000000
N	2.380425	2.380425	0.000000
N	-2.380425	2.380425	0.000000
N	-2.380425	-2.380425	0.000000
N	2.380425	-2.380425	0.000000
N	0.000000	1.989035	0.000000
C	1.117407	2.773655	0.000000
C	0.702697	4.152829	0.000000
C	-0.702697	4.152829	0.000000
C	-1.117407	2.773655	0.000000
N	-1.989035	0.000000	0.000000
C	-2.773655	1.117407	0.000000
C	-4.152829	0.702697	0.000000
C	-4.152829	-0.702697	0.000000
C	-2.773655	-1.117407	0.000000
N	0.000000	-1.989035	0.000000
C	-1.117407	-2.773655	0.000000
C	-0.702697	-4.152829	0.000000
C	0.702697	-4.152829	0.000000
C	1.117407	-2.773655	0.000000
N	1.989035	0.000000	0.000000
C	2.773655	-1.117407	0.000000

C	4.152829	-0.702697	0.000000
C	4.152829	0.702697	0.000000
C	2.773655	1.117407	0.000000
C	-5.342344	-1.410983	0.000000
C	-6.527566	-0.699329	0.000000
C	-6.527566	0.699329	0.000000
C	-5.342344	1.410983	0.000000
C	-1.410983	5.342344	0.000000
C	-0.699329	6.527566	0.000000
C	0.699329	6.527566	0.000000
C	1.410983	5.342344	0.000000
C	5.342344	1.410983	0.000000
C	6.527566	0.699329	0.000000
C	6.527566	-0.699329	0.000000
C	5.342344	-1.410983	0.000000
C	1.410983	-5.342344	0.000000
C	0.699329	-6.527566	0.000000
C	-0.699329	-6.527566	0.000000
C	-1.410983	-5.342344	0.000000
H	-5.325142	-2.504148	0.000000
H	-7.481291	-1.233810	0.000000
H	-7.481291	1.233810	0.000000
H	-5.325142	2.504148	0.000000
H	-2.504148	5.325142	0.000000
H	-1.233810	7.481291	0.000000
H	1.233810	7.481291	0.000000
H	2.504148	5.325142	0.000000
H	5.325142	2.504148	0.000000
H	7.481291	1.233810	0.000000
H	7.481291	-1.233810	0.000000
H	5.325142	-2.504148	0.000000
H	2.504148	-5.325142	0.000000
H	1.233810	-7.481291	0.000000
H	-1.233810	-7.481291	0.000000
H	-2.504148	-5.325142	0.000000

LS min

Mg	0.000000	0.000000	0.000000
N	2.389324	2.371886	0.000000
N	-2.389324	2.371886	0.000000
N	-2.389324	-2.371886	0.000000
N	2.389324	-2.371886	0.000000
N	0.000000	1.993977	0.000000
C	1.114701	2.777098	0.000000
C	0.705834	4.147941	0.000000
C	-0.705834	4.147941	0.000000
C	-1.114701	2.777098	0.000000
N	-1.982839	0.000000	0.000000
C	-2.768767	1.119542	0.000000
C	-4.157840	0.699252	0.000000
C	-4.157840	-0.699252	0.000000

C	-2.768767	-1.119542	0.000000
N	0.000000	-1.993977	0.000000
C	-1.114701	-2.777098	0.000000
C	-0.705834	-4.147941	0.000000
C	0.705834	-4.147941	0.000000
C	1.114701	-2.777098	0.000000
N	1.982839	0.000000	0.000000
C	2.768767	-1.119542	0.000000
C	4.157840	-0.699252	0.000000
C	4.157840	0.699252	0.000000
C	2.768767	1.119542	0.000000
C	-5.342426	-1.410102	0.000000
C	-6.529862	-0.697316	0.000000
C	-6.529862	0.697316	0.000000
C	-5.342426	1.410102	0.000000
C	-1.412460	5.342094	0.000000
C	-0.701232	6.524225	0.000000
C	0.701232	6.524225	0.000000
C	1.412460	5.342094	0.000000
C	5.342426	1.410102	0.000000
C	6.529862	0.697316	0.000000
C	6.529862	-0.697316	0.000000
C	5.342426	-1.410102	0.000000
C	1.412460	-5.342094	0.000000
C	0.701232	-6.524225	0.000000
C	-0.701232	-6.524225	0.000000
C	-1.412460	-5.342094	0.000000
H	-5.321824	-2.502853	0.000000
H	-7.483364	-1.231729	0.000000
H	-7.483364	1.231729	0.000000
H	-5.321824	2.502853	0.000000
H	-2.505470	5.326988	0.000000
H	-1.234479	7.478506	0.000000
H	1.234479	7.478506	0.000000
H	2.505470	5.326988	0.000000
H	5.321824	2.502853	0.000000
H	7.483364	1.231729	0.000000
H	7.483364	-1.231729	0.000000
H	5.321824	-2.502853	0.000000
H	2.505470	-5.326988	0.000000
H	1.234479	-7.478506	0.000000
H	-1.234479	-7.478506	0.000000
H	-2.505470	-5.326988	0.000000

LS TS

Mg	0.000002	-0.000001	0.000000
N	2.388073	2.388082	0.000000
N	-2.372506	2.372542	0.000000
N	-2.388081	-2.388088	0.000000
N	2.372508	-2.372535	0.000000
N	0.011233	1.988443	0.000000

C	1.117089	2.770140	0.000000
C	0.699122	4.153663	0.000000
C	-0.705695	4.152166	0.000000
C	-1.117946	2.776411	0.000000
N	-1.988450	-0.011216	0.000000
C	-2.776411	1.117972	0.000000
C	-4.152142	0.705694	0.000000
C	-4.153684	-0.699141	0.000000
C	-2.770143	-1.117073	0.000000
N	-0.011238	-1.988447	0.000000
C	-1.117093	-2.770145	0.000000
C	-0.699123	-4.153669	0.000000
C	0.705698	-4.152167	0.000000
C	1.117947	-2.776410	0.000000
N	1.988452	0.011221	0.000000
C	2.776413	-1.117967	0.000000
C	4.152143	-0.705689	0.000000
C	4.153681	0.699143	0.000000
C	2.770141	1.117073	0.000000
C	-5.338008	-1.412435	0.000000
C	-6.526971	-0.705500	0.000000
C	-6.527476	0.692991	0.000000
C	-5.346324	1.409803	0.000000
C	-1.409787	5.346335	0.000000
C	-0.692985	6.527481	0.000000
C	0.705497	6.526940	0.000000
C	1.412427	5.337968	0.000000
C	5.337999	1.412438	0.000000
C	6.526964	0.705509	0.000000
C	6.527474	-0.692981	0.000000
C	5.346323	-1.409796	0.000000
C	1.409794	-5.346337	0.000000
C	0.692995	-6.527485	0.000000
C	-0.705488	-6.526951	0.000000
C	-1.412425	-5.337981	0.000000
H	-5.313015	-2.505269	0.000000
H	-7.479451	-1.241384	0.000000
H	-7.482466	1.225248	0.000000
H	-5.335467	2.502704	0.000000
H	-2.502685	5.335472	0.000000
H	-1.225226	7.482474	0.000000
H	1.241400	7.479407	0.000000
H	2.505257	5.312969	0.000000
H	5.313000	2.505269	0.000000
H	7.479441	1.241396	0.000000
H	7.482464	-1.225235	0.000000
H	5.335468	-2.502696	0.000000
H	2.502692	-5.335472	0.000000
H	1.225240	-7.482477	0.000000
H	-1.241386	-7.479422	0.000000
H	-2.505257	-5.312987	0.000000

Cartesian coordinates for MnPc in HS and LS minimum structures obtained by LDA.

HS

Mn	0.000000	0.000000	0.000000
N	2.362463	2.362463	0.000000
N	-2.362463	2.362463	0.000000
N	-2.362463	-2.362463	0.000000
N	2.362463	-2.362463	0.000000
N	0.000000	1.916937	0.000000
C	1.110628	2.733992	0.000000
C	0.696744	4.106978	0.000000
C	-0.696744	4.106978	0.000000
C	-1.110628	2.733992	0.000000
N	-1.916937	0.000000	0.000000
C	-2.733992	1.110628	0.000000
C	-4.106978	0.696744	0.000000
C	-4.106978	-0.696744	0.000000
C	-2.733992	-1.110628	0.000000
N	0.000000	-1.916937	0.000000
C	-1.110628	-2.733992	0.000000
C	-0.696744	-4.106978	0.000000
C	0.696744	-4.106978	0.000000
C	1.110628	-2.733992	0.000000
N	1.916937	0.000000	0.000000
C	2.733992	-1.110628	0.000000
C	4.106978	-0.696744	0.000000
C	4.106978	0.696744	0.000000
C	2.733992	1.110628	0.000000
C	-5.289468	-1.414528	0.000000
C	-6.471333	-0.698379	0.000000
C	-6.471333	0.698379	0.000000
C	-5.289468	1.414528	0.000000
C	-1.414528	5.289468	0.000000
C	-0.698379	6.471333	0.000000
C	0.698379	6.471333	0.000000
C	1.414528	5.289468	0.000000
C	5.289468	1.414528	0.000000
C	6.471333	0.698379	0.000000
C	6.471333	-0.698379	0.000000
C	5.289468	-1.414528	0.000000
C	1.414528	-5.289468	0.000000
C	0.698379	-6.471333	0.000000
C	-0.698379	-6.471333	0.000000
C	-1.414528	-5.289468	0.000000
H	-5.273312	-2.506737	0.000000
H	-7.425400	-1.230362	0.000000
H	-7.425400	1.230362	0.000000
H	-5.273312	2.506737	0.000000
H	-2.506737	5.273312	0.000000

H	-1.230362	7.425400	0.000000
H	1.230362	7.425400	0.000000
H	2.506737	5.273312	0.000000
H	5.273312	2.506737	0.000000
H	7.425400	1.230362	0.000000
H	7.425400	-1.230362	0.000000
H	5.273312	-2.506737	0.000000
H	2.506737	-5.273312	0.000000
H	1.230362	-7.425400	0.000000
H	-1.230362	-7.425400	0.000000
H	-2.506737	-5.273312	0.000000

LS min

Mn	0.000000	0.000000	0.000000
N	2.367787	2.357219	0.000000
N	-2.367787	2.357219	0.000000
N	-2.367787	-2.357219	0.000000
N	2.367787	-2.357219	0.000000
N	0.000000	1.921394	0.000000
C	1.110962	2.733604	0.000000
C	0.698588	4.100287	0.000000
C	-0.698588	4.100287	0.000000
C	-1.110962	2.733604	0.000000
N	-1.912189	0.000000	0.000000
C	-2.734500	1.110339	0.000000
C	-4.113358	0.694734	0.000000
C	-4.113358	-0.694734	0.000000
C	-2.734500	-1.110339	0.000000
N	0.000000	-1.921394	0.000000
C	-1.110962	-2.733604	0.000000
C	-0.698588	-4.100287	0.000000
C	0.698588	-4.100287	0.000000
C	1.110962	-2.733604	0.000000
N	1.912189	0.000000	0.000000
C	2.734500	-1.110339	0.000000
C	4.113358	-0.694734	0.000000
C	4.113358	0.694734	0.000000
C	2.734500	1.110339	0.000000
C	-5.292593	-1.412902	0.000000
C	-6.477660	-0.696684	0.000000
C	-6.477660	0.696684	0.000000
C	-5.292593	1.412902	0.000000
C	-1.416287	5.286315	0.000000
C	-0.700297	6.464248	0.000000
C	0.700297	6.464248	0.000000
C	1.416287	5.286315	0.000000
C	5.292593	1.412902	0.000000
C	6.477660	0.696684	0.000000
C	6.477660	-0.696684	0.000000
C	5.292593	-1.412902	0.000000
C	1.416287	-5.286315	0.000000

C	0.700297	-6.464248	0.000000
C	-0.700297	-6.464248	0.000000
C	-1.416287	-5.286315	0.000000
H	-5.275478	-2.504883	0.000000
H	-7.430866	-1.229806	0.000000
H	-7.430866	1.229806	0.000000
H	-5.275478	2.504883	0.000000
H	-2.508237	5.270706	0.000000
H	-1.230663	7.419076	0.000000
H	1.230663	7.419076	0.000000
H	2.508237	5.270706	0.000000
H	5.275478	2.504883	0.000000
H	7.430866	1.229806	0.000000
H	7.430866	-1.229806	0.000000
H	5.275478	-2.504883	0.000000
H	2.508237	-5.270706	0.000000
H	1.230663	-7.419076	0.000000
H	-1.230663	-7.419076	0.000000
H	-2.508237	-5.270706	0.000000

LS TS

Mn	0.000000	0.000000	0.000000
N	0.000000	3.345902	0.000000
N	-3.338278	0.000000	0.000000
N	0.000000	-3.345902	0.000000
N	3.338278	0.000000	0.000000
N	-1.354121	1.356543	0.000000
C	-1.146518	2.718400	0.000000
C	-2.408593	3.398508	0.000000
C	-3.394259	2.413799	0.000000
C	-2.718595	1.148897	0.000000
N	-1.354121	-1.356543	0.000000
C	-2.718595	-1.148897	0.000000
C	-3.394259	-2.413799	0.000000
C	-2.408593	-3.398508	0.000000
C	-1.146518	-2.718400	0.000000
N	1.354121	-1.356543	0.000000
C	1.146518	-2.718400	0.000000
C	2.408593	-3.398508	0.000000
C	3.394259	-2.413799	0.000000
C	2.718595	-1.148897	0.000000
N	1.354121	1.356543	0.000000
C	2.718595	1.148897	0.000000
C	3.394259	2.413799	0.000000
C	2.408593	3.398508	0.000000
C	1.146518	2.718400	0.000000
C	-2.729511	-4.743948	0.000000
C	-4.069253	-5.080432	0.000000
C	-5.058528	-4.094108	0.000000
C	-4.736199	-2.750332	0.000000
C	-4.736199	2.750332	0.000000

C	-5.058528	4.094108	0.000000
C	-4.069253	5.080432	0.000000
C	-2.729511	4.743948	0.000000
C	2.729511	4.743948	0.000000
C	4.069253	5.080432	0.000000
C	5.058528	4.094108	0.000000
C	4.736199	2.750332	0.000000
C	4.736199	-2.750332	0.000000
C	5.058528	-4.094108	0.000000
C	4.069253	-5.080432	0.000000
C	2.729511	-4.743948	0.000000
H	-1.940631	-5.499220	0.000000
H	-4.364235	-6.131839	0.000000
H	-6.108517	-4.395485	0.000000
H	-5.502249	-1.972021	0.000000
H	-5.502249	1.972021	0.000000
H	-6.108517	4.395485	0.000000
H	-4.364235	6.131839	0.000000
H	-1.940631	5.499220	0.000000
H	1.940631	5.499220	0.000000
H	4.364235	6.131839	0.000000
H	6.108517	4.395485	0.000000
H	5.502249	1.972021	0.000000
H	5.502249	-1.972021	0.000000
H	6.108517	-4.395485	0.000000
H	4.364235	-6.131839	0.000000
H	1.940631	-5.499220	0.000000