ELECTRONIC SUPPLEMENTARY INFORMATION

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Assessment of Electronic Structure Methods for the Determination of the Ground Spin States of Fe(II), Fe(III) and Fe(IV) Complexes

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S1. Conversion of r_0 to r_e

The experimental r_0 values of FeO and FeO^+ were converted to r_e values so that a consistent comparison can be made with the theoretically calculated r_e values. Note that r_0 is the average value of the internuclear distance in the ground state, which is the same as the average value in an ideal 0 K gas, whereas r_e is the equilibrium internuclear distance, corresponding to classical equilibrium where the molecule is at the minimum-energy position of the potential energy curve.

The conversion was done using the following equations. The equation for mean displacements of bond length by vibration at temperature T is (see ref. 1),

$$\langle x_T \rangle \cong \tfrac{3}{2} a \langle x_T^2 \rangle \tag{S1}$$

where the parameter a is the Morse constant, which can be expressed as a function of the harmonic force constant (k_e) as

$$a = \sqrt{k_e / 2D_e} \tag{S2}$$

where D_e is the equilibrium dissociation energy of the molecule. The harmonic force constant and the harmonic vibrational frequency in wavenumbers are related by:

$$\omega_e = \frac{1}{2\pi c}\sqrt{k_e / \mu} \tag{S3}$$

The mean square amplitude of vibration at temperature T can be calculated for diatomic molecules by the general equation (see ref. 2),

$$\langle x_T^2 \rangle = \frac{1}{\mu}\frac{h}{8\pi^2 c\omega_e}\coth\left(\frac{hc\omega_e}{2k_B T}\right) \tag{S4}$$

where μ is the reduced mass of the diatomic molecule, and h, c, and k_B are Planck constant, the speed of light, and the Boltzmann constant, respectively. Since the temperature is 0 K, eq S4 can be simplified to

$$\langle x_0^2 \rangle = \frac{1}{\mu}\frac{h}{8\pi^2 c\omega_e} \tag{S5}$$

Then one can obtain r_e by using the equation:

$$r_e = r_0 - \langle x_0 \rangle \tag{S6}$$

We note that the rotational motions do not contribute to the bond lengthening due to the 0 K temperature.

S2. Relative energies (kcal/mol) of conformers of $[Fe(O)(TMC)(MeCN)]^{2+}$ and $[Fe(O)(TMCS)]^{+}$

Table S1. Relative energies (kcal/mol)[a] of the two conformers (parallel and crossed) of $[Fe(O)(TMC)(MeCN)]^{2+}$ and $[Fe(O)(TMCS)]^{+}$ in quintet and triplet spin states using the def2-TZVP basis set.

Functional	$[Fe(O)(TMC)(MeCN)]^{2+}$		$[Fe(O)(TMCS)]^{+}$	
	quintet	triplet	quintet	triplet
GVWN5	0.0	–0.3	1.7	2.7
BLYP	–0.9	–0.9	1.5	2.1
PBE	–0.6	–0.7	1.6	2.3
OPBE	–0.6	–0.8	1.8	2.3
OLYP	–0.8	–0.9	1.6	2.2
N12	–0.6	–0.6	1.7	2.5
GAM	–0.9	–1.0	1.5	2.0
M06-L	–0.3	–0.4	1.9	2.7
M11-L	0.0	–0.1	2.3	3.3
MN15-L	0.1	–0.5	2.4	3.1
B3LYP*	–0.7	–0.8	1.6	2.3
B3LYP	–0.7	–0.8	1.6	2.3
PBE0	–0.5	–0.7	1.8	2.5
B97-3	–0.6	–0.8	1.7	2.4
M06	–0.5	–0.9	1.6	2.3
PW6B95	0.0	–0.2	2.1	3.0
SOGGA11-X	–0.5	–0.6	1.7	2.5
MPW1B95	0.1	–0.1	2.2	3.0
MN15	0.3	–0.4	1.9	3.0
M08-SO	0.1	–0.2	2.1	3.1

[a]For a given spin state the relative energy is calculated as $E_{\text{parallel}} - E_{\text{crossed}}$. See Section S3 for a description of the two conformers. For Table 7 in the paper we used — for each functional — the conformer which the functional predicted to be lower in energy in the triplet state (in Table S1). For $[Fe(O)(TMC)(MeCN)]^{2+}$ it turns out to be the parallel conformer, and for $[Fe(O)(TMCS)]^{+}$ it turns out to be the crossed conformer.

S3. The conformers of $[Fe(O)(TMC)(MeCN)]^{2+}$ and $[Fe(O)(TMCS)]^{+}$

Oxoiron(IV) complexes bearing ligands of the TMC family have been extensively studied using computational approaches. For most studies involving complexes of this family the conformation of the macrocycle was based on the reported crystallographic data[3] for $[Fe^{IV}(O)(TMC)(MeCN)]^{2+}$ where the two *N*-CH_2-CH_2-*N* groups are oriented in a "parallel" fashion.[4-10] When the *trans* ligand is not covalently attached, the ligand has C_s symmetry in these cases. Based on this structural information a related conformation was considered in early computational studies involving $[Fe^{IV}(O)(TMCS)]^{+}$.[4-6,10] In later studies a conformation of the $[Fe^{IV}(O)(TMCS)]^{+}$ complex was considered where the two *N*-CH_2-CH_2-*N* groups are oriented in a "crossed" way.[7,8] In the absence of a tethered ligand this conformation has C_2 symmetry. Both types of conformations have been observed in oxoiron(IV) complexes of the TMC family crystallographically when tethered ligands are present.[11,12]

In the present study we consider the two conformations for both complexes studied, $[Fe^{IV}(O)(TMC)(MeCN)]^{2+}$ and $[Fe^{IV}(O)(TMCS)]^{+}$, that are derived from the crystallographic data available for tethered ligands. These are named "crossed" and "parallel", and they are shown in Fig. S1. For $[Fe^{IV}(O)(TMCS)]^{+}$ we obtain a very consistent picture with all functionals favoring a "crossed" conformation of the macrocyclic ligand in both spin states studied. For the $[Fe^{IV}(O)(TMC)(MeCN)]^{2+}$ complex we find the parallel conformation to be favored by all functionals in the triplet state as observed in the X-ray crystal structure, although both conformations are very close in energy (within 1 kcal/mol). In the quintet spin state the parallel conformation is predicted to be more stable by most functionals; however, there are some cases where the "crossed" conformation is favored. The findings provide a reminder that more than one conformation can be relevant when one considers molecules of this type.

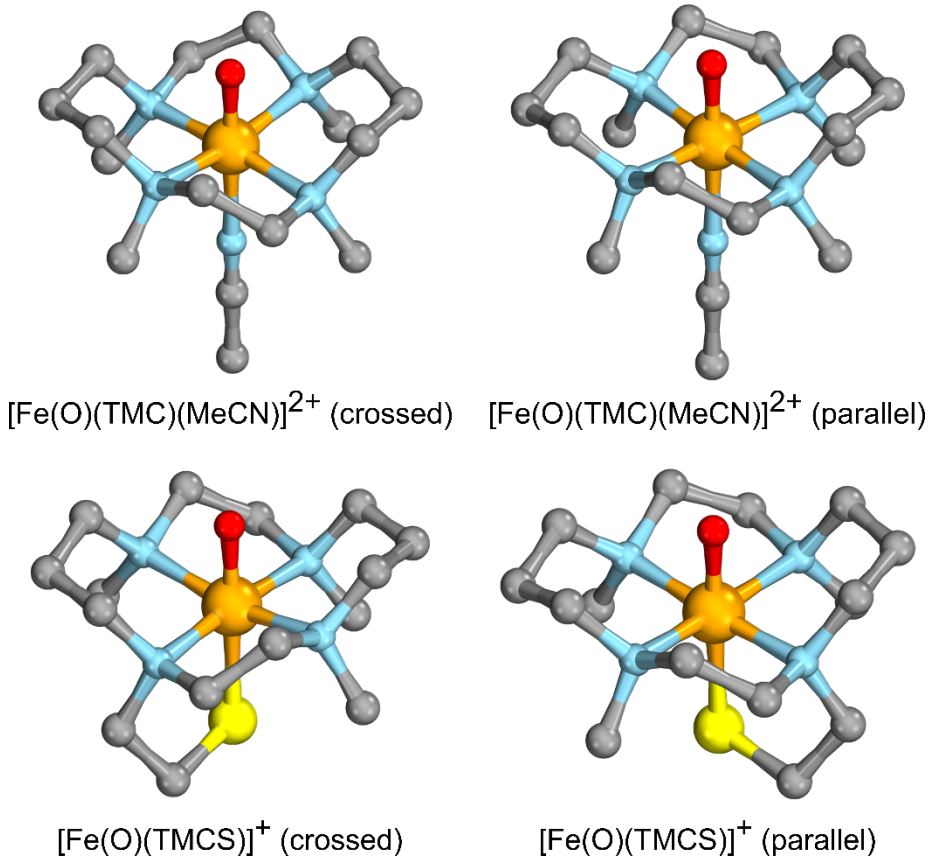

Figure S1. Depictions of the studied conformations of complexes **13** (top) and **14** (bottom) at the PW6B95/def2-TZVP level of theory for the triplet spin state. Structural depictions were generated using IboView.[13,14]

S4. The <S^2> values of Fe^{2+} ion, FeO, and the 14 complexes

Table S2. The <S^2> values of Fe^{2+} ion and FeO using 20 density functionals and the def2-TZVP basis set.[a]

Functional	Fe^{2+} ion			FeO[b]		
	singlet	triplet	quintet	quintet ($^5\Delta$)	quintet ($^5\Sigma$)	septet ($^7\Sigma$)
GVWN5	1.931	2.934	6.002	6.012	-	12.004
BLYP	1.927	2.933	6.002	6.016	-	12.007
PBE	1.937	2.945	6.001	6.017	-	12.005
OPBE	1.939	2.940	6.002	6.017	-	12.007
OLYP	1.931	2.931	6.003	6.016	6.172	12.010
N12	1.920	2.925	6.001	6.011	-	12.013
GAM	1.930	2.940	6.006	6.104	6.209	12.017
M06-L	1.901	2.932	6.006	6.126	6.231	12.015
M11-L	1.862	2.881	6.002	6.012	-	12.018
MN15-L	1.834	2.725	6.011	6.191	6.373	12.020
B3LYP*	1.927	2.934	6.002	6.030	6.152	12.013
B3LYP	1.927	2.936	6.002	6.038	6.183	12.016
PBE0	1.937	2.952	6.002	6.054	6.212	12.016
B97-3	1.922	2.930	6.003	6.040	6.205	12.019
M06	1.891	2.996	6.006	6.038	6.263	12.019
PW6B95	1.926	2.933	6.002	6.048	6.210	12.017
SOGGA11-X	1.920	2.927	6.002	6.073	6.217	12.025
MPW1B95	1.927	2.932	6.002	6.054	6.249	12.018
MN15	1.978	3.000	6.002	6.030	6.167	12.015
M08-SO	1.975	3.000	6.005	6.099	6.224	12.031

[a]The <S^2> values corresponding to Fe^{2+} ion and FeO reported in Tables 2 and 3, respectively, of the paper.

[b]The $^5\Sigma$ state was not determined for all the local functionals.

Table S3. The $\langle S^2 \rangle$ values of seven Fe(II) complexes using 20 density functionals and the def2-TZVP basis set.[a]

Functional	Spin state	1	2	3	4	5	6	7
GVWN5	singlet	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	triplet	2.026	2.021	2.024	2.010	2.007	2.072	2.074
	quintet	6.034	6.042	6.033	6.008	6.006	6.110	6.106
BLYP	singlet	-	0.000	-	-	0.885	-	-
	triplet	2.027	2.029	2.018	2.011	2.312	2.064	2.072
	quintet	6.019	6.025	6.016	6.006	6.004	6.053	6.033
PBE	singlet	-	0.000	-	-	0.995	-	-
	triplet	2.029	2.031	2.021	2.012	2.382	2.079	2.084
	quintet	6.024	6.031	6.019	6.006	6.004	6.069	6.055
OPBE	singlet	-	0.000	-	-	1.200	-	-
	triplet	2.045	2.047	2.033	2.020	2.470	2.129	2.130
	quintet	6.036	6.047	6.025	6.009	6.006	6.090	6.067
OLYP	singlet	-	0.000	-	-	1.061	-	-
	triplet	2.044	2.046	2.029	2.018	2.372	2.112	2.117
	quintet	6.032	6.041	6.022	6.008	6.006	6.076	6.043
N12	singlet	-	0.000	-	-	0.082	-	-
	triplet	2.020	2.022	2.015	2.009	2.011	2.045	2.052
	quintet	6.017	6.022	6.014	6.005	6.004	6.045	6.028
GAM	singlet	-	0.000	-	-	0.840	-	-
	triplet	2.072	2.077	2.044	2.028	2.293	2.169	2.167
	quintet	6.045	6.060	6.035	6.013	6.010	6.109	6.070
M06-L	singlet	-	0.000	-	-	0.715	-	-
	triplet	2.055	2.060	2.030	2.018	2.146	2.091	2.090
	quintet	6.043	6.057	6.036	6.013	6.010	6.118	6.063
	septet[b]	12.014	12.011	12.020	12.008	12.007		
M11-L	singlet	-	0.000	-	-	0.000	-	-
	triplet	2.020	2.019	2.012	2.013	2.008	2.021	2.020
	quintet	6.013	6.015	6.010	6.008	6.005	6.018	6.011
MN15-L	singlet	-	0.000	-	-	0.000	-	-
	triplet	2.096	2.101	2.051	2.031	2.016	2.150	2.140
	quintet	6.077	6.098	6.067	6.030	6.021	6.183	6.118
B3LYP*	singlet	-	0.000	-	-	0.991	-	-
	triplet	2.027	2.031	2.014	2.010	2.408	2.029	2.035
	quintet	6.016	6.021	6.013	6.006	6.004	6.026	6.012
B3LYP	singlet	-	0.000	-	-	1.120	-	0.122
	triplet	2.025	2.029	2.012	2.009	2.508	2.022	2.384
	quintet	6.014	6.019	6.011	6.006	6.004	6.011	6.010
PBE0	singlet	-	0.000	-	0.350	1.342	-	0.363
	triplet	2.029	2.034	2.014	2.167	2.656	2.025	2.027
	quintet	6.016	6.022	6.012	6.006	6.005	6.020	6.011
B97-3	singlet	-	0.000	-	-	1.202	-	0.243
	triplet	2.023	2.028	2.011	2.009	2.557	2.017	2.018
	quintet	6.013	6.018	6.010	6.006	6.004	6.009	6.010
M06	singlet	-	0.000	-	-	0.000	-	-
	triplet	2.0336	2.042	2.018	2.010	2.007	2.030	2.033
	quintet	6.0329	6.044	6.028	6.014	6.011	6.052	6.026
PW6B95	singlet	-	0.000	-	-	0.868	-	-

	triplet	2.022	2.026	2.010	2.008	2.390	2.016	2.017
	quintet	6.013	6.018	6.010	6.006	6.004	6.010	6.010
SOGGA11-X	singlet	-	0.000	-	-	1.037	-	0.306
	triplet	2.019	2.024	2.009	2.007	2.467	2.012	2.012
	quintet	6.013	6.017	6.011	6.007	6.005	6.009	6.010
MPW1B95	singlet	-	0.000	-	-	0.812	-	-
	triplet	2.023	2.028	2.011	2.008	2.359	2.017	2.017
	quintet	6.014	6.019	6.011	6.006	6.005	6.010	6.011
MN15	singlet	-	0.000	-	-	1.895	-	-
	triplet	2.010	2.012	2.005	2.003	2.754	2.008	2.010
	quintet	6.015	6.019	6.012	6.007	6.005	6.016	6.012
M08-SO	singlet	-	0.000	-	0.749	1.882	-	1.266
	triplet	2.018	2.023	2.009	2.006	2.796	2.012	2.025
	quintet	6.022	6.028	6.018	6.013	6.009	6.022	6.019

[a]The $\langle S^2 \rangle$ values correspond to the seven Fe(II) complexes reported in Table 5 of the paper. The singlet spin states for which $\langle S^2 \rangle$ values are missing turned out to be closed-shell calculations for which $\langle S^2 \rangle$ values were not printed in the output.

[b]The septet state was calculated only for complexes **1**–**5** with the M06-L exchange–correlation functional.

1 = $[Fe(CO)_6]^{2+}$, **2** = $[Fe(CNH)_6]^{2+}$, **3** = $[Fe(NCH)_6]^{2+}$, **4** = $[Fe(NH_3)_6]^{2+}$, **5** = $[Fe(H_2O)_6]^{2+}$, **6** = $[Fe(bipy)_3]^{2+}$, **7** = $Fe(amp)_2Cl_2$

Table S4. The $<S^2>$ values of five Fe(III) complexes using 20 density functionals and the def2-TZVP basis set.[a]

Functional	Spin state	8	9	10	11	12
GVWN5	doublet	0.758	0.757	0.755	0.757	0.759
	quartet	3.782	3.779	3.771	3.777	3.785
	sextet	8.753	8.754	8.754	8.753	8.755
BLYP	doublet	0.762	0.760	0.763	0.777	0.772
	quartet	3.790	3.784	3.773	3.790	3.802
	sextet	8.753	8.754	8.754	8.753	8.755
PBE	doublet	0.761	0.760	0.761	0.775	0.770
	quartet	3.791	3.785	3.775	3.791	3.802
	sextet	8.754	8.754	8.754	8.753	8.756
OPBE	doublet	0.765	0.764	0.760	0.771	0.772
	quartet	3.813	3.802	3.787	3.814	3.832
	sextet	8.755	8.755	8.754	8.754	8.757
OLYP	doublet	0.766	0.764	0.760	0.773	0.773
	quartet	3.814	3.802	3.786	3.814	3.833
	sextet	8.754	8.754	8.754	8.754	8.756
N12	doublet	0.758	0.758	0.759	0.766	0.764
	quartet	3.779	3.776	3.768	3.778	3.785
	sextet	8.755	8.755	8.754	8.754	8.756
GAM	doublet	0.781	0.776	0.765	0.780	0.789
	quartet	3.855	3.835	3.810	3.861	3.901
	sextet	8.757	8.757	8.755	8.756	8.759
M06-L	doublet	0.769	0.768	0.762	0.760	0.764
	quartet	3.837	3.823	3.793	3.823	3.846
	sextet	8.757	8.757	8.756	8.756	8.759
M11-L	doublet	0.786	0.779	0.792	0.811	0.801
	quartet	3.775	3.772	3.766	3.770	3.767
	sextet	8.759	8.759	8.757	8.758	8.760
MN15-L	doublet	0.795	0.788	0.778	0.787	0.799
	quartet	3.903	3.870	3.823	3.874	3.911
	sextet	8.757	8.757	8.756	8.757	8.760
B3LYP*	doublet	0.765	0.763	0.768	0.781	0.776
	quartet	3.800	3.791	3.775	3.799	3.817
	sextet	8.755	8.755	8.754	8.754	8.756
B3LYP	doublet	0.768	0.764	0.775	0.790	0.782
	quartet	3.806	3.795	3.776	3.807	3.826
	sextet	8.755	8.755	8.755	8.755	8.756
PBE0	doublet	0.770	0.767	0.785	0.804	0.789
	quartet	3.813	3.801	3.779	3.809	3.836
	sextet	8.755	8.755	8.755	8.755	8.756
B97-3	doublet	0.769	0.765	0.778	0.791	0.782
	quartet	3.812	3.799	3.776	3.808	3.834
	sextet	8.755	8.755	8.755	8.755	8.756
M06	doublet	0.788	0.781	0.834	0.767	0.776
	quartet	3.819	3.807	3.781	3.805	3.830
	sextet	8.757	8.757	8.756	8.756	8.758
PW6B95	doublet	0.767	0.764	0.771	0.781	0.775
	quartet	3.808	3.796	3.775	3.804	3.825

	sextet	8.755	8.755	8.755	8.755	8.756
SOGGA11-X	doublet	0.771	0.767	0.778	0.787	0.781
	quartet	3.817	3.804	3.775	3.808	3.837
	sextet	8.756	8.756	8.755	8.756	8.757
MPW1B95	doublet	0.767	0.764	0.768	0.777	0.773
	quartet	3.811	3.798	3.776	3.804	3.827
	sextet	8.755	8.755	8.755	8.755	8.756
MN15	doublet	0.847	0.813	1.119	1.148	0.985
	quartet	3.771	3.768	3.760	3.767	3.773
	sextet	8.754	8.754	8.754	8.753	8.754
M08-SO	doublet	0.912	0.843	1.257	1.193	1.015
	quartet	3.817	3.803	3.772	3.803	3.832
	sextet	8.756	8.756	8.755	8.755	8.757

[a]The $\langle S^2 \rangle$ values correspond to the five Fe(III) complexes reported in Table 6 of the paper.

8 = $[Fe(CO)_6]^{3+}$, **9** = $[Fe(CNH)_6]^{3+}$, **10** = $[Fe(NCH)_6]^{3+}$, **11** = $[Fe(NH_3)_6]^{3+}$, **12** = $[Fe([9]aneN_3)_2]^{3+}$

Table S5. The $<S^2>$ values of the two conformations of two Fe(IV) complexes using 20 density functionals and the def2-TZVP basis set.[a]

Functional	Spin state	13 (parallel)	13 (crossed)	14 (parallel)	14 (crossed)
GVWN5	triplet	2.015	2.015	2.018	2.018
	quintet	6.027	6.027	6.035	6.036
BLYP	triplet	2.021	2.021	2.022	2.021
	quintet	6.033	6.033	6.044	6.045
PBE	triplet	2.021	2.020	2.021	2.021
	quintet	6.034	6.035	6.044	6.045
OPBE	triplet	2.036	2.036	2.037	2.036
	quintet	6.052	6.053	6.067	6.069
OLYP	triplet	2.038	2.038	2.039	2.038
	quintet	6.052	6.052	6.069	6.071
N12	triplet	2.018	2.018	2.019	2.019
	quintet	6.022	6.023	6.032	6.032
GAM	triplet	2.074	2.073	2.080	2.077
	quintet	6.090	6.092	6.117	6.119
M06-L	triplet	2.032	2.032	2.035	2.034
	quintet	6.075	6.077	6.093	6.094
M11-L	triplet	2.021	2.021	2.019	2.019
	quintet	6.019	6.019	6.027	6.027
MN15-L	triplet	2.087	2.087	2.096	2.096
	quintet	6.147	6.148	6.168	6.169
B3LYP*	triplet	2.029	2.028	2.031	2.030
	quintet	6.050	6.052	6.069	6.070
B3LYP	triplet	2.032	2.031	2.034	2.034
	quintet	6.062	6.064	6.082	6.083
PBE0	triplet	2.036	2.036	2.039	2.039
	quintet	6.081	6.082	6.095	6.096
B97-3	triplet	2.035	2.035	2.038	2.038
	quintet	6.082	6.084	6.100	6.101
M06	triplet	2.038	2.038	2.052	2.053
	quintet	6.093	6.095	6.125	6.127
PW6B95	triplet	2.032	2.032	2.036	2.036
	quintet	6.074	6.076	6.094	6.095
SOGGA11-X	triplet	2.038	2.037	2.043	2.044
	quintet	6.186	6.187	6.140	6.144
MPW1B95	triplet	2.034	2.034	2.039	2.039
	quintet	6.083	6.085	6.101	6.102
MN15	triplet	2.028	2.028	2.040	2.040
	quintet	6.035	6.034	6.056	6.059
M08-SO	triplet	2.200	2.205	2.129	2.140
	quintet	6.391	6.384	6.218	6.233

[a]The $<S^2>$ values correspond to the Fe(IV) complexes reported in Table S1.

13 = $[Fe(O)(TMC)(MeCN)]^{2+}$, **14** = $[Fe(O)(TMCS)]^{+}$

S5. Geometries (in Å) and energies (in hartrees) of 14 Fe complexes using PW6B95/def2-TZVP

1, $[Fe(CO)_6]^{2+}$

E = –1944.850464 (M_S = 0)

26	0.000001	-0.000001	0.000002
6	-0.907942	1.147469	1.270330
8	-1.427798	1.804463	1.997592
6	-1.440705	0.264574	-1.268590
8	-2.265566	0.416069	-1.994850
6	1.440706	-0.264577	1.268594
8	2.265567	-0.416073	1.994854
6	-0.924714	-1.538876	0.729131
8	-1.454199	-2.419895	1.146571
6	0.907942	-1.147478	-1.270321
8	1.427785	-1.804443	-1.997619
6	0.924717	1.538875	-0.729128
8	1.454204	2.419893	-1.146565

E = –1944.799257 (M_S = 1)

26	-0.000001	-0.000008	0.000057
6	2.216653	0.013191	0.002387
8	3.325013	0.020233	0.003187
6	-0.013178	2.212500	0.000057
8	-0.020223	3.320838	0.000051
6	0.013183	-2.212518	0.000071
8	0.020232	-3.320857	0.000071
6	-0.002451	-0.000016	1.955520
8	-0.003894	-0.000022	3.065029
6	-2.216653	-0.013208	-0.002492
8	-3.325014	-0.020128	-0.003705
6	0.002454	-0.000001	-1.955410
8	0.003881	0.000003	-3.064919

E = –1944.806351 (M_S = 2)

26	0.000021	0.000000	0.000001
6	0.001444	-2.293667	0.009338
8	0.002442	-3.402462	0.013910
6	2.342896	0.001445	-0.001119
8	3.450992	0.002349	-0.001127
6	-2.342869	-0.001445	0.001117
8	-3.450965	-0.002349	0.001124

6	0.001317	0.009315	2.292241
8	0.000948	0.013934	3.401041
6	-0.001382	2.293667	-0.009333
8	-0.002401	3.402462	-0.013918
6	-0.001388	-0.009316	-2.292238
8	-0.001098	-0.013934	-3.401038

2, $[Fe(CNH)_6]^{2+}$

E = –1825.458740 (M_S = 0)

26	0.000002	0.000001	-0.000002
6	1.322934	-0.535699	-1.278721
6	0.131762	1.808073	-0.621152
6	-0.131757	-1.808072	0.621147
6	1.380137	0.340874	1.285024
6	-1.322930	0.535701	1.278716
6	-1.380133	-0.340874	-1.285028
7	2.114089	-0.856075	-2.043399
7	-2.205629	-0.544680	-2.053351
7	0.210603	2.889349	-0.992537
7	2.205630	0.544674	2.053351
7	-0.210609	-2.889344	0.992543
7	-2.114086	0.856073	2.043396
1	2.805800	-1.136437	-2.711696
1	0.279541	3.834732	-1.316862
1	-2.927823	-0.722775	-2.724474
1	-2.805799	1.136409	2.711701
1	-0.279644	-3.834688	1.316959
1	2.927816	0.722741	2.724491

E = –1825.396662 (M_S = 1)

26	-0.000001	-0.000001	0.000008
6	0.000013	-0.000758	1.933265
6	-0.000105	-2.107130	-0.000728
6	0.000106	2.107127	0.000744
6	2.231522	-0.000126	-0.000003
6	-0.000014	0.000766	-1.933249
6	-2.231523	0.000121	0.000018
7	-0.000002	-0.001247	3.079481
7	-3.378481	0.000202	0.000011
7	-0.000188	-3.252586	-0.001137
7	3.378480	-0.000187	0.000001
7	0.000192	3.252583	0.001116

7	0.000001	0.001197	-3.079466
1	-0.000138	-0.001861	4.081005
1	-0.000508	-4.255401	-0.002055
1	-4.380953	0.000576	-0.000146
1	0.000140	0.001729	-4.080989
1	0.000523	4.255398	0.001492
1	4.380953	-0.000164	0.000171

E = –1825.392569 (M_S = 2)

26	0.000000	0.000001	0.000012
6	0.000257	-2.234191	0.201599
6	-0.020387	0.201643	2.232838
6	0.020387	-0.201641	-2.232825
6	-2.285448	-0.002097	-0.020168
6	-0.000257	2.234193	-0.201574
6	2.285449	0.002094	0.020135
7	0.000029	-3.376440	0.304699
7	3.431017	0.002905	0.031458
7	-0.032144	0.304840	3.375025
7	-3.431016	-0.002911	-0.031532
7	0.032144	-0.304839	-3.375012
7	-0.000029	3.376443	-0.304673
1	0.000625	-4.374576	0.394974
1	-0.042445	0.394933	4.373125
1	4.433821	0.004120	0.041613
1	-0.000626	4.374575	-0.394981
1	0.042423	-0.394934	-4.373112
1	-4.433820	-0.004133	-0.041717

3, $[Fe(NCH)_6]^{2+}$

E = –1825.493036 (M_S = 0)

26	0.000001	0.000000	0.000002
7	-1.152843	-0.267290	-1.566494
7	1.576055	-0.440819	-1.084561
7	0.204051	1.894389	-0.473449
7	1.152845	0.267290	1.566496
7	-0.204050	-1.894389	0.473454
7	-1.576052	0.440820	1.084566
6	2.488118	-0.695952	-1.712102
1	3.346929	-0.936264	-2.303195
6	0.322199	2.990635	-0.747390
1	0.433540	4.022996	-1.005323

6	-0.322199	-2.990634	0.747396
1	-0.433470	-4.023009	1.005305
6	-1.819924	-0.422010	-2.473038
1	-2.448134	-0.567714	-3.326748
6	1.819927	0.422010	2.473039
1	2.448112	0.567809	3.326751
6	-2.488120	0.695949	1.712102
1	-3.347059	0.936171	2.303045

E = –1825.473929 (M_S = 1)

26	-0.000005	0.000007	-0.000007
7	-1.755022	1.229461	-0.000736
7	-1.229456	-1.755008	-0.000092
7	0.000587	-0.000303	-1.951579
7	1.755014	-1.229447	0.000721
7	-0.000596	0.000315	1.951564
7	1.229447	1.755021	0.000074
6	-1.881666	-2.686864	-0.000113
1	-2.495197	-3.563669	0.000003
6	0.000937	-0.000492	-3.087534
1	0.001385	-0.001032	-4.157479
6	-0.000948	0.000495	3.087519
1	-0.001542	0.000627	4.157465
6	-2.686874	1.881678	-0.001107
1	-3.563530	2.495422	-0.000525
6	2.686867	-1.881661	0.001099
1	3.563604	-2.495289	0.000817
6	1.881666	2.686871	0.000093
1	2.495699	3.563325	0.000506

E = –1825.500329 (M_S = 2)

26	-0.000148	-0.000185	-0.000027
7	-1.057067	-1.915246	-0.050815
7	1.329635	-0.688286	-1.589585
7	-1.377309	0.795397	-1.497696
7	1.056846	1.914757	0.050965
7	1.377442	-0.795196	1.497538
7	-1.329541	0.688583	1.589570
6	2.031287	-1.050796	-2.408738
1	2.690849	-1.391759	-3.179243
6	-2.102521	1.213758	-2.268145
1	-2.784318	1.607142	-2.993056

6	2.102898	-1.213329	2.267875
1	2.784945	-1.606529	2.992647
6	-1.607924	-2.909953	-0.075473
1	-2.126591	-3.846109	-0.098066
6	1.607768	2.909412	0.075906
1	2.126482	3.845516	0.098805
6	-2.031026	1.051510	2.408684
1	-2.690460	1.392874	3.179122

4, $[Fe(NH_3)_6]^{2+}$

E = –1603.916342 (M_S = 0)

26	0.000005	-0.000001	-0.000179
7	1.107370	-1.775084	-0.115539
7	1.186916	0.836284	-1.510938
7	-1.110659	1.776485	0.051479
7	-1.181846	-0.780767	1.543878
7	1.329590	0.731862	1.444936
7	-1.331385	-0.788805	-1.413473
1	-0.979536	-0.808721	-2.364952
1	-1.588511	-1.751143	-1.219589
1	-2.215418	-0.294866	-1.478174
1	1.464501	1.791727	-1.311327
1	2.058905	0.345460	-1.679520
1	0.742442	0.887775	-2.421579
1	-1.360332	2.113014	-0.872727
1	-1.993822	1.705371	0.546114
1	-0.636832	2.561330	0.486228
1	2.236273	1.005196	1.080380
1	1.001132	1.547707	1.950938
1	1.538179	0.052748	2.169568
1	2.034978	-1.718344	0.291893
1	0.677406	-2.574295	0.338231
1	1.264416	-2.081174	-1.070226
1	-1.315871	-0.126297	2.307752
1	-2.120841	-1.042383	1.261881
1	-0.807104	-1.612901	1.987359

E = –1603.906912 (M_S = 1)

26	-0.000673	-0.014207	0.000022
7	-0.040828	-0.043696	-2.064673
7	-1.714536	-1.475445	0.053204
7	0.035660	-0.044357	2.064807

7	1.651303	1.539720	0.002498
7	−1.475607	1.708237	−0.004850
7	1.545626	−1.651071	−0.051010
1	1.171104	−2.558664	−0.306126
1	2.277663	−1.475801	−0.730892
1	2.035068	−1.809784	0.822894
1	−2.420494	−1.224990	0.737103
1	−2.221960	−1.577081	−0.818952
1	−1.439017	−2.419117	0.303461
1	−0.005033	−0.982834	2.448005
1	0.870221	0.368542	2.467253
1	−0.737314	0.448402	2.498911
1	−2.419705	1.432851	−0.253753
1	−1.574747	2.202940	0.874858
1	−1.229193	2.427941	−0.675797
1	−0.829765	0.450556	−2.467462
1	0.777574	0.367660	−2.500271
1	−0.095438	−0.982220	−2.446019
1	1.481552	2.285250	0.669013
1	2.559412	1.165631	0.256487
1	1.806250	2.016383	−0.879108

E = −1603.936138 (M_S = 2)

26	0.000124	−0.004605	0.000284
7	1.675441	−1.577058	−0.033490
7	−1.523421	−1.723713	0.044572
7	−1.719030	1.517473	0.142861
7	1.571307	1.668463	−0.154126
7	−0.138421	0.049468	−2.251839
7	0.133614	0.078084	2.251503
1	−0.621856	−0.398932	2.731466
1	0.983950	−0.325195	2.629567
1	0.109866	1.028808	2.604164
1	−2.480228	−1.447693	−0.145970
1	−1.317856	−2.450701	−0.631954
1	−1.565071	−2.208944	0.934161
1	−2.399422	1.280054	0.856431
1	−1.434042	2.466222	0.358708
1	−2.259987	1.596821	−0.711363
1	−0.948321	−0.431588	−2.627715
1	−0.200001	0.995788	−2.611771
1	0.657731	−0.360887	−2.727683

1	1.761143	-2.062851	-0.919679
1	2.603107	-1.213166	0.153779
1	1.538365	-2.315300	0.648230
1	2.101752	1.804616	0.699498
1	2.271365	1.488820	-0.865527
1	1.199834	2.584830	-0.378098

5, $[Fe(H_2O)_6]^{2+}$

E = –1723.213256 (M_S = 0)

26	0.000000	0.000000	0.000000
8	1.235312	1.206791	1.101643
1	1.060693	1.572540	1.973887
1	1.975046	1.688109	0.718150
8	-1.237958	-0.350102	1.594025
1	-1.977001	0.223728	1.818696
1	-1.064275	-0.922371	2.347298
8	1.237958	0.350102	-1.594025
1	1.977001	-0.223729	-1.818696
1	1.064276	0.922372	-2.347298
8	1.235987	-1.556774	0.495477
1	1.974500	-1.465264	1.105531
8	-1.235987	1.556775	-0.495477
1	-1.974501	1.465264	-1.105529
8	-1.235311	-1.206792	-1.101643
1	-1.975045	-1.688111	-0.718150
1	1.061470	-2.495054	0.376160
1	-1.061471	2.495054	-0.376161
1	-1.060695	-1.572537	-1.973889

E = –1723.216702 (M_S = 1)

26	0.000000	0.000000	0.000000
8	0.152333	1.762472	1.066025
1	0.378883	1.883217	1.993274
1	-0.048398	2.627877	0.695442
8	0.387751	-1.148196	1.629331
1	-0.266240	-1.427068	2.277772
1	1.262697	-1.244121	2.018749
8	-0.387751	1.148196	-1.629331
1	0.266240	1.427068	-2.277772
1	-1.262697	1.244121	-2.018749
8	2.170562	0.076752	-0.364352
1	2.751741	0.817769	-0.167600

8	-2.170562	-0.076752	0.364352
1	-2.751741	-0.817769	0.167600
8	-0.152333	-1.762472	-1.066025
1	0.048398	-2.627877	-0.695442
1	2.703695	-0.578658	-0.824627
1	-2.703695	0.578658	0.824627
1	-0.378883	-1.883217	-1.993274

E = –1723.260552 (M_S = 2)

26	0.000010	-0.000004	0.000000
8	0.539001	1.603708	1.317221
1	0.843615	2.478744	1.057416
1	0.521649	1.580570	2.279067
8	0.458411	1.279884	-1.636548
1	1.318813	1.382283	-2.055643
1	-0.146981	1.888329	-2.072097
8	-0.458419	-1.279881	1.636549
1	-1.318837	-1.382249	2.055620
1	0.146942	-1.888341	2.072120
8	-2.050987	0.705433	-0.020121
1	-2.444114	1.340773	0.585932
8	2.050997	-0.705435	0.020121
1	2.444144	-1.340726	-0.585971
8	-0.539027	-1.603701	-1.317221
1	-0.521693	-1.580557	-2.279067
1	-2.740401	0.444609	-0.638311
1	2.740393	-0.444658	0.638352
1	-0.843582	-2.478756	-1.057414

6, $[Fe(bipy)_3]^{2+}$

E = –2752.747151 (M_S = 0)

26	0.000584	0.001300	0.002781
7	-0.818654	-1.507091	-1.038145
7	0.732943	-1.553244	1.041337
6	-0.527522	-2.736559	-0.578726
6	0.373877	-2.763264	0.578223
6	-1.630485	-1.393952	-2.088128
6	-2.185174	-2.482297	-2.728951
6	-1.889747	-3.747726	-2.260304
6	-1.050960	-3.873991	-1.171770
6	0.834206	-3.929717	1.166959
6	1.680247	-3.853635	2.254542

6	2.046053	-2.608085	2.726708
6	1.551474	-1.488565	2.090260
1	-1.837486	-0.393293	-2.427774
1	-2.834361	-2.332589	-3.575302
1	-2.305103	-4.623099	-2.732897
1	2.047348	-4.752179	2.723581
1	2.703644	-2.497307	3.572565
1	1.813621	-0.501952	2.432886
7	0.981353	1.412030	1.040976
7	1.715299	0.046708	-1.038592
6	2.207571	1.708576	0.575734
6	0.516094	2.086308	2.090998
6	2.635429	0.913333	-0.580480
6	2.021336	-0.715138	-2.087327
6	2.985594	2.692912	1.163047
6	1.236643	3.076266	2.726496
1	-0.468307	1.816873	2.434516
6	3.882718	1.024997	-1.173314
6	3.241335	-0.654598	-2.728182
1	1.257036	-1.394380	-2.424958
6	2.496283	3.386090	2.251597
1	0.812041	3.589340	3.573034
6	4.191140	0.232570	-2.260368
1	3.435658	-1.293364	-3.573376
1	3.089334	4.155222	2.719462
1	5.157540	0.307236	-2.732260
1	0.576586	1.793800	-2.423652
1	-3.504284	-1.093514	3.578646
6	-2.058378	-0.597188	2.093373
7	-1.709975	0.143295	1.042626
6	-2.307031	3.508755	-2.259548
6	-3.822421	1.236383	1.169288
1	-2.859082	4.304690	-2.732711
6	-0.394771	2.112525	-2.085359
1	-5.137046	0.593477	2.727772
6	-2.581700	1.056145	0.579720
6	-4.174993	0.465625	2.258443
6	-2.109996	1.824161	-0.577545
6	-1.061783	3.135464	-2.726898
7	-0.898344	1.464771	-1.036256
1	-1.332425	-1.315370	2.435130
6	-2.835336	2.844175	-1.171465

1	-0.608026	3.624330	-3.572632
6	-3.274671	-0.469217	2.731503
1	-3.802065	3.122538	-0.789357
1	0.540149	-4.890226	0.781082
1	-4.510858	1.967593	0.782705
1	4.610218	1.719618	-0.790873
1	-0.811011	-4.850415	-0.788404
1	3.963151	2.921777	0.775720

E = −2752.723986 (M_S = 1)

26	0.063155	0.006720	0.009476
7	-1.763364	0.763733	-0.957361
7	-1.598373	-1.042920	0.977420
6	-2.925660	0.286747	-0.496247
6	-2.827267	-0.787077	0.512400
6	-1.779602	1.732229	-1.868283
6	-2.945222	2.272453	-2.371507
6	-4.148773	1.789648	-1.894857
6	-4.138587	0.788070	-0.945166
6	-3.928627	-1.503148	0.957680
6	-3.758145	-2.489503	1.907947
6	-2.488205	-2.741956	2.389989
6	-1.439957	-1.997202	1.890172
1	-0.817903	2.083542	-2.208968
1	-2.904817	3.052284	-3.113436
1	-5.083945	2.188552	-2.253662
1	-4.605243	-3.054055	2.263077
1	-2.307656	-3.500558	3.133046
1	-0.431297	-2.166033	2.234085
7	1.636800	-0.992133	1.049342
7	0.305576	-1.619203	-1.125790
6	2.033463	-2.119813	0.440957
6	2.273883	-0.586779	2.143851
6	1.267579	-2.486840	-0.760297
6	-0.429961	-1.891704	-2.203457
6	3.094231	-2.865424	0.929443
6	3.333789	-1.279983	2.691797
1	1.917158	0.326111	2.594637
6	1.498795	-3.646190	-1.483007
6	-0.249393	-3.024366	-2.968494
1	-1.187697	-1.169227	-2.455412
6	3.750179	-2.440649	2.068020

1	3.817808	−0.914228	3.581789
6	0.734928	−3.920006	−2.599233
1	−0.871850	−3.194048	−3.830904
1	4.577294	−3.009729	2.461163
1	0.906271	−4.819207	−3.168680
1	1.913233	−0.025432	−2.577815
1	−1.365138	3.025642	3.849378
6	−0.722221	1.804138	2.226096
7	0.034540	1.654533	1.139288
6	3.230917	3.031360	−2.119767
6	0.855842	3.864241	1.461474
1	3.936435	3.732918	−2.535220
6	2.108889	0.943102	−2.145300
1	0.087368	4.932588	3.146033
6	0.823291	2.674712	0.752431
6	0.070633	4.011014	2.586932
6	1.625209	2.435250	−0.457065
6	3.019200	1.805265	−2.720933
7	1.427188	1.245839	−1.044528
1	−1.337177	0.961765	2.494538
6	2.527685	3.350585	−0.974683
1	3.547048	1.517907	−3.614737
6	−0.734232	2.959336	2.978980
1	2.687943	4.300751	−0.495829
1	−4.909755	−1.305433	0.562770
1	1.485714	4.674513	1.138452
1	2.266485	−4.335179	−1.177283
1	−5.068075	0.412888	−0.554028
1	3.413221	−3.765054	0.432783

E = −2752.742577 (M_S = 2)

26	0.011426	0.004816	0.002171
7	−1.363309	−1.329269	−1.111305
7	0.011545	−1.922262	1.078760
6	−1.559824	−2.554800	−0.609386
6	−0.744923	−2.905797	0.572507
6	−2.061817	−0.947852	−2.176522
6	−2.989530	−1.759267	−2.797113
6	−3.201217	−3.022765	−2.280981
6	−2.478920	−3.424817	−1.174818
6	−0.743740	−4.171641	1.136799
6	0.043529	−4.421213	2.243583

6	0.816052	-3.400639	2.763108
6	0.769693	-2.168967	2.144051
1	-1.867164	0.048268	-2.542949
1	-3.529490	-1.404502	-3.658930
1	-3.920252	-3.688515	-2.730673
1	0.053789	-5.402140	2.691139
1	1.444421	-3.551142	3.624792
1	1.360307	-1.343567	2.509336
7	1.672145	0.919369	1.129743
7	1.842372	-0.479742	-1.130771
6	2.896516	0.793794	0.600285
6	1.510797	1.664243	2.219878
6	2.999755	-0.050541	-0.609580
6	1.865167	-1.241593	-2.220928
6	3.990257	1.430954	1.165151
6	2.552213	2.321619	2.841824
1	0.504935	1.733125	2.604308
6	4.214271	-0.393467	-1.182873
6	3.033689	-1.616211	-2.851472
1	0.905883	-1.560972	-2.597712
6	3.816304	2.201597	2.298055
1	2.371510	2.911865	3.724462
6	4.231050	-1.183059	-2.315948
1	3.000642	-2.232903	-3.733906
1	4.658741	2.703232	2.746690
1	5.169202	-1.457505	-2.771119
1	0.970500	1.640909	-2.507114
1	-3.751722	0.486493	3.679994
6	-2.227445	0.407707	2.186589
7	-1.654246	0.949930	1.116221
6	-1.087666	4.282436	-2.254505
6	-3.257358	2.700403	1.187872
1	-1.329280	5.230250	-2.708258
6	0.189885	2.290968	-2.144165
1	-4.706993	2.598742	2.754924
6	-2.154404	2.086603	0.615623
6	-3.847990	2.132697	2.299541
6	-1.460071	2.627283	-0.571892
6	-0.080483	3.489971	-2.770032
7	-0.478897	1.866029	-1.075243
1	-1.787600	-0.507506	2.551576
6	-1.783568	3.847417	-1.143827

1	0.487464	3.790624	-3.634341
6	-3.323803	0.963120	2.814060
1	-2.563361	4.461342	-0.728708
1	-1.341352	-4.962191	0.718279
1	-3.662003	3.607020	0.773456
1	5.142001	-0.061173	-0.751317
1	-2.641788	-4.403442	-0.758701
1	4.968752	1.340995	0.727211

7, $Fe(amp)_2Cl_2$
E = –2872.779803 (M_S = 0)

26	0.000000	0.000000	0.000001
17	-0.026666	-1.400054	-1.880635
7	1.987264	-0.235364	0.089757
7	0.595580	1.525346	-1.208687
6	2.643368	-1.338862	0.431467
1	2.039881	-2.204997	0.645425
6	4.018535	-1.407512	0.486030
1	4.499192	-2.326653	0.776819
6	4.750364	-0.285558	0.146009
1	5.828451	-0.301321	0.171901
6	4.074260	0.848665	-0.253652
1	4.605260	1.736049	-0.559255
6	2.691821	0.839110	-0.269638
6	1.877813	2.014029	-0.701096
1	1.662860	2.624665	0.173609
1	2.428607	2.611262	-1.427668
1	-0.046353	2.295208	-1.316495
1	0.690076	1.054549	-2.103299
17	0.026666	1.400055	1.880636
7	-1.987264	0.235364	-0.089756
7	-0.595581	-1.525345	1.208689
6	-2.643368	1.338862	-0.431466
1	-2.039882	2.204997	-0.645423
6	-4.018535	1.407510	-0.486032
1	-4.499193	2.326652	-0.776821
6	-4.750364	0.285556	-0.146012
1	-5.828451	0.301318	-0.171906
6	-4.074260	-0.848667	0.253649
1	-4.605259	-1.736051	0.559251
6	-2.691821	-0.839110	0.269637
6	-1.877813	-2.014029	0.701097

1	−1.662859	−2.624665	−0.173608
1	−2.428607	−2.611262	1.427668
1	0.046352	−2.295207	1.316499
1	−0.690078	−1.054546	2.103300

E = −2872.773892 (M_S = 1)

26	0.000000	0.000001	−0.000001
17	−0.051386	−1.327376	−1.964970
7	1.984797	−0.221529	0.055541
7	0.760982	1.737892	−1.242676
6	2.572300	−1.376694	0.352178
1	1.909155	−2.211477	0.505683
6	3.939725	−1.518874	0.435731
1	4.366501	−2.475885	0.685252
6	4.734008	−0.417277	0.178808
1	5.809024	−0.488740	0.229705
6	4.126539	0.771116	−0.169440
1	4.709526	1.646052	−0.408886
6	2.745758	0.837825	−0.221662
6	2.021022	2.089506	−0.603722
1	1.780017	2.633568	0.308559
1	2.671793	2.711014	−1.220858
1	0.197846	2.557276	−1.405242
1	0.891675	1.250032	−2.120535
17	0.051384	1.327377	1.964971
7	−1.984797	0.221528	−0.055544
7	−0.760978	−1.737884	1.242684
6	−2.572302	1.376690	−0.352191
1	−1.909160	2.211473	−0.505704
6	−3.939728	1.518867	−0.435743
1	−4.366506	2.475875	−0.685272
6	−4.734009	0.417271	−0.178810
1	−5.809025	0.488732	−0.229707
6	−4.126537	−0.771119	0.169445
1	−4.709523	−1.646054	0.408899
6	−2.745757	−0.837824	0.221667
6	−2.021019	−2.089503	0.603734
1	−1.780015	−2.633570	−0.308544
1	−2.671789	−2.711008	1.220875
1	−0.197842	−2.557267	1.405258
1	−0.891670	−1.250014	2.120538

E = –2872.802613 (M_S = 2)

26	0.000000	-0.000001	0.000003
17	-0.104011	-1.392048	-1.928768
7	2.248502	-0.286542	0.059297
7	0.915509	1.647211	-1.249788
6	2.879814	-1.399612	0.407715
1	2.253037	-2.252867	0.619232
6	4.253690	-1.489009	0.483896
1	4.722904	-2.414550	0.773790
6	4.999900	-0.368336	0.168010
1	6.077612	-0.396336	0.208946
6	4.345396	0.782695	-0.218326
1	4.894358	1.669675	-0.492927
6	2.960229	0.788736	-0.258480
6	2.191565	2.015914	-0.652342
1	1.969257	2.578874	0.253644
1	2.812385	2.636018	-1.300710
1	0.336936	2.460628	-1.387136
1	1.025308	1.170400	-2.135953
17	0.104010	1.392046	1.928774
7	-2.248500	0.286542	-0.059296
7	-0.915514	-1.647208	1.249797
6	-2.879810	1.399612	-0.407720
1	-2.253032	2.252866	-0.619234
6	-4.253686	1.489009	-0.483910
1	-4.722899	2.414549	-0.773809
6	-4.999898	0.368336	-0.168026
1	-6.077610	0.396336	-0.208969
6	-4.345396	-0.782694	0.218316
1	-4.894361	-1.669674	0.492915
6	-2.960230	-0.788735	0.258479
6	-2.191568	-2.015912	0.652348
1	-1.969258	-2.578876	-0.253635
1	-2.812391	-2.636013	1.300717
1	-0.336944	-2.460626	1.387153
1	-1.025315	-1.170390	2.135957

8, $[Fe(CO)_6]^{3+}$

E = –1944.103743 (M_S = 1/2)

26	-0.000027	-0.000019	0.000000
6	-1.204382	1.176496	-1.113604
8	-1.863301	1.820095	-1.722872

6	-0.420282	-1.632065	-1.111106
8	-0.650058	-2.525011	-1.718925
6	0.420127	1.632055	1.111098
8	0.649817	2.525039	1.718895
6	-1.620730	-0.451224	1.115617
8	-2.507463	-0.697913	1.725901
6	1.204346	-1.176809	1.113241
8	1.863497	-1.820402	1.722264
6	1.620808	0.451418	-1.115264
8	2.507679	0.698350	-1.725250

E = –1944.078349 (M_S = 3/2)

26	0.000002	-0.000011	-0.000012
6	0.000431	1.450824	-1.486258
8	0.000670	2.221961	-2.276329
6	0.000072	1.486238	1.450824
8	0.000113	2.276311	2.221958
6	-0.000073	-1.486257	-1.450845
8	-0.000116	-2.276330	-2.221979
6	2.346717	-0.000312	0.000280
8	3.452369	-0.000444	0.000411
6	-0.000432	-1.450852	1.486228
8	-0.000673	-2.222012	2.276276
6	-2.346715	0.000365	-0.000223
8	-3.452368	0.000545	-0.000304

E = –1944.085011 (M_S = 5/2)

26	0.000009	-0.000004	-0.000003
6	1.541930	-0.944930	-1.385954
8	2.289667	-1.403181	-2.058074
6	0.773454	2.071011	-0.551280
8	1.148514	3.075369	-0.818580
6	-0.773464	-2.071005	0.551284
8	-1.148541	-3.075355	0.818589
6	1.488637	-0.097263	1.722087
8	2.210617	-0.144410	2.557177
6	-1.542037	0.944633	1.386013
8	-2.289852	1.402657	2.058202
6	-1.488518	0.097578	-1.722164
8	-2.210437	0.144915	-2.557296

9, $[Fe(CNH)_6]^{3+}$

E = –1824.872685 (M_S = 1/2)

26	0.000000	0.000009	0.000024
6	-1.107667	1.207791	-1.092769
6	0.493889	1.563258	1.091858
6	-0.493890	-1.563233	-1.091842
6	1.599307	0.353768	-1.094044
6	1.107685	-1.207829	1.092724
6	-1.599339	-0.353752	1.094035
7	-1.745809	1.903481	-1.729469
7	-2.520647	-0.557563	1.731413
7	0.778374	2.463801	1.728006
7	2.520611	0.557588	-1.731424
7	-0.778366	-2.463774	-1.727998
7	1.745829	-1.903565	1.729371
1	-2.312552	2.521458	-2.297423
1	1.030982	3.263777	2.295365
1	-3.339090	-0.738600	2.299780
1	2.312476	-2.521589	2.297370
1	-1.030899	-3.263821	-2.295290
1	3.339235	0.738753	-2.299491

E = –1824.832957 (M_S = 3/2)

26	0.000009	0.000003	0.000002
6	-0.000003	1.248500	1.589501
6	-2.277764	-0.000211	0.000175
6	2.277771	0.000209	-0.000171
6	0.000295	-1.589490	1.248508
6	-0.000011	-1.248495	-1.589497
6	-0.000293	1.589496	-1.248504
7	-0.000010	1.951492	2.484537
7	-0.000463	2.484529	-1.951499
7	-3.419590	-0.000320	0.000260
7	0.000461	-2.484534	1.951490
7	3.419597	0.000311	-0.000256
7	-0.000021	-1.951486	-2.484534
1	-0.000015	2.577324	3.281306
1	-4.430641	-0.000537	0.000373
1	-0.000607	3.281326	-2.577295
1	-0.000032	-2.577313	-3.281306
1	4.430648	0.000493	-0.000404
1	0.000614	-3.281386	2.577215

E = –1824.826615 (M_S = 5/2)

26	0.000091	0.000007	0.000022
6	-0.046998	-1.766996	1.329797
6	-2.136389	-0.308220	-0.484954
6	2.136524	0.308253	0.484990
6	0.572745	-1.294515	-1.699669
6	0.046942	1.766977	-1.329811
6	-0.572737	1.294511	1.699671
7	-0.070671	-2.677944	2.015260
7	-0.868980	1.961578	2.575748
7	-3.237353	-0.468040	-0.735146
7	0.868687	-1.961603	-2.575831
7	3.237485	0.468081	0.735184
7	0.070490	2.677906	-2.015304
1	-0.091670	-3.486330	2.623652
1	-4.214527	-0.609575	-0.956877
1	-1.131364	2.553967	3.353117
1	0.091399	3.486273	-2.623724
1	4.214657	0.609579	0.956955
1	1.131011	-2.554004	-3.353211

10, $[Fe(NCH)_6]^{3+}$

E = –1824.914054 (M_S = 1/2)

26	-0.000044	0.000042	-0.000037
7	1.458281	-0.660482	1.100524
7	0.159488	-1.593423	-1.099484
7	-1.302916	-0.934318	1.097230
7	-1.458272	0.660538	-1.100651
7	1.302740	0.934363	-1.097405
7	-0.159427	1.593272	1.099739
6	0.251609	-2.518794	-1.752594
1	0.339057	-3.397521	-2.371822
6	-2.060368	-1.476708	1.747947
1	-2.778799	-1.992474	2.365273
6	2.059999	1.476918	-1.748207
1	2.778986	1.991898	-2.365541
6	2.305025	-1.045238	1.753468
1	3.108797	-1.410784	2.372804
6	-2.304971	1.045312	-1.753644
1	-3.109172	1.410971	-2.372359
6	-0.251161	2.518548	1.753040
1	-0.337780	3.396935	2.372868

E = –1824.903904 (M_S = 3/2)

26	0.000011	0.000005	-0.000001
7	2.150032	0.000070	0.000064
7	0.000091	-1.255972	-1.507465
7	0.000004	-1.507460	1.255976
7	-2.150024	-0.000061	-0.000076
7	0.000002	1.507471	-1.255980
7	-0.000099	1.255981	1.507462
6	0.000145	-1.983667	-2.380889
1	0.000113	-2.674463	-3.209808
6	0.000001	-2.380887	1.983667
1	-0.000045	-3.209855	2.674404
6	-0.000005	2.380897	-1.983673
1	-0.000061	3.210021	-2.674222
6	3.289262	0.000099	0.000094
1	4.366439	-0.000154	0.000133
6	-3.289254	-0.000095	-0.000119
1	-4.366430	-0.000291	-0.000114
6	-0.000174	1.983669	2.380893
1	-0.000186	2.674324	3.209930

E = –1824.930171 (M_S = 5/2)

26	-0.000007	0.000012	0.000007
7	0.096705	1.414469	1.539679
7	0.125689	-1.542682	1.408928
7	-2.087534	-0.027362	0.156162
7	-0.096713	-1.414444	-1.539658
7	2.087524	0.027370	-0.156151
7	-0.125699	1.542702	-1.408915
6	0.193548	-2.382369	2.175589
1	0.257639	-3.176975	2.901476
6	-3.223366	-0.042102	0.240522
1	-4.298456	-0.056214	0.320507
6	3.223361	0.042049	-0.240451
1	4.298447	0.056157	-0.320482
6	0.148968	2.184089	2.377767
1	0.198643	2.913174	3.170470
6	-0.148959	-2.184065	-2.377748
1	-0.198146	-2.912905	-3.170707
6	-0.193514	2.382272	-2.175708
1	-0.257985	3.176844	-2.901599

11, $[Fe(NH_3)_6]^{3+}$

E = –1603.363940 (M_S = 1/2)

26	-0.000071	-0.002763	-0.000039
7	-0.843971	-1.439575	-1.191991
7	-0.893021	1.480676	-1.101779
7	0.882806	1.485198	1.103773
7	0.852831	-1.437115	1.188608
7	1.672005	-0.036841	-1.189117
7	-1.670592	-0.049934	1.190495
1	-2.494100	0.388829	0.782031
1	-1.973300	-0.992991	1.428917
1	-1.561667	0.412444	2.092180
1	-0.276968	1.963308	-1.754023
1	-1.676185	1.169414	-1.674456
1	-1.279749	2.226791	-0.525863
1	0.262811	1.964382	1.754843
1	1.666596	1.178177	1.677881
1	1.266655	2.233384	0.528603
1	1.568180	0.442535	-2.082466
1	2.496611	0.390063	-0.770411
1	1.970528	-0.977009	-1.443730
1	-0.769303	-1.220398	-2.185084
1	-0.425922	-2.364760	-1.111057
1	-1.839869	-1.591185	-1.041506
1	0.784252	-1.217067	2.181931
1	0.435015	-2.362713	1.111320
1	1.847851	-1.588219	1.031984

E = –1603.355570 (M_S = 3/2)

26	-0.000130	0.001018	-0.007162
7	2.287688	-0.041910	0.048360
7	-0.038735	1.352919	1.553014
7	-2.288129	0.027002	0.054376
7	-0.095116	-1.312937	-1.594756
7	0.039198	-1.589494	1.309293
7	0.095456	1.561921	-1.352814
1	0.459324	2.430517	-0.964804
1	0.690182	1.362100	-2.155745
1	-0.810332	1.808390	-1.750317
1	-0.372901	0.972312	2.436436
1	0.877126	1.748312	1.762966

1	-0.640582	2.154620	1.370757
1	-2.724453	0.854160	-0.349189
1	-2.739491	-0.746517	-0.430694
1	-2.675917	-0.013237	0.995401
1	0.387992	-1.361277	2.238385
1	-0.879037	-2.004327	1.464147
1	0.629122	-2.356961	0.991425
1	2.675925	-0.121767	0.986666
1	2.718594	-0.815174	-0.455458
1	2.743775	0.783276	-0.336851
1	-0.703102	-0.988125	-2.345236
1	0.808146	-1.475683	-2.038438
1	-0.443537	-2.239612	-1.355552

E = –1603.369399 (M_S = 5/2)

26	-0.000151	0.000185	-0.000206
7	1.229303	-0.845864	-1.615950
7	1.242296	-1.047025	1.482752
7	-1.235987	0.682874	1.686164
7	-1.235450	1.189719	-1.377254
7	-1.348423	-1.715752	-0.283030
7	1.348635	1.735658	0.107786
1	2.258538	1.536401	0.520506
1	1.562537	2.139863	-0.802723
1	0.987184	2.517067	0.652716
1	0.812737	-1.881764	1.878789
1	2.141531	-1.367535	1.126872
1	1.475941	-0.474337	2.292448
1	-0.804831	1.407025	2.258775
1	-2.136924	1.074383	1.415915
1	-1.465754	-0.058329	2.346460
1	-0.983192	-2.600501	0.066258
1	-2.255365	-1.617569	0.170669
1	-1.568961	-1.901463	-1.260297
1	1.392600	-1.846948	-1.519375
1	0.829432	-0.743566	-2.547513
1	2.160644	-0.439970	-1.692381
1	-1.398063	2.142831	-1.055821
1	-0.839498	1.301274	-2.309423
1	-2.167226	0.811055	-1.539784

12, $[Fe([9]aneN_3)_2]^{3+}$

E = –2068.659949 (M_S = 1/2)

26	0.000000	0.000000	0.005346
7	0.000000	1.479999	-1.372421
7	0.056869	1.518448	1.342656
7	-1.992096	0.366566	0.033765
6	-1.391668	1.892222	-1.749672
6	-2.370167	0.823650	-1.329113
6	-2.353316	1.359812	1.096346
6	-1.226868	1.478037	2.093477
6	0.782203	2.592141	-0.762989
6	0.272294	2.827757	0.639636
1	-1.450716	2.079118	-2.817889
1	-1.193403	0.627200	2.769535
1	-1.344927	2.366610	2.710931
1	0.805647	1.405570	2.016083
1	-2.337934	-0.037011	-1.993002
1	-1.611264	2.834977	-1.259913
1	0.965094	3.445761	1.203283
1	-3.278320	1.070386	1.586514
1	0.479886	1.205513	-2.221529
1	-0.671964	3.361435	0.623679
1	-3.391533	1.199198	-1.348868
1	-2.513921	-0.481690	0.223757
1	0.700114	3.497399	-1.361743
1	-2.546278	2.312540	0.614955
1	1.831557	2.306619	-0.769403
7	1.992096	-0.366566	0.033765
7	0.000000	-1.479999	-1.372421
7	-0.056869	-1.518448	1.342656
6	2.353316	-1.359812	1.096346
6	2.370167	-0.823650	-1.329113
1	2.513921	0.481690	0.223757
6	-0.782203	-2.592141	-0.762989
6	1.391668	-1.892222	-1.749672
1	-0.479886	-1.205513	-2.221529
6	1.226868	-1.478037	2.093477
6	-0.272294	-2.827757	0.639636
1	-0.805647	-1.405570	2.016083
1	3.278320	-1.070386	1.586514
1	2.546278	-2.312540	0.614955
1	3.391533	-1.199198	-1.348868
1	2.337934	0.037011	-1.993002

1	-1.831557	-2.306619	-0.769403
1	-0.700114	-3.497399	-1.361743
1	1.450716	-2.079118	-2.817889
1	1.611264	-2.834977	-1.259913
1	1.193403	-0.627200	2.769535
1	1.344927	-2.366610	2.710931
1	-0.965094	-3.445761	1.203283
1	0.671964	-3.361435	0.623679

E = –2068.640031 (M_S = 3/2)

26	-0.000074	-0.000072	0.017128
7	-1.302632	-0.802651	1.376516
7	-1.304655	-0.845117	-1.332799
7	-1.546251	1.592587	-0.049507
6	-2.417079	0.142045	1.724973
6	-2.093825	1.565918	1.326292
6	-2.543836	1.267397	-1.104631
6	-1.976454	0.254732	-2.078414
6	-1.785122	-2.067616	0.751888
6	-2.271369	-1.761756	-0.643008
1	-2.620181	0.086412	2.790620
1	-1.237396	0.708811	-2.734682
1	-2.761948	-0.145518	-2.717228
1	-0.782547	-1.392930	-2.007560
1	-1.348303	2.001293	1.989639
1	-3.313390	-0.204416	1.222306
1	-2.396126	-2.675732	-1.216596
1	-2.841978	2.163348	-1.641643
1	-0.828691	-1.047740	2.238771
1	-3.240501	-1.275262	-0.623430
1	-2.988920	2.179785	1.416928
1	-1.195769	2.526671	-0.222099
1	-2.573311	-2.518061	1.352976
1	-3.444075	0.887651	-0.631878
1	-0.952970	-2.767310	0.738666
7	1.546752	-1.592806	-0.049485
7	1.302418	0.802644	1.376494
7	1.304495	0.845019	-1.332804
6	2.544230	-1.267213	-1.104582
6	2.094189	-1.565850	1.326364
1	1.196675	-2.527042	-0.222069
6	1.784748	2.067654	0.751834

6	2.417024	-0.141862	1.725003
1	0.828442	1.047719	2.238735
6	1.976473	-0.254757	-2.078375
6	2.271088	1.761791	-0.643026
1	0.782349	1.392760	-2.007595
1	2.842709	-2.163052	-1.641593
1	3.444324	-0.887131	-0.631822
1	2.989451	-2.179455	1.417114
1	1.348741	-2.001402	1.989678
1	0.952495	2.767228	0.738546
1	2.572855	2.518232	1.352929
1	2.620071	-0.086153	2.790656
1	3.313286	0.204790	1.222379
1	1.237490	-0.709054	-2.734577
1	2.761830	0.145644	-2.717261
1	2.395758	2.675756	-1.216650
1	3.240273	1.275404	-0.623395

E = –2068.641263 (M_S = 5/2)

26	0.000000	0.000000	0.001340
7	0.000000	1.618632	-1.443373
7	0.149867	1.694770	1.346880
7	-2.087972	0.580274	0.097168
6	-1.393944	2.071403	-1.736042
6	-2.408811	1.044652	-1.279793
6	-2.304513	1.620917	1.147730
6	-1.131657	1.684747	2.103345
6	0.854265	2.668416	-0.824854
6	0.390117	2.959174	0.586807
1	-1.512267	2.258706	-2.799398
1	-1.116789	0.817110	2.761044
1	-1.214353	2.563768	2.740395
1	0.899103	1.586876	2.020956
1	-2.400596	0.171625	-1.930469
1	-1.554385	3.022983	-1.240670
1	1.128775	3.569665	1.098185
1	-3.217197	1.413558	1.698937
1	0.434199	1.354127	-2.320153
1	-0.529162	3.535222	0.583291
1	-3.412578	1.463923	-1.325025
1	-2.697595	-0.203305	0.301401
1	0.841564	3.580685	-1.418979

1	-2.457665	2.575523	0.655627
1	1.879305	2.301171	-0.830439
7	2.087972	-0.580274	0.097168
7	0.000000	-1.618632	-1.443373
7	-0.149867	-1.694770	1.346880
6	2.304513	-1.620917	1.147730
6	2.408811	-1.044652	-1.279793
1	2.697595	0.203305	0.301401
6	-0.854265	-2.668416	-0.824854
6	1.393944	-2.071403	-1.736042
1	-0.434199	-1.354127	-2.320153
6	1.131657	-1.684747	2.103345
6	-0.390117	-2.959174	0.586807
1	-0.899103	-1.586876	2.020956
1	3.217197	-1.413558	1.698937
1	2.457665	-2.575523	0.655627
1	3.412578	-1.463923	-1.325025
1	2.400596	-0.171625	-1.930469
1	-1.879305	-2.301171	-0.830439
1	-0.841564	-3.580685	-1.418979
1	1.512267	-2.258706	-2.799398
1	1.554385	-3.022983	-1.240670
1	1.116789	-0.817110	2.761044
1	1.214353	-2.563768	2.740395
1	-1.128775	-3.569665	1.098185
1	0.529162	-3.535222	0.583291

13, $[Fe(O)(TMC)(MeCN)]^{2+}$ (parallel)
E = –2245.246448 (M_S = 1)

26	-0.026012	0.000007	-0.213715
8	-0.028969	0.000042	-1.818764
7	-1.396200	1.560084	-0.334451
7	1.424831	1.543096	-0.180897
7	1.424825	-1.543088	-0.180967
7	-1.396208	-1.560059	-0.334521
6	-0.626173	2.599469	-1.063648
6	0.694861	2.825656	-0.399100
6	2.330673	1.299440	-1.341464
6	3.109108	0.000021	-1.288126
6	2.330659	-1.299386	-1.341529
6	0.694851	-2.825637	-0.399223
6	-0.626184	-2.599417	-1.063759

6	-2.582183	-1.249372	-1.174478
6	-3.330717	0.000025	-0.784463
6	-2.582185	1.249446	-1.174412
6	-1.864236	2.093988	0.957688
6	2.250242	1.762943	1.024622
6	2.250250	-1.762988	1.024533
6	-1.864266	-2.094019	0.957587
1	-1.198871	3.526585	-1.095515
1	-0.492663	2.245679	-2.079401
1	0.559211	3.300667	0.566514
1	1.310155	3.498403	-0.994008
1	3.041841	2.126044	-1.372288
1	1.724914	1.341916	-2.239371
1	3.752386	0.000040	-2.166618
1	3.798902	-0.000004	-0.447482
1	1.724892	-1.341809	-2.239433
1	3.041818	-2.125996	-1.372400
1	1.310141	-3.498361	-0.994160
1	0.559202	-3.300688	0.566372
1	-1.198885	-3.526530	-1.095663
1	-0.492673	-2.245587	-2.079497
1	-3.239463	-2.118311	-1.139337
1	-2.226489	-1.141013	-2.194598
1	-3.623372	-0.000004	0.262878
1	-4.265215	0.000039	-1.341730
1	-2.226505	1.141145	-2.194542
1	-3.239465	2.118383	-1.139214
1	-2.496433	2.963594	0.786232
1	-1.026851	2.383884	1.578331
1	-2.437807	1.340344	1.483224
1	2.897668	2.623562	0.861155
1	2.872927	0.911387	1.244733
1	1.613051	1.967718	1.874963
1	2.897697	-2.623581	0.861007
1	1.613072	-1.967836	1.874865
1	2.872913	-0.911428	1.244689
1	-2.496480	-2.963604	0.786079
1	-2.437829	-1.340389	1.483153
1	-1.026895	-2.383964	1.578223
7	-0.064112	-0.000041	1.891391
6	-0.087105	-0.000067	3.035547
6	-0.118689	-0.000144	4.476919

1	0.895516	−0.002364	4.868196
1	−0.640761	−0.884570	4.833549
1	−0.636961	0.886437	4.833738

E = −2245.237637 (M_S = 2)

26	−0.042329	−0.000017	−0.198116
8	−0.004020	−0.000105	−1.800094
7	−1.421473	1.663336	−0.370948
7	1.481509	1.610557	−0.143853
7	1.481277	−1.610761	−0.143702
7	−1.421691	−1.663232	−0.370761
6	−0.588439	2.642966	−1.106951
6	0.737309	2.868684	−0.422040
6	2.409740	1.311198	−1.270360
6	3.171916	−0.000273	−1.164798
6	2.409548	−1.311642	−1.270239
6	0.736942	−2.868840	−0.421744
6	−0.588785	−2.643039	−1.106667
6	−2.573672	−1.275470	−1.226166
6	−3.283864	0.000152	−0.813174
6	−2.573504	1.275631	−1.226315
6	−1.915197	2.247467	0.884545
6	2.257444	1.834447	1.088061
6	2.257174	−1.834541	1.088256
6	−1.915471	−2.247166	0.884798
1	−1.117819	3.593446	−1.185481
1	−0.441841	2.256171	−2.108943
1	0.585330	3.377502	0.524115
1	1.351372	3.528929	−1.033581
1	3.136962	2.124062	−1.317523
1	1.827664	1.333541	−2.185481
1	3.866232	−0.000365	−2.003804
1	3.813427	−0.000285	−0.286825
1	1.827464	−1.333991	−2.185355
1	3.136652	−2.124615	−1.317321
1	1.350923	−3.529215	−1.033228
1	0.584916	−3.377545	0.524464
1	−1.118282	−3.593463	−1.185093
1	−0.442151	−2.256365	−2.108701
1	−3.276272	−2.109614	−1.230986
1	−2.195103	−1.157359	−2.237125
1	−3.531308	0.000231	0.246778

1	-4.244367	0.000185	-1.324400
1	-2.194952	1.157354	-2.237261
1	-3.275993	2.109868	-1.231228
1	-2.510611	3.135256	0.673907
1	-1.088678	2.523941	1.527833
1	-2.533529	1.529349	1.410056
1	2.942451	2.670904	0.949000
1	2.836947	0.961989	1.350951
1	1.587106	2.069521	1.906220
1	2.942196	-2.670999	0.949289
1	1.586810	-2.069552	1.906411
1	2.836649	-0.962049	1.351097
1	-2.510986	-3.134913	0.674265
1	-2.533717	-1.528919	1.410236
1	-1.088979	-2.523656	1.528113
7	-0.152580	0.000106	1.879418
6	-0.214892	0.000208	3.022011
6	-0.293496	0.000340	4.460560
1	0.708224	0.000022	4.883111
1	-0.825233	-0.885425	4.799336
1	-0.824600	0.886549	4.799179

13, $[Fe(O)(TMC)(MeCN)]^{2+}$ (crossed)
E = –2245.246162 (M_S = 1)

26	0.000036	0.001871	-0.209193
7	0.000346	-0.013648	1.897174
8	-0.000011	0.013146	-1.815045
7	1.585500	1.378470	-0.080212
7	1.228252	-1.668693	-0.418126
7	-1.585453	-1.376178	-0.099265
7	-1.228364	1.675245	-0.394910
6	2.522167	1.118359	-1.209263
6	3.205032	-0.231376	-1.140086
6	2.311969	-1.418783	-1.411455
6	0.300505	-2.644473	-1.049294
6	-0.977542	-2.725829	-0.274165
6	-2.521949	-1.100645	-1.224823
6	-3.205030	0.247888	-1.136911
6	-2.312130	1.439081	-1.391577
6	-0.300631	2.659474	-1.012840
6	0.977488	2.730332	-0.236862
6	1.806327	-2.251008	0.804487

6	−2.382813	−1.427326	1.146365
6	−1.806038	2.240650	0.835778
6	2.382449	1.412967	1.166175
1	1.962004	1.210947	−2.133715
1	3.278607	1.903311	−1.185747
1	3.765334	−0.346696	−0.215710
1	3.959647	−0.237447	−1.924631
1	2.914470	−2.325836	−1.468446
1	1.827647	−1.279331	−2.371214
1	0.110721	−2.300959	−2.059738
1	0.776127	−3.623597	−1.105289
1	−0.800014	−3.142519	0.711506
1	−1.684716	−3.386425	−0.773245
1	−1.961611	−1.180296	−2.150370
1	−3.278249	−1.885982	−1.212350
1	−3.959558	0.264811	−1.921378
1	−3.765450	0.350204	−0.211078
1	−2.914749	2.346763	−1.435931
1	−1.827790	1.313054	−2.353199
1	−0.776244	3.639275	−1.055484
1	−0.110935	2.329763	−2.027885
1	0.799987	3.133661	0.754349
1	1.684645	3.397611	−0.726994
1	2.334683	−3.171469	0.561070
1	2.508635	−1.561419	1.254182
1	1.030880	−2.472019	1.526676
1	−3.243189	−2.077583	0.995335
1	−1.784358	−1.831500	1.950550
1	−2.733390	−0.446049	1.429756
1	−2.332718	3.165464	0.605630
1	−2.509686	1.545776	1.275069
1	−1.030684	2.449348	1.561676
1	1.783178	1.804851	1.975831
1	2.734127	0.428339	1.436050
1	3.241986	2.066460	1.024640
6	0.000229	−0.023874	3.041525
6	−0.000267	−0.038117	4.483265
1	0.357266	0.916211	4.861868
1	−1.009217	−0.210468	4.849593
1	0.651195	−0.830364	4.843446

E = −2245.237605 (M_S = 2)

26	-0.000260	0.001361	-0.215350
7	0.002348	-0.008585	1.881217
8	-0.001739	0.008181	-1.821468
7	1.843266	1.241035	-0.060366
7	0.996638	-1.872421	-0.432554
7	-1.843921	-1.239481	-0.067563
7	-0.997794	1.876615	-0.414734
6	2.709052	0.788953	-1.182061
6	3.151040	-0.663993	-1.093763
6	2.112366	-1.723494	-1.410261
6	-0.069918	-2.687348	-1.070305
6	-1.370883	-2.626742	-0.304337
6	-2.711836	-0.778082	-1.183840
6	-3.153631	0.674066	-1.082473
6	-2.115378	1.736183	-1.391556
6	0.067372	2.697025	-1.047745
6	1.369766	2.630196	-0.284823
6	1.480194	-2.518743	0.795916
6	-2.625226	-1.228705	1.180685
6	-1.479050	2.512668	0.820055
6	2.626969	1.220285	1.186232
1	2.167884	0.956690	-2.108050
1	3.595887	1.425316	-1.190439
1	3.652039	-0.865856	-0.150245
1	3.928071	-0.787896	-1.846316
1	2.604089	-2.693823	-1.491883
1	1.659997	-1.501350	-2.370582
1	-0.203994	-2.307052	-2.076811
1	0.257986	-3.724793	-1.143169
1	-1.257593	-3.105911	0.662736
1	-2.129762	-3.192782	-0.844717
1	-2.172424	-0.938008	-2.112227
1	-3.598675	-1.414376	-1.195853
1	-3.931830	0.804403	-1.832729
1	-3.653137	0.867918	-0.136487
1	-2.607171	2.707221	-1.463768
1	-1.664860	1.522456	-2.354637
1	-0.260855	3.734977	-1.111296
1	0.199577	2.325138	-2.057630
1	1.258231	3.101398	0.686358
1	2.127638	3.200658	-0.821950
1	1.908908	-3.492506	0.561958

1	2.241843	-1.906704	1.263791
1	0.667553	-2.652702	1.499415
1	-3.548987	-1.792591	1.050328
1	-2.053154	-1.687898	1.976671
1	-2.876131	-0.217265	1.473289
1	-1.908004	3.488407	0.594964
1	-2.240051	1.896921	1.284081
1	-0.665458	2.640531	1.523519
1	2.055735	1.672036	1.987102
1	2.879595	0.206812	1.470028
1	3.549777	1.786458	1.059041
6	0.004427	-0.015817	3.025459
6	0.006665	-0.025299	4.466467
1	0.578922	0.820344	4.839716
1	-1.013416	0.042838	4.836149
1	0.457114	-0.946905	4.826595

14, [Fe(O)(TMCS)]$^{+}$ (parallel)
E = –2549.887388 (M_S = 1)

26	0.084479	0.049539	-0.080185
8	0.254224	0.257557	-1.707118
7	1.498821	-1.496204	-0.285654
7	-1.327875	-1.409640	-0.349574
7	-1.419550	1.612827	-0.036593
7	1.462088	1.591385	0.145871
6	0.759024	-2.435384	-1.155269
1	1.310885	-3.371984	-1.250633
1	0.683734	-1.972961	-2.133205
6	-0.605176	-2.685468	-0.586508
1	-0.529358	-3.210452	0.358185
1	-1.189722	-3.316035	-1.255238
6	-2.119472	-1.080977	-1.564347
1	-2.844481	-1.885110	-1.709647
1	-1.423641	-1.093688	-2.395895
6	-2.879411	0.236181	-1.548419
1	-3.350328	0.310959	-2.527584
1	-3.711340	0.179180	-0.851009
6	-2.108428	1.531157	-1.345580
1	-1.364853	1.650134	-2.123517
1	-2.814492	2.363189	-1.406112
6	-0.631501	2.863631	0.074564
1	-1.162351	3.675614	-0.424401

1	-0.585925	3.117386	1.128955
6	0.750219	2.728586	-0.480431
1	1.310928	3.650555	-0.315386
1	0.713631	2.530324	-1.545563
6	2.701310	1.404464	-0.644545
1	3.355205	2.251744	-0.430432
1	2.414962	1.453343	-1.690601
6	3.429241	0.103931	-0.412948
1	3.654717	-0.060764	0.637588
1	4.394130	0.186061	-0.909519
6	2.701278	-1.065278	-1.031510
1	2.374734	-0.788266	-2.028828
1	3.364610	-1.927908	-1.113786
6	1.942074	-2.191125	0.935723
1	2.643340	-2.980202	0.661488
1	1.102556	-2.617851	1.463969
1	2.416757	-1.493936	1.612137
6	-2.211380	-1.603972	0.823829
1	-2.788238	-2.520931	0.675189
1	-2.911233	-0.784695	0.852702
6	-1.429863	-1.645806	2.114765
6	-2.446255	1.747342	1.019785
1	-2.911316	2.729533	0.926347
1	-1.983549	1.642233	1.991823
1	-3.226275	1.009737	0.920916
6	1.826782	1.907539	1.536609
1	2.480485	2.779741	1.558928
1	2.336061	1.061308	1.981641
1	0.941826	2.100456	2.128915
16	-0.215349	-0.302923	2.188816
1	-2.118609	-1.541264	2.948553
1	-0.932520	-2.604658	2.252048

E = –2549.888075 (M_S = 2)

26	0.105189	0.063619	-0.072572
8	0.220298	0.275516	-1.708431
7	1.793454	-1.369355	-0.303828
7	-1.117499	-1.652266	-0.329825
7	-1.741663	1.460482	-0.033153
7	1.185687	1.891464	0.126919
6	1.132152	-2.342579	-1.187986
1	1.764827	-3.220843	-1.335008

1	0.981653	-1.861129	-2.148031
6	-0.196110	-2.782169	-0.610389
1	-0.035607	-3.320034	0.316876
1	-0.679176	-3.476398	-1.297648
6	-1.985620	-1.418917	-1.512556
1	-2.576521	-2.324569	-1.672006
1	-1.318915	-1.296621	-2.360145
6	-2.950772	-0.240833	-1.447630
1	-3.489874	-0.270016	-2.393821
1	-3.716118	-0.422261	-0.697151
6	-2.409441	1.178000	-1.319439
1	-1.697651	1.371973	-2.113701
1	-3.248085	1.871667	-1.434215
6	-1.121169	2.801110	-0.022781
1	-1.739818	3.502453	-0.587010
1	-1.123369	3.146075	1.006693
6	0.285166	2.840545	-0.566540
1	0.677316	3.854618	-0.464152
1	0.291731	2.572769	-1.616841
6	2.449294	1.814416	-0.648471
1	3.003421	2.736444	-0.461176
1	2.173180	1.796105	-1.698132
6	3.332441	0.615059	-0.358586
1	3.482737	0.480754	0.710524
1	4.315916	0.853142	-0.759204
6	2.880115	-0.675264	-1.022331
1	2.518394	-0.451502	-2.021141
1	3.725439	-1.361138	-1.113173
6	2.343652	-2.037503	0.878935
1	3.109768	-2.754015	0.576236
1	1.566418	-2.552344	1.425970
1	2.775856	-1.311269	1.554800
6	-1.907457	-1.952799	0.883187
1	-2.364966	-2.941101	0.781055
1	-2.705712	-1.227719	0.943065
6	-1.067918	-1.863837	2.134482
6	-2.730759	1.469117	1.053387
1	-3.395216	2.328590	0.940987
1	-2.221699	1.519073	2.008084
1	-3.341292	0.578199	1.041861
6	1.468104	2.337155	1.497645
1	1.933979	3.323195	1.481761

1	2.134159	1.633410	1.982756
1	0.555512	2.376294	2.079711
16	-0.106226	-0.323556	2.181845
1	-1.720781	-1.878062	3.002983
1	-0.403113	-2.718353	2.237643

14, [Fe(O)(TMCS)]$^{+}$ (crossed)
E = –2549.892147 (M_S = 1)

26	-0.055105	0.048413	-0.081923
6	1.797295	2.314269	0.984285
1	2.231110	3.291882	0.770416
1	2.588011	1.630876	1.261484
1	1.126932	2.378183	1.829219
7	-1.684068	1.298856	0.349665
7	1.091075	1.821820	-0.208046
6	-2.385074	1.140629	1.640404
1	-2.720868	0.124709	1.780630
1	-3.243018	1.813457	1.665782
6	-1.130467	2.675973	0.337949
1	-0.826162	2.910603	1.352461
1	-1.911658	3.384717	0.061995
6	-2.680602	1.149847	-0.739228
1	-3.469733	1.883325	-0.560083
1	-2.186693	1.390322	-1.674629
6	-3.301221	-0.230513	-0.824806
1	-4.108258	-0.162999	-1.552554
1	-3.785647	-0.501495	0.109756
6	-2.380874	-1.325682	-1.314552
1	-2.955235	-2.241437	-1.467904
1	-1.956691	-1.025595	-2.264978
6	-1.735599	-2.418950	0.733746
1	-2.258630	-3.309364	0.382847
1	-2.412995	-1.816773	1.322699
1	-0.918893	-2.702483	1.382581
7	1.571028	-1.204166	-0.239463
7	-1.242588	-1.654214	-0.421298
16	0.195104	-0.274665	2.198090
6	2.401022	-1.275255	0.990733
1	2.947888	-0.347356	1.075824
1	3.129949	-2.081151	0.865961
6	1.562679	-1.452676	2.225712
1	2.175417	-1.266183	3.103173

1	1.182788	-2.467701	2.327080
6	-0.300095	-2.485189	-1.202861
6	1.022946	-2.560459	-0.500172
1	0.915198	-3.068789	0.450254
1	1.736973	-3.133951	-1.090341
6	2.424355	-0.798469	-1.383444
1	3.233734	-1.527307	-1.463059
1	1.810329	-0.865956	-2.276144
6	3.025167	0.590339	-1.283300
6	2.042968	1.737940	-1.342253
1	-1.716308	1.384712	2.454954
6	0.039260	2.789388	-0.592960
1	-0.259241	2.553991	-1.608209
1	0.440508	3.804004	-0.573931
1	1.449872	1.645715	-2.243757
1	2.591408	2.681165	-1.385587
1	3.674683	0.700259	-2.150504
1	3.689096	0.677793	-0.427533
1	-0.184966	-2.012401	-2.171648
1	-0.711796	-3.485313	-1.347605
8	-0.193092	0.244153	-1.714951

E = –2549.891432 (M_S = 2)

26	-0.053819	0.047749	-0.073574
6	1.810398	2.433161	0.965946
1	2.258314	3.404847	0.748782
1	2.587047	1.747169	1.280859
1	1.118732	2.523405	1.793210
7	-1.730814	1.378169	0.352525
7	1.130582	1.914287	-0.222788
6	-2.412986	1.258916	1.651435
1	-2.745440	0.243770	1.819483
1	-3.271790	1.931499	1.681859
6	-1.151415	2.739499	0.265820
1	-0.872362	3.033431	1.272539
1	-1.914709	3.442206	-0.072045
6	-2.712015	1.153636	-0.736755
1	-3.525952	1.869787	-0.596341
1	-2.217123	1.376031	-1.676722
6	-3.303810	-0.248137	-0.788696
1	-4.142117	-0.191853	-1.481591
1	-3.750517	-0.516702	0.165307

6	-2.411299	-1.359821	-1.312009
1	-3.021362	-2.248983	-1.489426
1	-1.985115	-1.049370	-2.258772
6	-1.771625	-2.518155	0.710234
1	-2.299374	-3.408948	0.364196
1	-2.442638	-1.915734	1.309527
1	-0.950241	-2.809735	1.351728
7	1.625561	-1.272571	-0.223381
7	-1.282777	-1.745078	-0.433598
16	0.197360	-0.269571	2.192975
6	2.409148	-1.351737	1.028950
1	2.964530	-0.428375	1.130236
1	3.131047	-2.169987	0.950596
6	1.519683	-1.504000	2.233729
1	2.105149	-1.347517	3.135440
1	1.093094	-2.501567	2.310621
6	-0.304739	-2.525844	-1.215633
6	1.040194	-2.601576	-0.523769
1	0.943121	-3.141704	0.410927
1	1.732575	-3.169436	-1.145846
6	2.478708	-0.817360	-1.347161
1	3.306893	-1.524095	-1.444370
1	1.873141	-0.877559	-2.246833
6	3.054085	0.587138	-1.219108
6	2.091503	1.755916	-1.337665
1	-1.729671	1.517993	2.450379
6	0.051773	2.828360	-0.646233
1	-0.224830	2.555124	-1.658553
1	0.413122	3.859150	-0.655269
1	1.509426	1.639276	-2.244177
1	2.670021	2.679459	-1.421850
1	3.749060	0.691545	-2.051380
1	3.675855	0.680465	-0.332600
1	-0.199050	-2.036964	-2.177716
1	-0.675276	-3.539629	-1.382449
8	-0.180688	0.231380	-1.712282

S6. Geometries (in Å) and energies (in hartrees) of 14 Fe complexes using M06-L/def2-TZVP

1, $[Fe(CO)_6]^{2+}$

E = –1943.262870 (M_S = 0)

26	0.000001	-0.000004	0.000003
6	-1.372258	0.418294	1.286660
8	-2.169040	0.661253	2.033537
6	-1.260242	0.272306	-1.432133
8	-1.991993	0.430359	-2.263546
6	1.260244	-0.272312	1.432136
8	1.991995	-0.430372	2.263549
6	-0.492709	-1.861263	0.079626
8	-0.778964	-2.941814	0.125959
6	1.372284	-0.418325	-1.286623
8	2.168990	-0.661185	-2.033613
6	0.492721	1.861254	-0.079609
8	0.778978	2.941805	-0.125939

E = –1943.196938 (M_S = 1)

26	0.000005	-0.000004	0.000006
6	-1.390648	-1.713613	0.001108
8	-2.093863	-2.580893	0.001574
6	-0.000896	-0.000727	-1.926922
8	-0.001435	-0.001163	-3.047018
6	0.000914	0.000712	1.926935
8	0.001458	0.001144	3.047031
6	1.713650	-1.390650	-0.000252
8	2.581018	-2.093757	-0.000345
6	1.390650	1.713611	-0.001126
8	2.093769	2.580969	-0.001609
6	-1.713628	1.390632	0.000257
8	-2.580996	2.093739	0.000345

E = –1943.193922 (M_S = 2)

26	-0.000012	0.000001	0.000019
6	0.000342	-2.263575	0.051386
8	0.000428	-3.380254	0.076543
6	-1.643846	0.036486	1.614987
8	-2.466360	0.053867	2.369337
6	1.643845	-0.036484	-1.614957

8	2.466358	−0.053869	−2.369307
6	−1.643936	−0.036943	−1.614889
8	−2.466460	−0.054554	−2.369221
6	−0.000337	2.263576	−0.051341
8	−0.000571	3.380256	−0.076468
6	1.644002	0.036941	1.614804
8	2.466592	0.054551	2.369065

E = −1943.046008 (M_S = 3)

26	−0.000454	−0.000931	0.219886
6	1.154369	−1.102614	−1.428746
8	1.690004	−1.690327	−2.215831
6	−1.556617	−1.577154	−0.179648
8	−2.197744	−2.492812	−0.286227
6	1.556900	1.578022	−0.166573
8	2.198338	2.494242	−0.266259
6	−1.151976	1.112868	−1.422388
8	−1.685865	1.706468	−2.206246
6	−1.725142	0.710434	1.402057
8	−2.309907	1.107001	2.280897
6	1.722893	−0.719994	1.399180
8	2.306329	−1.122719	2.276127

2, $[Fe(CNH)_6]^{2+}$

E = −1823.972987 (M_S = 0)

26	0.000003	0.000001	−0.000002
6	−1.401859	0.045983	−1.299480
6	−1.210956	−0.742294	1.280033
6	1.210948	0.742298	−1.280046
6	−0.473652	1.761531	0.573307
6	1.401858	−0.045988	1.299483
6	0.473669	−1.761529	−0.573301
7	−2.247316	0.073650	−2.082771
7	0.759336	−2.823568	−0.919086
7	−1.941073	−1.189929	2.051818
7	−0.759325	2.823568	0.919094
7	1.941060	1.189937	−2.051834
7	2.247306	−0.073662	2.082783
1	−2.983110	0.097863	−2.763088
1	−2.575843	−1.579499	2.722711
1	1.008364	−3.746836	−1.219696
1	2.983087	−0.097879	2.763115

1	2.575879	1.579512	-2.722679
1	-1.008416	3.746829	1.219675

E = –1823.899096 (M_S = 1)

26	-0.000001	0.000000	0.000000
6	-1.780950	-1.232027	0.000304
6	0.000049	0.000407	1.913373
6	-0.000050	-0.000407	-1.913373
6	-1.232059	1.780847	-0.000342
6	1.780952	1.232027	-0.000300
6	1.232064	-1.780843	0.000338
7	-2.728288	-1.888550	0.000501
7	1.888677	-2.728118	0.000487
7	0.000145	0.000717	3.067684
7	-1.888669	2.728124	-0.000498
7	-0.000153	-0.000722	-3.067683
7	2.728291	1.888550	-0.000492
1	-3.553787	-2.459913	0.001122
1	0.000714	0.001383	4.069498
1	2.460192	-3.553512	0.000342
1	3.553790	2.459912	-0.001110
1	-0.000767	-0.001420	-4.069498
1	-2.460183	3.553519	-0.000357

E = –1823.887748 (M_S = 2)

26	-0.000016	0.000003	0.000014
6	0.002251	2.215915	0.088417
6	1.606285	0.061846	-1.582753
6	-1.606285	-0.061847	1.582782
6	-1.606384	0.065076	-1.582546
6	-0.002282	-2.215913	-0.088394
6	1.606433	-0.065076	1.582491
7	0.003583	3.368920	0.133955
7	2.450768	-0.097345	2.366592
7	2.450536	0.092307	-2.367016
7	-2.450673	0.097341	-2.366696
7	-2.450530	-0.092316	2.367050
7	-0.003619	-3.368919	-0.133927
1	0.005357	4.371444	0.173739
1	3.185406	0.118979	-3.050253
1	3.185203	-0.125591	3.050227
1	-0.005425	-4.371444	-0.173675

1	-3.185510	-0.118987	3.050169
1	-3.185177	0.125590	-3.050256

E = –1823.753433 (M_S = 3)

26	-0.000375	0.000825	-0.001289
6	1.437763	1.559583	-0.548304
6	-1.432755	1.555518	-0.572070
6	1.436120	-1.257048	-1.073493
6	1.430554	-0.302318	1.629531
6	-1.436367	-0.280388	1.629122
6	-1.433988	-1.272476	-1.059278
7	2.108753	2.451170	-0.863316
7	-2.101468	-1.998256	-1.668748
7	-2.100446	2.445046	-0.899000
7	2.099032	-0.479244	2.560051
7	2.103638	-1.979491	-1.687571
7	-2.109593	-0.443440	2.558840
1	2.730465	3.193230	-1.125514
1	-2.716826	3.187243	-1.173245
1	-2.718423	-2.604010	-2.176796
1	-2.729657	-0.579102	3.335329
1	2.722476	-2.580199	-2.199355
1	2.714341	-0.626341	3.338261

3, $[Fe(NCH)_6]^{2+}$

E = –1824.007285 (M_S = 0)

26	-0.000001	0.000007	-0.000006
7	0.142639	-1.944818	-0.076093
7	1.392092	0.048686	1.366503
7	1.360234	0.154301	-1.390529
7	-0.142640	1.944833	0.076081
7	-1.360233	-0.154286	1.390518
7	-1.392087	-0.048675	-1.366517
6	2.207883	0.077326	2.167661
1	2.973061	0.104208	2.918815
6	2.157764	0.244745	-2.205355
1	2.905483	0.328919	-2.969738
6	-2.157757	-0.244754	2.205348
1	-2.905208	-0.329580	2.969921
6	0.226473	-3.084630	-0.120710
1	0.305514	-4.153513	-0.161913
6	-0.226485	3.084644	0.120706

1	-0.305643	4.153508	0.162163
6	-2.207872	-0.077315	-2.167682
1	-2.973249	-0.104111	-2.918637

E = –1823.978733 (M_S = 1)

26	-0.000004	0.000012	0.000004
7	-0.316094	-2.108321	0.000247
7	2.108386	-0.316095	0.000370
7	0.000337	-0.000256	-1.928159
7	0.316102	2.108335	-0.000236
7	-0.000343	0.000288	1.928165
7	-2.108390	0.316105	-0.000360
6	3.240149	-0.486810	0.000732
1	4.301555	-0.646771	0.001290
6	0.000716	-0.000481	-3.072403
1	0.001083	-0.001385	-4.144786
6	-0.000726	0.000452	3.072408
1	-0.001042	0.000184	4.144790
6	-0.486820	-3.240087	0.000348
1	-0.647054	-4.301454	-0.000062
6	0.486841	3.240100	-0.000349
1	0.647024	4.301473	-0.000792
6	-3.240153	0.486836	-0.000713
1	-4.301500	0.647198	-0.000865

E = –1824.002831 (M_S = 2)

26	0.000094	0.000119	0.000167
7	-0.082670	-2.155365	-0.171676
7	-1.613781	-0.054180	1.447445
7	1.467926	-0.182484	1.583236
7	0.083135	2.155555	0.171835
7	-1.468038	0.182703	-1.582754
7	1.613324	0.053933	-1.447794
6	-2.455848	-0.084805	2.222172
1	-3.245680	-0.113985	2.948522
6	2.231043	-0.279172	2.430883
1	2.946353	-0.369736	3.226041
6	-2.230977	0.279446	-2.430544
1	-2.946120	0.370489	-3.225777
6	-0.126223	-3.296229	-0.262369
1	-0.166885	-4.365148	-0.347307
6	0.126969	3.296413	0.262399

1	0.168403	4.365334	0.346922
6	2.454815	0.083863	−2.223200
1	3.243548	0.111727	−2.950820

E = −1823.870035 (M_S = 3)

26	−0.006904	0.001252	0.134985
7	0.505206	−0.120852	−2.020984
7	0.098416	−2.142492	0.105079
7	2.118364	0.092525	0.464702
7	−0.536436	0.129915	1.912345
7	−2.042752	−0.116950	−0.597260
7	−0.010494	2.127707	−0.188597
6	0.123492	−3.282047	0.201814
1	0.147343	−4.352605	0.293525
6	3.217213	0.142809	0.780137
1	4.248271	0.189764	1.079215
6	−3.164963	−0.152331	−0.818633
1	−4.218722	−0.185059	−1.025457
6	0.773561	−0.184391	−3.131610
1	1.025790	−0.244121	−4.174139
6	−1.087220	0.260459	3.023803
1	−0.613165	0.108447	4.014880
6	−0.065322	3.268977	−0.243785
1	−0.116715	4.341202	−0.294989

4, $[Fe(NH_3)_6]^{2+}$

E = −1602.733559 (M_S = 0)

26	0.000010	−0.000009	0.000234
7	1.228146	−1.703670	0.134558
7	1.168351	0.717164	−1.595954
7	−1.229950	1.696612	−0.197950
7	−1.171935	−0.654109	1.620688
7	1.251255	1.003167	1.362737
7	−1.245904	−1.059125	−1.324453
1	−0.863296	−1.209211	−2.255317
1	−1.470480	−1.997266	−1.000337
1	−2.154183	−0.633951	−1.497056
1	1.403867	1.703374	−1.509054
1	2.068915	0.257969	−1.712996
1	0.736634	0.650799	−2.514955
1	−1.493208	1.891992	−1.161328
1	−2.118694	1.644910	0.295015

1	−0.820952	2.571141	0.123460
1	2.160930	1.270319	0.992954
1	0.877743	1.868412	1.746369
1	1.473159	0.448135	2.186363
1	2.140850	−1.545028	0.555681
1	0.841739	−2.478273	0.669405
1	1.442415	−2.117014	−0.770351
1	−1.353605	0.077241	2.304621
1	−2.098100	−0.993604	1.370674
1	−0.773730	−1.409997	2.173397

E = −1602.719680 (M_S = 1)

26	−0.001877	0.011211	0.000088
7	1.798180	−1.374658	0.001794
7	0.040240	0.048081	−2.068986
7	−1.851372	1.309108	−0.063053
7	−0.055285	0.039047	2.069172
7	1.381918	1.795526	0.059454
7	−1.309015	−1.844597	0.001569
1	−1.392224	−2.346335	−0.878914
1	−0.985905	−2.552099	0.656798
1	−2.271991	−1.670460	0.278575
1	−0.091801	0.979684	−2.455950
1	0.912599	−0.276568	−2.479341
1	−0.677505	−0.515600	−2.517998
1	−2.545824	0.979380	−0.728812
1	−2.365866	1.398654	0.809457
1	−1.675959	2.269754	−0.346968
1	1.853621	2.025777	−0.811450
1	0.930259	2.664411	0.333863
1	2.137772	1.688686	0.731378
1	2.664715	−0.925019	−0.283404
1	2.031422	−1.822629	0.884296
1	1.695621	−2.150989	−0.647102
1	−0.194471	0.970401	2.454243
1	−0.800358	−0.519479	2.478713
1	0.792043	−0.296620	2.520659

E = −1602.750499 (M_S = 2)

26	0.005983	−0.000081	−0.000398
7	−1.620794	0.015780	1.590561
7	−0.062493	2.300639	0.009764

7	1.662389	0.063360	-1.548533
7	-0.023777	-2.301411	-0.015653
7	-1.626752	-0.042384	-1.583940
7	1.663308	-0.035807	1.548497
1	2.223998	0.809951	1.611843
1	1.327573	-0.187203	2.495963
1	2.343422	-0.777616	1.402889
1	0.274875	2.745897	-0.839704
1	-1.003785	2.667691	0.124033
1	0.464757	2.748259	0.754828
1	2.328124	0.818193	-1.403421
1	2.238774	-0.772016	-1.608757
1	1.325512	0.206266	-2.496903
1	-1.962672	0.866793	-1.890625
1	-1.326392	-0.502391	-2.439309
1	-2.468924	-0.545300	-1.316044
1	-2.481144	0.484531	1.318477
1	-1.923837	-0.898508	1.915690
1	-1.331765	0.501499	2.435565
1	0.359273	-2.744234	0.815507
1	-0.962969	-2.684074	-0.088411
1	0.476453	-2.736882	-0.786121

E = –1602.581784 (M_S = 3)

26	0.000234	-0.000219	-0.000391
7	1.271954	1.750211	0.241592
7	-1.284261	1.371067	-1.100418
7	-1.275232	-1.645262	-0.637559
7	1.284656	-1.078962	1.387653
7	-1.276379	0.262324	1.744093
7	1.278744	-0.658807	-1.634481
1	0.880264	-0.413192	-2.551257
1	2.216116	-0.242880	-1.614203
1	1.420973	-1.676511	-1.643497
1	-2.221205	0.996780	-1.284790
1	-1.427392	2.262453	-0.609560
1	-0.888029	1.606905	-2.020729
1	-1.415099	-1.669053	-1.655346
1	-0.876129	-2.557910	-0.377969
1	-2.213610	-1.620368	-0.224272
1	-2.215499	0.606301	1.516729
1	-1.414244	-0.609293	2.270715

1	-0.879402	0.942351	2.407000
1	0.871450	2.420583	0.912246
1	2.210804	1.529631	0.590668
1	1.410752	2.266127	-0.636224
1	2.223759	-1.263084	1.018660
1	1.422444	-0.578539	2.274510
1	0.891580	-1.998614	1.631337

5, $[Fe(H_2O)_6]^{2+}$

E = –1721.890238 (M_S = 0)

26	0.000001	0.000001	-0.000004
8	1.264054	-1.322432	0.923778
1	1.047783	-2.220244	1.201353
1	1.963881	-1.007532	1.509303
8	-1.257296	-1.464792	-0.686726
1	-1.958817	-1.815291	-0.123922
1	-1.037727	-2.153485	-1.324938
8	1.257290	1.464792	0.686733
1	1.958839	1.815269	0.123949
1	1.037678	2.153521	1.324893
8	1.263922	-0.134246	-1.606962
1	1.966651	-0.795749	-1.626031
8	-1.263922	0.134237	1.606955
1	-1.966601	0.795792	1.626069
8	-1.264055	1.322444	-0.923761
1	-1.963932	1.007523	-1.509215
1	1.047368	0.072960	-2.523487
1	-1.047362	-0.073023	2.523467
1	-1.047722	2.220199	-1.201475

E = –1721.890445 (M_S = 1)

26	0.000000	0.000000	0.000000
8	0.003818	-1.855995	-0.915526
1	0.003576	-2.089923	-1.850866
1	0.007440	-2.682326	-0.417265
8	-0.006791	1.013486	-1.736079
1	-0.786067	1.051030	-2.304501
1	0.770287	1.057434	-2.307044
8	0.006790	-1.013486	1.736079
1	0.786068	-1.051036	2.304499
1	-0.770286	-1.057430	2.307047
8	2.198972	0.006264	-0.003604

1	2.779704	-0.722958	-0.249018
8	-2.198971	-0.006264	0.003603
1	-2.779704	0.722960	0.249011
8	-0.003818	1.855995	0.915526
1	-0.007440	2.682326	0.417266
1	2.777357	0.738196	0.239276
1	-2.777357	-0.738199	-0.239270
1	-0.003571	2.089923	1.850867

E = –1721.938902 (M_S = 2)

26	-0.000001	-0.000055	-0.000004
8	1.755706	0.100307	1.231676
1	2.672293	0.133220	0.934878
1	1.778619	0.119796	2.195265
8	1.278832	0.019854	-1.690679
1	1.681039	-0.746563	-2.116521
1	1.615524	0.798932	-2.149084
8	-1.278838	-0.019889	1.690675
1	-1.680835	0.746612	2.116564
1	-1.615752	-0.798902	2.149026
8	-0.093135	2.158382	-0.041400
1	0.369093	2.768682	0.544642
8	0.093169	-2.158444	0.041403
1	-0.368820	-2.768764	-0.544807
8	-1.755732	-0.100043	-1.231668
1	-1.778648	-0.119778	-2.195252
1	-0.602073	2.704546	-0.651504
1	0.601884	-2.704598	0.651702
1	-2.672308	-0.133108	-0.934854

E = –1721.758859 (M_S = 3)

26	0.019996	0.000007	0.000182
8	-1.245821	0.550062	-1.564219
1	-2.001178	1.156452	-1.533112
1	-1.003467	0.429327	-2.495619
8	-1.247825	1.077306	1.258904
1	-2.001531	0.745346	1.769764
1	-1.006408	1.944447	1.620337
8	1.185368	-0.950607	-1.349281
1	2.152736	-0.706602	-1.097216
1	1.164770	-1.883928	-1.637482
8	1.182785	1.645653	-0.149077

1	1.159862	2.362765	-0.812229
8	-1.243398	-1.631804	0.305179
1	-1.000055	-2.377402	0.875863
8	1.186811	-0.690738	1.497864
1	1.166239	-0.474805	2.450494
1	2.150756	1.306850	-0.065771
1	-1.998669	-1.909227	-0.235025
1	2.153691	-0.592378	1.160302

6, $[Fe(bipy)_3]^{2+}$
E = –2749.891901 (M_S = 0)

26	0.001785	0.000187	-0.004079
7	-1.248991	1.154212	1.042232
7	0.188222	1.698357	-1.037618
6	-1.375715	2.424884	0.586536
6	-0.548748	2.737861	-0.574198
6	-1.971663	0.784442	2.108349
6	-2.834988	1.639866	2.764359
6	-2.967347	2.939558	2.302691
6	-2.228963	3.331926	1.202671
6	-0.498539	3.986548	-1.181215
6	0.317094	4.182338	-2.279269
6	1.069416	3.117458	-2.748346
6	0.977305	1.900670	-2.101546
1	-1.841678	-0.235491	2.444600
1	-3.390577	1.286032	3.620966
1	-3.635077	3.636045	2.791077
1	0.365589	5.149744	-2.760151
1	1.722083	3.220909	-3.603316
1	1.548016	1.047569	-2.443176
7	1.379195	-0.998127	-1.049254
7	1.624608	0.491376	1.049813
6	2.647341	-0.887171	-0.582500
6	1.161384	-1.763183	-2.127522
6	2.787909	-0.034560	0.593231
6	1.663676	1.284688	2.129004
6	3.704965	-1.542002	-1.201251
6	2.170500	-2.437579	-2.786561
1	0.137677	-1.825502	-2.471489
6	3.997461	0.231375	1.222964
6	2.833541	1.584831	2.798890
1	0.715631	1.682965	2.464862

6	3.468474	−2.325376	−2.314705
1	1.935212	−3.038290	−3.653408
6	4.024647	1.047911	2.337371
1	2.803398	2.228638	3.666218
1	4.283147	−2.840088	−2.805477
1	4.959523	1.261861	2.837089
1	1.108657	−1.489770	2.446965
1	−3.597762	−0.121801	−3.653920
6	−2.104629	−0.103949	−2.129606
7	−1.551926	−0.683791	−1.055312
6	−1.102038	−4.030906	2.299216
6	−3.192075	−2.419053	−1.216253
1	−1.384390	−4.952399	2.789739
6	0.286916	−2.105419	2.106693
1	−4.607614	−2.254994	−2.816938
6	−2.092740	−1.839042	−0.595766
6	−3.751894	−1.813366	−2.324814
6	−1.423432	−2.399414	0.573550
6	−0.038350	−3.275104	2.765117
7	−0.383428	−1.661688	1.034465
1	−1.643152	0.814333	−2.467576
6	−1.798332	−3.585695	1.191949
1	0.536895	−3.581658	3.626941
6	−3.196081	−0.632622	−2.790566
1	−2.630275	−4.157296	0.806566
1	−1.093474	4.800859	−0.793496
1	−3.607358	−3.339593	−0.832259
1	4.912198	−0.198776	0.841340
1	−2.314788	4.339117	0.821132
1	4.707371	−1.439119	−0.811369

E = −2749.858244 (M_S = 1)

26	0.027224	0.000283	−0.000172
7	−1.696901	0.859713	−1.001847
7	−1.695845	−0.861345	1.001518
6	−2.910017	0.507264	−0.530879
6	−2.909383	−0.510609	0.530317
6	−1.622256	1.780657	−1.966794
6	−2.734465	2.389972	−2.515331
6	−3.984397	2.034952	−2.033839
6	−4.071499	1.086723	−1.032083
6	−4.070151	−1.091686	1.031295

6	-3.981957	-2.039701	2.033157
6	-2.731631	-2.392884	2.514971
6	-1.620158	-1.782105	1.966572
1	-0.624860	2.028891	-2.312043
1	-2.618860	3.125216	-3.298784
1	-4.880232	2.492703	-2.431200
1	-4.877234	-2.498691	2.430343
1	-2.615134	-3.127865	3.298537
1	-0.622518	-2.029034	2.312044
7	1.502122	-1.088072	1.074145
7	0.156958	-1.635574	-1.106627
6	1.847524	-2.244226	0.466698
6	2.136922	-0.725525	2.192169
6	1.085659	-2.559259	-0.742205
6	-0.585020	-1.872483	-2.199570
6	2.853006	-3.053046	0.984739
6	3.139451	-1.485285	2.763792
1	1.819487	0.208952	2.640560
6	1.272884	-3.717782	-1.486092
6	-0.442225	-3.005230	-2.974681
1	-1.312590	-1.112916	-2.451040
6	3.503419	-2.670169	2.142955
1	3.621669	-1.152764	3.671797
6	0.506939	-3.947731	-2.612656
1	-1.068824	-3.139411	-3.844734
1	4.286588	-3.290860	2.557278
1	0.646635	-4.847481	-3.195965
1	1.820087	-0.206629	-2.640659
1	-1.075276	3.140832	3.841955
6	-0.588565	1.873325	2.198096
7	0.154783	1.636427	1.106088
6	3.504992	2.671319	-2.139542
6	1.268363	3.719923	1.485407
1	4.289157	3.291678	-2.552473
6	2.137449	0.727476	-2.191441
1	0.639145	4.850182	3.193823
6	1.083051	2.560728	0.742099
6	0.500996	3.949878	2.611001
6	1.846430	2.245708	-0.465844
6	3.141182	1.486906	-2.761373
7	1.501284	1.089929	-1.074157
1	-1.315698	1.113239	2.449262

6	2.853143	3.054128	-0.982115
1	3.624455	1.154482	-3.668852
6	-0.447633	3.006689	2.972649
1	3.126381	3.974498	-0.486726
1	-5.035886	-0.811805	0.636219
1	2.011066	4.442313	1.179403
1	2.016086	-4.439566	-1.179867
1	-5.036927	0.805378	-0.637290
1	3.126337	-3.973837	0.490188

E = –2749.873891 (M_S = 2)

26	-0.015876	-0.055155	0.002118
7	0.910062	1.570690	-1.085639
7	-0.640186	1.719381	1.062468
6	0.682710	2.813515	-0.603104
6	-0.179918	2.896230	0.580795
6	1.686001	1.433310	-2.168129
6	2.267933	2.500131	-2.822004
6	2.041896	3.776778	-2.330348
6	1.244247	3.931478	-1.213476
6	-0.522267	4.100374	1.189462
6	-1.341598	4.099885	2.301424
6	-1.810105	2.889510	2.789709
6	-1.435879	1.731455	2.139253
1	1.839080	0.419018	-2.518217
1	2.884385	2.330869	-3.693184
1	2.481433	4.640459	-2.810651
1	-1.612056	5.031303	2.780112
1	-2.454347	2.840608	3.655836
1	-1.780336	0.764232	2.486718
7	-1.340641	-1.404086	1.078154
7	-1.866887	-0.086865	-1.170252
6	-2.570310	-1.589811	0.554657
6	-0.979098	-2.100938	2.159272
6	-2.883894	-0.808663	-0.653683
6	-2.081238	0.625004	-2.280364
6	-3.460845	-2.488271	1.132554
6	-1.813571	-3.009018	2.781608
1	0.020385	-1.910240	2.534132
6	-4.140874	-0.806388	-1.248449
6	-3.299292	0.659035	-2.932071
1	-1.233541	1.188211	-2.654621

6	-3.080570	-3.201404	2.254731
1	-1.476596	-3.547836	3.655416
6	-4.351020	-0.067772	-2.398419
1	-3.417831	1.247468	-3.830608
1	-3.766133	-3.903488	2.710284
1	-5.324387	-0.059049	-2.870137
1	-0.352150	-1.916611	-2.501271
1	3.536055	0.704960	3.849654
6	2.123070	0.296363	2.296018
7	1.804841	-0.370757	1.183016
6	2.545262	-3.620380	-2.253289
6	3.944570	-1.424840	1.260309
1	3.124841	-4.407309	-2.717256
6	0.614800	-2.243916	-2.135412
1	5.225858	-0.869944	2.884978
6	2.702145	-1.236139	0.664788
6	4.262838	-0.730056	2.412723
6	2.275300	-1.960176	-0.544260
6	1.310737	-3.256358	-2.766765
7	1.078536	-1.605644	-1.057143
1	1.369562	0.979154	2.672761
6	3.029580	-2.969485	-1.133368
1	0.894615	-3.742234	-3.637497
6	3.331641	0.144553	2.948635
1	3.984633	-3.254051	-0.716964
1	-0.151830	5.035507	0.796175
1	4.661891	-2.107144	0.828206
1	-4.952843	-1.373011	-0.816603
1	1.059713	4.919517	-0.818427
1	-4.441208	-2.639418	0.705118

7, $Fe(amp)_2Cl_2$
E = –2870.353117 (M_S = 0)

26	0.000001	0.000003	0.000003
17	-0.009070	-1.355086	-1.920144
7	1.964289	-0.227369	0.095793
7	0.577440	1.557229	-1.178601
6	2.626682	-1.340357	0.430729
1	2.019144	-2.208036	0.650475
6	4.003504	-1.413311	0.477409
1	4.481882	-2.339234	0.763840
6	4.743356	-0.291785	0.139290

1	5.824720	-0.313149	0.160752
6	4.067357	0.851306	-0.250845
1	4.602627	1.741927	-0.553309
6	2.683761	0.853431	-0.262277
6	1.871010	2.034801	-0.671104
1	1.657221	2.638699	0.214240
1	2.417190	2.654174	-1.388311
1	-0.063282	2.335882	-1.264146
1	0.666732	1.121289	-2.095765
17	0.009068	1.355098	1.920149
7	-1.964290	0.227369	-0.095790
7	-0.577441	-1.557218	1.178616
6	-2.626687	1.340351	-0.430735
1	-2.019154	2.208034	-0.650480
6	-4.003510	1.413296	-0.477427
1	-4.481891	2.339215	-0.763864
6	-4.743357	0.291766	-0.139311
1	-5.824721	0.313124	-0.160781
6	-4.067353	-0.851319	0.250832
1	-4.602620	-1.741944	0.553293
6	-2.683757	-0.853435	0.262276
6	-1.871003	-2.034800	0.671111
1	-1.657204	-2.638698	-0.214232
1	-2.417185	-2.654175	1.388314
1	0.063281	-2.335869	1.264190
1	-0.666746	-1.121257	2.095769

E = –2870.341969 (M_S = 1)

26	-0.000001	0.000000	-0.000005
17	-0.033708	-1.304646	-1.991023
7	1.960206	-0.218427	0.065289
7	0.727935	1.754928	-1.220939
6	2.562689	-1.378281	0.358624
1	1.902412	-2.219040	0.520870
6	3.932451	-1.514129	0.432505
1	4.362900	-2.473871	0.680922
6	4.727758	-0.409549	0.171338
1	5.806386	-0.478869	0.216923
6	4.111479	0.780203	-0.174199
1	4.692208	1.660357	-0.417661
6	2.729534	0.849627	-0.219739
6	2.000830	2.100544	-0.590252

1	1.763646	2.647859	0.326519
1	2.645630	2.736233	-1.205976
1	0.172747	2.585261	-1.374934
1	0.860051	1.294930	-2.117708
17	0.033708	1.304643	1.991016
7	-1.960206	0.218426	-0.065295
7	-0.727933	-1.754928	1.220934
6	-2.562690	1.378281	-0.358623
1	-1.902414	2.219039	-0.520876
6	-3.932454	1.514131	-0.432489
1	-4.362904	2.473875	-0.680900
6	-4.727759	0.409552	-0.171314
1	-5.806388	0.478874	-0.216887
6	-4.111478	-0.780201	0.174214
1	-4.692207	-1.660355	0.417681
6	-2.729533	-0.849627	0.219739
6	-2.000827	-2.100545	0.590243
1	-1.763639	-2.647851	-0.326533
1	-2.645625	-2.736241	1.205961
1	-0.172752	-2.585263	1.374942
1	-0.860054	-1.294921	2.117698

E = –2870.367282 (M_S = 2)

26	0.000010	0.000026	0.000042
17	-0.073284	-1.446825	-1.883403
7	2.224562	-0.274543	0.069773
7	0.907724	1.647105	-1.262590
6	2.855642	-1.395939	0.416186
1	2.219457	-2.247304	0.631398
6	4.230863	-1.494571	0.489995
1	4.695584	-2.427263	0.777597
6	4.987784	-0.374421	0.180888
1	6.068667	-0.408966	0.226015
6	4.339276	0.783841	-0.205126
1	4.896333	1.670780	-0.479267
6	2.951851	0.800860	-0.252437
6	2.188416	2.023048	-0.664250
1	1.958262	2.605992	0.232325
1	2.813368	2.644414	-1.314324
1	0.340742	2.468712	-1.419222
1	1.030482	1.175925	-2.153859
17	0.073273	1.446891	1.883473

7	-2.224572	0.274553	-0.069731
7	-0.907721	-1.647024	1.262698
6	-2.855678	1.395908	-0.416225
1	-2.219515	2.247302	-0.631391
6	-4.230897	1.494467	-0.490171
1	-4.695639	2.427128	-0.777838
6	-4.987788	0.374282	-0.181116
1	-6.068668	0.408768	-0.226352
6	-4.339256	-0.783938	0.204984
1	-4.896294	-1.670900	0.479089
6	-2.951835	-0.800883	0.252428
6	-2.188381	-2.023030	0.664331
1	-1.958184	-2.606012	-0.232207
1	-2.813340	-2.644377	1.314415
1	-0.340736	-2.468611	1.419424
1	-1.030524	-1.175773	2.153924

8, $[Fe(CO)_6]^{3+}$

E = –1942.518838 (M_S = 1/2)

26	0.000006	0.000008	-0.000003
6	1.180422	-1.205515	-1.107222
8	1.831518	-1.870092	-1.719644
6	0.454968	1.625210	-1.106423
8	0.705582	2.521394	-1.718538
6	-0.454923	-1.625183	1.106468
8	-0.705503	-2.521357	1.718612
6	1.634168	0.418307	1.107814
8	2.535101	0.649322	1.720683
6	-1.180409	1.205632	1.107084
8	-1.831599	1.870204	1.719409
6	-1.634188	-0.418413	-1.107718
8	-2.535145	-0.649525	-1.720515

E = –1942.491003 (M_S = 3/2)

26	-0.000001	0.000033	-0.000048
6	0.000865	1.784118	1.072383
8	0.001279	2.738232	1.645941
6	0.000741	-1.072398	1.784027
8	0.001205	-1.645990	2.738123
6	-0.000750	1.072459	-1.784114
8	-0.001221	1.646050	-2.738210
6	2.371362	-0.000362	-0.000968

8	3.485293	-0.000542	-0.001313
6	-0.000875	-1.784044	-1.072493
8	-0.001225	-2.738161	-1.646047
6	-2.371375	0.000231	0.001158
8	-3.485305	0.000301	0.001666

E = –1942.505000 (M_S = 5/2)

26	0.000012	-0.000015	-0.000016
6	1.029694	-0.396124	-2.013583
8	1.529139	-0.587655	-2.989913
6	0.306333	2.257205	-0.287119
8	0.454849	3.351780	-0.425646
6	-0.306364	-2.257214	0.287135
8	-0.454913	-3.351782	0.425685
6	2.030210	-0.139496	1.064895
8	3.014309	-0.207428	1.580915
6	-1.029813	0.395454	2.013617
8	-1.529195	0.586640	2.990048
6	-2.030121	0.140176	-1.064973
8	-3.014182	0.208492	-1.581016

9, $[Fe(CNH)_6]^{3+}$

E = –1823.383602 (M_S = 1/2)

26	-0.000007	0.000002	-0.000038
6	1.365340	0.905937	-1.088311
6	1.466636	-0.728702	1.089355
6	-1.466674	0.728714	-1.089368
6	0.102803	-1.635222	-1.088320
6	-1.365311	-0.905928	1.088323
6	-0.102814	1.635192	1.088323
7	2.157623	1.431874	-1.726958
7	-0.162910	2.584011	1.727321
7	2.317656	-1.151303	1.729165
7	0.162932	-2.584041	-1.727316
7	-2.317712	1.151325	-1.729150
7	-2.157551	-1.431852	1.727034
1	2.857522	1.895792	-2.293511
1	3.069063	-1.524117	2.296996
1	-0.216195	3.421327	2.294858
1	-2.857384	-1.895773	2.293668
1	-3.069041	1.524184	-2.297053
1	0.216064	-3.421507	-2.294646

E = –1823.342255 (M_S = 3/2)

26	-0.000010	-0.000015	-0.000018
6	-2.302441	0.000038	0.000514
6	0.000338	1.448641	1.409081
6	-0.000323	-1.448667	-1.409108
6	-0.000305	1.409077	-1.448671
6	2.302432	0.000035	-0.000448
6	0.000292	-1.409109	1.448634
7	-3.450649	0.000052	0.000739
7	0.000485	-2.207412	2.269321
7	0.000536	2.269367	2.207345
7	-0.000507	2.207369	-2.269370
7	-0.000482	-2.269384	-2.207380
7	3.450640	0.000063	-0.000609
1	-4.462433	-0.000029	0.000879
1	0.000773	2.996055	2.913591
1	0.000925	-2.913967	2.995709
1	4.462424	-0.000036	-0.000472
1	-0.000535	-2.995969	-2.913733
1	-0.001009	2.913851	-2.995830

E = –1823.344970 (M_S = 5/2)

26	0.000190	-0.000177	0.000077
6	-1.351790	-1.756364	-0.207375
6	-1.621904	1.334919	-0.735934
6	1.622187	-1.335084	0.736087
6	0.705107	-0.295701	-2.090056
6	1.351576	1.756517	0.207261
6	-0.705169	0.295741	2.090013
7	-2.048624	-2.660901	-0.314553
7	-1.068595	0.448114	3.167022
7	-2.457408	2.023150	-1.114775
7	1.068270	-0.447854	-3.167181
7	2.457692	-2.023294	1.114954
7	2.048098	2.661310	0.314299
1	-2.663518	-3.459655	-0.409467
1	-3.195016	2.630960	-1.448847
1	-1.389707	0.582775	4.117741
1	2.662728	3.460276	0.409143
1	3.195188	-2.631242	1.449032
1	1.389323	-0.582366	-4.117940

10, $[Fe(NCH)_6]^{3+}$

E = –1823.426543 (M_S = 1/2)

26	-0.000001	-0.000011	0.000009
7	1.559242	0.366794	1.105278
7	1.098939	-1.164908	-1.105593
7	-0.460857	-1.535976	1.102530
7	-1.559248	-0.366819	-1.105260
7	0.460861	1.535956	-1.102510
7	-1.098939	1.164896	1.105602
6	1.740600	-1.844836	-1.763921
1	2.347592	-2.488044	-2.386949
6	-0.730022	-2.433000	1.758526
1	-0.984120	-3.281626	2.379491
6	0.730028	2.433019	-1.758449
1	0.984113	3.281411	-2.379739
6	2.469838	0.581132	1.762772
1	3.331484	0.784414	2.384542
6	-2.469846	-0.581152	-1.762752
1	-3.331350	-0.783901	-2.384893
6	-1.740584	1.844843	1.763920
1	-2.347771	2.488386	2.386410

E = –1823.417966 (M_S = 3/2)

26	0.000004	0.000006	-0.000027
7	0.000025	1.442677	-1.337221
7	-2.154176	0.000073	-0.000010
7	-0.000060	-1.337187	-1.442689
7	-0.000010	-1.442663	1.337170
7	0.000039	1.337200	1.442639
7	2.154179	-0.000065	-0.000066
6	-3.300600	0.000158	-0.000030
1	-4.381351	0.000660	0.000543
6	-0.000148	-2.115083	-2.281390
1	-0.000582	-2.852281	-3.073927
6	0.000005	2.115134	2.281307
1	0.000007	2.850295	3.075735
6	0.000070	2.281418	-2.115077
1	0.001129	3.075081	-2.851063
6	-0.000020	-2.281410	2.115016
1	-0.000092	-3.074874	2.851215
6	3.300602	-0.000110	-0.000088

1	4.381349	0.000087	0.001008

E = –1823.457680 (M_S = 5/2)

26	0.000039	-0.000012	-0.000025
7	0.581649	1.819331	0.871641
7	-1.718352	0.921935	-0.778222
7	1.057339	0.497620	-1.744113
7	-0.581548	-1.819368	-0.871687
7	-1.057272	-0.497616	1.744066
7	1.718421	-0.921992	0.778146
6	-2.655933	1.425280	-1.203936
1	-3.540718	1.900813	-1.605182
6	1.635244	0.769362	-2.695884
1	2.180902	1.025973	-3.593830
6	-1.635496	-0.769104	2.695715
1	-2.181139	-1.026462	3.593456
6	0.898630	2.812756	1.347308
1	1.197208	3.750323	1.796597
6	-0.898499	-2.812802	-1.347357
1	-1.197925	-3.750235	-1.796362
6	2.655823	-1.425311	1.204286
1	3.540397	-1.900527	1.606370

11, $[Fe(NH_3)_6]^{3+}$

E = –1602.191591 (M_S = 1/2)

26	0.000035	-0.000039	0.003436
7	-0.190803	-1.406246	-1.489585
7	-2.073702	0.214772	0.052022
7	0.128359	1.470044	1.439737
7	2.074136	-0.216054	0.036881
7	0.182015	1.429429	-1.468554
7	-0.120112	-1.491807	1.417864
1	-1.055327	-1.867773	1.579236
1	0.452955	-2.305430	1.189224
1	0.208062	-1.217058	2.344838
1	-2.436452	1.064154	-0.381790
1	-2.597396	-0.533896	-0.402698
1	-2.459676	0.244332	0.996471
1	-0.193934	1.180914	2.364365
1	1.064486	1.843830	1.600937
1	-0.446306	2.286913	1.227247
1	-0.687127	1.703813	-1.927807

1	0.588636	2.308246	-1.144639
1	0.795293	1.138649	-2.231404
1	-0.810986	-1.104724	-2.242608
1	0.675232	-1.670959	-1.960250
1	-0.592741	-2.291193	-1.176622
1	2.465498	-0.257387	0.978669
1	2.433972	-1.060241	-0.409465
1	2.595660	0.537873	-0.411587

E = –1602.183017 (M_S = 3/2)

26	-0.000229	-0.001183	-0.008001
7	-0.051498	1.643835	1.273267
7	0.105736	1.277028	-1.650447
7	-0.105584	-1.616376	-1.320642
7	0.051474	-1.319781	1.607379
7	-2.290643	0.042154	0.050995
7	2.291035	-0.024054	0.058801
1	2.749732	0.729100	-0.454905
1	2.681172	0.055330	0.998521
1	2.735377	-0.866065	-0.308654
1	-0.796763	1.434902	-2.101423
1	0.462246	2.210241	-1.442438
1	0.710630	0.925033	-2.393753
1	0.798137	-1.878158	-1.717557
1	-0.470070	-2.476286	-0.909464
1	-0.703341	-1.438944	-2.129044
1	-2.728906	0.807546	-0.462283
1	-2.754387	-0.787992	-0.319303
1	-2.681517	0.136391	0.988878
1	-0.637102	2.404863	0.927034
1	-0.410650	1.446674	2.207654
1	0.866141	2.064901	1.426652
1	0.654012	-2.127818	1.445919
1	0.390091	-0.914773	2.480463
1	-0.862497	-1.713820	1.836257

E = –1602.209219 (M_S = 5/2)

26	-0.000480	0.000527	-0.000030
7	1.331921	1.413632	1.047389
7	1.208538	0.230569	-1.830990
7	-1.337551	-1.285232	-1.196033
7	-1.211516	-0.426472	1.793576

7	-1.285044	1.737809	-0.445780
7	1.294777	-1.671478	0.631808
1	2.195809	-1.719622	0.154648
1	1.537778	-1.651739	1.623102
1	0.891949	-2.599634	0.495847
1	0.793209	0.829411	-2.545874
1	2.137365	0.627454	-1.683695
1	1.387112	-0.647958	-2.319240
1	-0.962075	-2.209831	-1.411247
1	-2.242638	-1.479003	-0.765653
1	-1.573905	-0.896912	-2.110064
1	-0.915627	2.371460	-1.155860
1	-2.219453	1.503983	-0.783626
1	-1.454503	2.342435	0.359081
1	1.522871	2.267016	0.520761
1	0.977589	1.751496	1.943224
1	2.257469	1.045009	1.269688
1	-1.417607	-1.417528	1.925483
1	-0.782906	-0.144674	2.676244
1	-2.127830	0.023130	1.808169

12, $[Fe([9]aneN_3)_2]^{3+}$
E = –2066.802559 (M_S = 1/2)

26	0.000000	0.000000	0.008250
7	0.000000	1.506413	-1.366899
7	0.024571	1.535317	1.351307
7	-2.027052	0.353996	0.020905
6	-1.403089	1.900922	-1.755788
6	-2.377001	0.822626	-1.351110
6	-2.392161	1.351311	1.088931
6	-1.271599	1.469451	2.091204
6	0.771653	2.623953	-0.740154
6	0.237498	2.855565	0.650277
1	-1.453147	2.097512	-2.825886
1	-1.227342	0.608100	2.759702
1	-1.402332	2.346766	2.728409
1	0.774840	1.424573	2.029508
1	-2.330379	-0.039087	-2.018874
1	-1.635115	2.844039	-1.263901
1	0.909656	3.484386	1.232486
1	-3.323882	1.065766	1.575295
1	0.494580	1.239300	-2.214805

1	-0.717831	3.376769	0.623352
1	-3.404436	1.190210	-1.397151
1	-2.566041	-0.489879	0.196864
1	0.702820	3.530626	-1.345176
1	-2.586488	2.308322	0.607410
1	1.823834	2.337154	-0.731838
7	2.027052	-0.353996	0.020905
7	0.000000	-1.506413	-1.366899
7	-0.024571	-1.535317	1.351307
6	2.392161	-1.351311	1.088931
6	2.377001	-0.822626	-1.351110
1	2.566041	0.489879	0.196864
6	-0.771653	-2.623953	-0.740154
6	1.403089	-1.900922	-1.755788
1	-0.494580	-1.239300	-2.214805
6	1.271599	-1.469451	2.091204
6	-0.237498	-2.855565	0.650277
1	-0.774840	-1.424573	2.029508
1	3.323882	-1.065766	1.575295
1	2.586488	-2.308322	0.607410
1	3.404436	-1.190210	-1.397151
1	2.330379	0.039087	-2.018874
1	-1.823834	-2.337154	-0.731838
1	-0.702820	-3.530626	-1.345176
1	1.453147	-2.097512	-2.825886
1	1.635115	-2.844039	-1.263901
1	1.227342	-0.608100	2.759702
1	1.402332	-2.346766	2.728409
1	-0.909656	-3.484386	1.232486
1	0.717831	-3.376769	0.623352

E = –2066.784158 (M_S = 3/2)

26	-0.000001	-0.000012	0.042826
7	-1.358675	-0.784014	1.400575
7	-1.323876	-0.864084	-1.322294
7	-1.578954	1.596127	-0.077454
6	-2.478335	0.177352	1.715387
6	-2.136265	1.589567	1.300361
6	-2.566587	1.252698	-1.144341
6	-1.981555	0.230007	-2.094785
6	-1.824286	-2.061896	0.777001
6	-2.300818	-1.774959	-0.622405

1	-2.705793	0.135280	2.779876
1	-1.223770	0.672580	-2.743976
1	-2.753042	-0.175876	-2.753294
1	-0.787829	-1.425040	-1.980442
1	-1.383567	2.026296	1.960764
1	-3.370058	-0.175551	1.200721
1	-2.429389	-2.695893	-1.189995
1	-2.868924	2.142553	-1.694978
1	-0.900407	-1.018544	2.278228
1	-3.272068	-1.283538	-0.617996
1	-3.022797	2.222794	1.386199
1	-1.228341	2.531435	-0.260090
1	-2.610856	-2.523636	1.378785
1	-3.474358	0.875043	-0.675565
1	-0.979938	-2.752898	0.781971
7	1.578982	-1.596124	-0.077458
7	1.358665	0.784005	1.400576
7	1.323861	0.864080	-1.322293
6	2.566605	-1.252681	-1.144349
6	2.136298	-1.589561	1.300356
1	1.228381	-2.531436	-0.260095
6	1.824257	2.061894	0.777002
6	2.478340	-0.177343	1.715391
1	0.900393	1.018531	2.278228
6	1.981553	-0.229998	-2.094790
6	2.300794	1.774964	-0.622403
1	0.787806	1.425034	-1.980436
1	2.868953	-2.142530	-1.694989
1	3.474374	-0.875012	-0.675578
1	3.022841	-2.222772	1.386190
1	1.383609	-2.026309	1.960757
1	0.979898	2.752883	0.781971
1	2.610819	2.523646	1.378787
1	2.705792	-0.135271	2.779881
1	3.370059	0.175578	1.200730
1	1.223774	-0.672580	-2.743980
1	2.753032	0.175900	-2.753300
1	2.429353	2.695901	-1.189991
1	3.272050	1.283554	-0.617995

E = –2066.796304 (M_S = 5/2)

26	0.000000	0.000000	0.002185

7	0.000000	1.597127	-1.501431
7	0.365924	1.749748	1.272826
7	-2.043176	0.766169	0.228967
6	-1.380966	2.146660	-1.706654
6	-2.422083	1.204628	-1.147531
6	-2.099865	1.856317	1.258411
6	-0.859311	1.844648	2.121431
6	0.981802	2.592046	-0.975569
6	0.637908	2.971858	0.446203
1	-1.564987	2.322574	-2.765634
1	-0.855575	0.982016	2.792246
1	-0.827975	2.732057	2.757839
1	1.153427	1.614907	1.901114
1	-2.507952	0.304720	-1.761448
1	-1.436172	3.123454	-1.229076
1	1.447645	3.553226	0.885032
1	-2.988492	1.745773	1.878367
1	0.348725	1.282419	-2.402776
1	-0.241212	3.612971	0.481754
1	-3.406958	1.677374	-1.151436
1	-2.702297	0.042491	0.502765
1	1.018597	3.480234	-1.610573
1	-2.213113	2.808847	0.743553
1	1.970776	2.130541	-1.030412
7	2.043176	-0.766169	0.228967
7	0.000000	-1.597127	-1.501431
7	-0.365924	-1.749748	1.272826
6	2.099865	-1.856317	1.258411
6	2.422083	-1.204628	-1.147531
1	2.702297	-0.042491	0.502765
6	-0.981802	-2.592046	-0.975569
6	1.380966	-2.146660	-1.706654
1	-0.348725	-1.282419	-2.402776
6	0.859311	-1.844648	2.121431
6	-0.637908	-2.971858	0.446203
1	-1.153427	-1.614907	1.901114
1	2.988492	-1.745773	1.878367
1	2.213113	-2.808847	0.743553
1	3.406958	-1.677374	-1.151436
1	2.507952	-0.304720	-1.761448
1	-1.970776	-2.130541	-1.030412
1	-1.018597	-3.480234	-1.610573

1	1.564987	−2.322574	−2.765634
1	1.436172	−3.123454	−1.229076
1	0.855575	−0.982016	2.792246
1	0.827975	−2.732057	2.757839
1	−1.447645	−3.553226	0.885032
1	0.241212	−3.612971	0.481754

13, $[Fe(O)(TMC)(MeCN)]^{2+}$ (parallel)
E = −2243.194193 (M_S = 1)

26	−0.027974	0.000032	−0.204295
8	−0.031626	0.000014	−1.833419
7	−1.410156	1.586677	−0.337367
7	1.439082	1.563071	−0.181900
7	1.439524	−1.562784	−0.181870
7	−1.409841	−1.586976	−0.337362
6	−0.623663	2.623198	−1.068891
6	0.696542	2.848111	−0.402351
6	2.347528	1.303059	−1.346327
6	3.120312	0.000360	−1.282994
6	2.347883	−1.302556	−1.346304
6	0.697170	−2.847920	−0.402337
6	−0.623063	−2.623271	−1.068903
6	−2.597667	−1.257683	−1.178957
6	−3.331237	−0.000354	−0.782084
6	−2.597951	1.257151	−1.178928
6	−1.876801	2.116814	0.960391
6	2.259135	1.769276	1.032566
6	2.259677	−1.769038	1.032518
6	−1.876429	−2.117246	0.960352
1	−1.193359	3.555807	−1.112380
1	−0.495070	2.262578	−2.087242
1	0.560426	3.320111	0.569215
1	1.314019	3.530655	−0.989905
1	3.060269	2.132492	−1.388803
1	1.736416	1.345184	−2.245581
1	3.782496	0.000447	−2.150141
1	3.802652	0.000469	−0.431343
1	1.736792	−1.344871	−2.245563
1	3.060858	−2.131790	−1.388776
1	1.314773	−3.530386	−0.989853
1	0.561114	−3.319920	0.569237
1	−1.192526	−3.556020	−1.112472

1	-0.494512	-2.262557	-2.087226
1	-3.266302	-2.122708	-1.148583
1	-2.238697	-1.157716	-2.202772
1	-3.606784	-0.000403	0.274268
1	-4.282497	-0.000452	-1.314891
1	-2.238994	1.157297	-2.202758
1	-3.266766	2.122035	-1.148496
1	-2.513779	2.988942	0.799425
1	-1.037284	2.408078	1.583881
1	-2.449926	1.359109	1.487832
1	2.930065	2.617917	0.881908
1	2.863416	0.901087	1.260806
1	1.617013	1.985664	1.880744
1	2.930378	-2.617858	0.881853
1	1.617635	-1.985158	1.880820
1	2.864251	-0.901000	1.260567
1	-2.513208	-2.989510	0.799336
1	-2.449741	-1.359688	1.487797
1	-1.036883	-2.408334	1.583883
7	-0.065147	-0.000072	1.882660
6	-0.089496	-0.000019	3.034854
6	-0.121605	0.000075	4.467750
1	0.891965	0.010164	4.867962
1	-0.633381	-0.890223	4.832807
1	-0.650723	0.880443	4.832200

E = –2243.188826 (M_S = 2)

26	-0.050151	0.000180	-0.195173
8	-0.015311	0.000859	-1.821018
7	-1.432158	1.683332	-0.365599
7	1.490240	1.623530	-0.149377
7	1.490121	-1.623407	-0.150752
7	-1.432287	-1.682790	-0.367039
6	-0.590756	2.665746	-1.102895
6	0.736017	2.886850	-0.420074
6	2.414591	1.314063	-1.286629
6	3.172501	0.000425	-1.179415
6	2.414444	-1.313033	-1.287778
6	0.735791	-2.886436	-0.422481
6	-0.590948	-2.664652	-1.105142
6	-2.590083	-1.280992	-1.220985
6	-3.287454	0.000521	-0.801725

6	-2.590057	1.282397	-1.219821
6	-1.920494	2.257257	0.900254
6	2.270921	1.833253	1.085225
6	2.270865	-1.834234	1.083622
6	-1.920789	-2.257782	0.898262
1	-1.120031	3.619936	-1.184467
1	-0.453341	2.277477	-2.109914
1	0.587464	3.388019	0.535308
1	1.351281	3.559443	-1.022741
1	3.142098	2.130549	-1.346133
1	1.821189	1.338392	-2.199110
1	3.878148	0.000756	-2.011803
1	3.813189	0.000000	-0.296011
1	1.820993	-1.336474	-2.200250
1	3.141860	-2.129545	-1.348054
1	1.351001	-3.558603	-1.025679
1	0.587172	-3.388364	0.532493
1	-1.120299	-3.618730	-1.187532
1	-0.453484	-2.275558	-2.111834
1	-3.300035	-2.113584	-1.226374
1	-2.211260	-1.172447	-2.236770
1	-3.520866	0.000043	0.265712
1	-4.262182	0.000759	-1.290495
1	-2.211334	1.174806	-2.235745
1	-3.299968	2.115029	-1.224352
1	-2.522182	3.148672	0.707139
1	-1.089355	2.531393	1.544656
1	-2.536121	1.531696	1.426183
1	2.971992	2.661962	0.956226
1	2.840075	0.948443	1.346586
1	1.603231	2.074053	1.908256
1	2.971980	-2.662781	0.953823
1	1.603222	-2.075865	1.906451
1	2.839976	-0.949632	1.345782
1	-2.522667	-3.148885	0.704298
1	-2.536285	-1.532570	1.424835
1	-1.089736	-2.532700	1.542440
7	-0.144496	-0.000884	1.874746
6	-0.197145	-0.001683	3.025587
6	-0.262358	-0.002782	4.456071
1	0.742401	-0.023576	4.877873
1	-0.808667	-0.878532	4.806236

1	-0.773250	0.892891	4.809286

13, [Fe(O)(TMC)(MeCN)]$^{2+}$ (crossed)
E = –2243.193587 (M_S = 1)

26	-0.001418	0.001126	-0.202303
7	0.007550	-0.009912	1.887732
8	-0.007075	0.008511	-1.832450
7	1.611846	1.386606	-0.087765
7	1.223180	-1.701150	-0.423466
7	-1.613944	-1.384698	-0.088937
7	-1.227508	1.705234	-0.399690
6	2.544829	1.098606	-1.222455
6	3.205423	-0.262577	-1.147506
6	2.310288	-1.448023	-1.422455
6	0.273756	-2.672147	-1.047867
6	-1.002884	-2.741993	-0.269667
6	-2.554574	-1.086999	-1.214673
6	-3.214993	0.273260	-1.123076
6	-2.321891	1.461357	-1.393045
6	-0.282773	2.681861	-1.022386
6	0.999465	2.745331	-0.252990
6	1.797645	-2.268961	0.810494
6	-2.398660	-1.424323	1.168078
6	-1.792466	2.261641	0.843774
6	2.405159	1.416156	1.163993
1	1.978930	1.200988	-2.147266
1	3.313987	1.876623	-1.210388
1	3.759341	-0.382417	-0.215200
1	3.974916	-0.278503	-1.920502
1	2.911088	-2.359972	-1.486472
1	1.818517	-1.311523	-2.383300
1	0.090642	-2.327469	-2.063531
1	0.740119	-3.659296	-1.109554
1	-0.827562	-3.157803	0.721360
1	-1.718133	-3.405650	-0.760559
1	-1.994956	-1.180915	-2.144182
1	-3.323459	-1.865312	-1.204336
1	-3.989425	0.296026	-1.890946
1	-3.762925	0.384485	-0.186190
1	-2.923192	2.373794	-1.444038
1	-1.837146	1.334082	-2.358725
1	-0.749776	3.669393	-1.071931

1	-0.106979	2.346336	-2.042380
1	0.831345	3.153156	0.742592
1	1.711145	3.412942	-0.743679
1	2.337493	-3.191630	0.587174
1	2.493136	-1.566511	1.261000
1	1.016490	-2.488201	1.532817
1	-3.264745	-2.077026	1.039073
1	-1.789576	-1.819776	1.973208
1	-2.749715	-0.437061	1.447028
1	-2.332577	3.187192	0.633407
1	-2.485734	1.555707	1.292203
1	-1.006069	2.472380	1.562876
1	1.801091	1.803813	1.976778
1	2.759393	0.427077	1.432184
1	3.269450	2.071224	1.034841
6	0.015217	-0.016611	3.040052
6	0.025526	-0.024459	4.473232
1	0.502252	0.879771	4.851465
1	-0.993374	-0.069166	4.857456
1	0.577198	-0.889386	4.841050

E = –2243.188310 (M_S = 2)

26	-0.000517	0.001728	-0.213932
7	0.002676	-0.011782	1.872066
8	-0.002505	0.010985	-1.843271
7	1.845525	1.263575	-0.060553
7	1.012057	-1.890316	-0.438012
7	-1.846341	-1.261280	-0.070537
7	-1.013449	1.896061	-0.414200
6	2.720199	0.799672	-1.181048
6	3.160967	-0.653217	-1.082015
6	2.138176	-1.723504	-1.411897
6	-0.060042	-2.705559	-1.082671
6	-1.361508	-2.651469	-0.318650
6	-2.723409	-0.784878	-1.183911
6	-3.164182	0.666706	-1.067344
6	-2.142085	1.740758	-1.387002
6	0.056902	2.718437	-1.052644
6	1.360083	2.656333	-0.292336
6	1.490747	-2.528340	0.799958
6	-2.616330	-1.254659	1.188240
6	-1.488672	2.520294	0.832150

6	2.618260	1.243523	1.196353
1	2.179697	0.968709	-2.111828
1	3.607436	1.441478	-1.192600
1	3.647992	-0.850519	-0.125653
1	3.959923	-0.777849	-1.814452
1	2.639862	-2.692398	-1.497291
1	1.683494	-1.507942	-2.376881
1	-0.186429	-2.318233	-2.091762
1	0.270393	-3.744993	-1.166577
1	-1.250020	-3.134683	0.651164
1	-2.122525	-3.222682	-0.857014
1	-2.184803	-0.943168	-2.117678
1	-3.610547	-1.426700	-1.200871
1	-3.964574	0.799654	-1.796745
1	-3.649351	0.853020	-0.107835
1	-2.643881	2.710638	-1.459633
1	-1.689926	1.536665	-2.355638
1	-0.274002	3.758618	-1.124566
1	0.180990	2.341910	-2.066102
1	1.250739	3.128952	0.682932
1	2.119861	3.233400	-0.826186
1	1.929868	-3.504802	0.582048
1	2.247598	-1.907465	1.273101
1	0.672090	-2.663985	1.501958
1	-3.542255	-1.824488	1.074061
1	-2.031722	-1.709710	1.982165
1	-2.872630	-0.241244	1.484350
1	-1.926744	3.499872	0.626499
1	-2.245543	1.895198	1.299589
1	-0.668593	2.646398	1.534219
1	2.034290	1.687687	1.996947
1	2.877491	0.227319	1.479937
1	3.542636	1.816821	1.087025
6	0.005490	-0.021522	3.023983
6	0.008693	-0.034139	4.456234
1	0.484791	0.868319	4.839435
1	-1.012673	-0.079433	4.833984
1	0.557539	-0.901592	4.822546

14, [Fe(O)(TMCS)]$^{+}$ (parallel)
E = –2547.625532 (M_S = 1)

26	0.085941	0.053727	-0.070805

8	0.259822	0.261235	-1.724216
7	1.491464	-1.541785	-0.299463
7	-1.359573	-1.415027	-0.358593
7	-1.397696	1.663825	-0.034321
7	1.490257	1.606762	0.142849
6	0.728403	-2.453016	-1.191161
1	1.267040	-3.398202	-1.314617
1	0.665611	-1.965205	-2.162185
6	-0.639900	-2.697380	-0.629332
1	-0.574607	-3.248956	0.306221
1	-1.233744	-3.311529	-1.310319
6	-2.164982	-1.049409	-1.561488
1	-2.898740	-1.847884	-1.720709
1	-1.474944	-1.055866	-2.403683
6	-2.906398	0.276036	-1.507143
1	-3.425328	0.360342	-2.463516
1	-3.712023	0.228529	-0.772982
6	-2.114348	1.561495	-1.336159
1	-1.375290	1.660376	-2.127452
1	-2.806650	2.408828	-1.404356
6	-0.590766	2.916500	0.033274
1	-1.113446	3.720652	-0.492798
1	-0.547417	3.211972	1.080734
6	0.790738	2.745685	-0.512734
1	1.368192	3.665417	-0.371494
1	0.761300	2.521878	-1.577154
6	2.744112	1.381546	-0.627183
1	3.419882	2.213752	-0.403766
1	2.476871	1.446467	-1.681454
6	3.428873	0.059646	-0.380945
1	3.610766	-0.114209	0.681097
1	4.420334	0.123175	-0.830555
6	2.708505	-1.100947	-1.027085
1	2.392734	-0.816290	-2.030047
1	3.373566	-1.966319	-1.115886
6	1.914087	-2.262485	0.918119
1	2.603446	-3.065965	0.643040
1	1.062308	-2.682453	1.439225
1	2.402433	-1.583440	1.608697
6	-2.231407	-1.618281	0.830836
1	-2.817615	-2.533512	0.681503
1	-2.937793	-0.797593	0.868919

6	-1.433126	-1.670902	2.109800
6	-2.397813	1.798525	1.049045
1	-2.936729	2.741826	0.921775
1	-1.899412	1.779748	2.012633
1	-3.124505	0.997314	1.028736
6	1.832357	1.934447	1.540470
1	2.483369	2.812138	1.574456
1	2.341051	1.092362	2.002001
1	0.934978	2.127310	2.121047
16	-0.222765	-0.319306	2.203929
1	-2.111556	-1.595924	2.959185
1	-0.924046	-2.631808	2.222308

E = −2547.630300 (M_S = 2)

26	0.110266	0.065780	-0.064636
8	0.230792	0.276595	-1.721974
7	1.761141	-1.428049	-0.313630
7	-1.170721	-1.643750	-0.338837
7	-1.697853	1.524281	-0.035100
7	1.239403	1.890430	0.126018
6	1.070794	-2.380515	-1.210591
1	1.685410	-3.273239	-1.371644
1	0.939333	-1.882678	-2.169541
6	-0.267925	-2.794479	-0.639755
1	-0.122991	-3.351956	0.283796
1	-0.769962	-3.474182	-1.333037
6	-2.044829	-1.369315	-1.516521
1	-2.660807	-2.260316	-1.687790
1	-1.376592	-1.259277	-2.369872
6	-2.970860	-0.162833	-1.428394
1	-3.542868	-0.178122	-2.357941
1	-3.724830	-0.319701	-0.655596
6	-2.388228	1.240661	-1.318670
1	-1.673245	1.411578	-2.121066
1	-3.206636	1.962483	-1.437232
6	-1.047785	2.859896	-0.043444
1	-1.653660	3.569234	-0.617070
1	-1.050552	3.222345	0.984082
6	0.361369	2.861807	-0.579901
1	0.780733	3.869532	-0.486761
1	0.373925	2.586011	-1.632274
6	2.513173	1.766553	-0.639212

1	3.101370	2.670213	-0.445704
1	2.244728	1.769402	-1.694937
6	3.344413	0.531277	-0.342913
1	3.465370	0.384849	0.732713
1	4.350432	0.738009	-0.709497
6	2.870603	-0.744640	-1.022171
1	2.517762	-0.511449	-2.026024
1	3.703682	-1.450186	-1.117831
6	2.290557	-2.117611	0.871046
1	3.048305	-2.849522	0.573495
1	1.498898	-2.626000	1.410731
1	2.733797	-1.403424	1.558358
6	-1.959019	-1.939015	0.884897
1	-2.434301	-2.923012	0.783195
1	-2.757854	-1.206901	0.946040
6	-1.108967	-1.864804	2.129344
6	-2.671208	1.539977	1.069004
1	-3.374048	2.370282	0.943336
1	-2.149317	1.641388	2.016440
1	-3.245099	0.621287	1.105136
6	1.518293	2.325519	1.504460
1	2.003638	3.305657	1.506147
1	2.169075	1.605474	1.994510
1	0.599038	2.377621	2.082294
16	-0.123181	-0.334494	2.198293
1	-1.752254	-1.891282	3.008470
1	-0.448917	-2.730508	2.216479

14, [Fe(O)(TMCS)]$^{+}$ (crossed)
E = –2547.629873 (M_S = 1)

26	-0.055351	0.049108	-0.072561
6	1.775838	2.350996	0.983932
1	2.226660	3.325869	0.776673
1	2.557286	1.656163	1.274830
1	1.096084	2.428532	1.825349
7	-1.715721	1.301847	0.352934
7	1.074850	1.859585	-0.215238
6	-2.408728	1.134334	1.650239
1	-2.732232	0.109857	1.792653
1	-3.279975	1.794193	1.687977
6	-1.169748	2.691125	0.327060
1	-0.873521	2.937827	1.345668

1	-1.960173	3.394257	0.049600
6	-2.712577	1.121304	-0.740606
1	-3.517434	1.845237	-0.570156
1	-2.219382	1.373076	-1.678425
6	-3.304721	-0.272668	-0.818880
1	-4.131660	-0.220879	-1.528618
1	-3.772620	-0.551452	0.126563
6	-2.381357	-1.360506	-1.320036
1	-2.951876	-2.281686	-1.480565
1	-1.957143	-1.058254	-2.274325
6	-1.717159	-2.453512	0.734980
1	-2.255659	-3.343906	0.397793
1	-2.382802	-1.843339	1.336971
1	-0.892235	-2.748055	1.374567
7	1.599808	-1.204719	-0.243916
7	-1.233362	-1.690621	-0.428634
16	0.211656	-0.275878	2.218503
6	2.427877	-1.268435	0.996495
1	2.971532	-0.332282	1.078138
1	3.171800	-2.066016	0.873924
6	1.585462	-1.454010	2.226326
1	2.196902	-1.286354	3.112282
1	1.203691	-2.474006	2.314666
6	-0.270519	-2.508690	-1.213493
6	1.056624	-2.570829	-0.516896
1	0.963090	-3.090499	0.434214
1	1.777415	-3.137626	-1.111475
6	2.448267	-0.770754	-1.389744
1	3.271186	-1.488679	-1.480169
1	1.832022	-0.849550	-2.285047
6	3.022569	0.629298	-1.281057
6	2.033724	1.771227	-1.352223
1	-1.737247	1.385959	2.464781
6	0.000973	2.813785	-0.601612
1	-0.288836	2.569788	-1.621875
1	0.387783	3.837963	-0.592958
1	1.437149	1.674261	-2.255809
1	2.575988	2.721599	-1.404945
1	3.692239	0.749143	-2.134235
1	3.674929	0.724475	-0.412196
1	-0.169704	-2.029311	-2.185376
1	-0.669188	-3.516452	-1.368505

8	-0.198703	0.243595	-1.731796

E = –2547.633264 (M_S = 2)

26	-0.055901	0.048134	-0.067964
6	1.732776	2.493087	0.970361
1	2.173403	3.473974	0.764624
1	2.516691	1.814885	1.296847
1	1.029077	2.574946	1.793294
7	-1.782253	1.348914	0.353847
7	1.072063	1.963340	-0.228456
6	-2.452389	1.213384	1.661002
1	-2.762065	0.187287	1.832605
1	-3.330546	1.864649	1.706192
6	-1.238952	2.732758	0.251592
1	-0.974529	3.045272	1.261174
1	-2.025334	3.413582	-0.088568
6	-2.763298	1.077289	-0.735372
1	-3.603363	1.769181	-0.599691
1	-2.276957	1.318463	-1.679962
6	-3.301317	-0.346742	-0.776296
1	-4.161877	-0.323951	-1.446812
1	-3.721192	-0.629628	0.190423
6	-2.384924	-1.432231	-1.313057
1	-2.971479	-2.340330	-1.494863
1	-1.967977	-1.110828	-2.264856
6	-1.696440	-2.577712	0.712398
1	-2.211844	-3.484201	0.379107
1	-2.375873	-1.987186	1.321077
1	-0.860719	-2.853723	1.348334
7	1.674139	-1.242895	-0.229498
7	-1.235213	-1.793993	-0.440068
16	0.218837	-0.267413	2.210362
6	2.456815	-1.310779	1.032378
1	3.002325	-0.375709	1.132526
1	3.200500	-2.114322	0.954044
6	1.564657	-1.484197	2.231156
1	2.144518	-1.340256	3.142134
1	1.150139	-2.492655	2.293300
6	-0.230973	-2.546944	-1.230649
6	1.118421	-2.590403	-0.546049
1	1.044581	-3.145222	0.387492
1	1.827551	-3.137693	-1.173278

6	2.518409	-0.744351	-1.350678
1	3.372483	-1.424447	-1.454487
1	1.916991	-0.825613	-2.256238
6	3.040418	0.679866	-1.208036
6	2.048819	1.822725	-1.341454
1	-1.766830	1.486935	2.457940
6	-0.036993	2.849874	-0.657425
1	-0.298458	2.564259	-1.674678
1	0.297743	3.893005	-0.676229
1	1.470056	1.691420	-2.252829
1	2.601895	2.765320	-1.429693
1	3.758192	0.810883	-2.019696
1	3.641147	0.789568	-0.303999
1	-0.148962	-2.048292	-2.194553
1	-0.576647	-3.571329	-1.407863
8	-0.188989	0.228447	-1.728942

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