

Electronic Supporting Information

A Computational Protocol for the Calculation of Standard Reduction Potential of Iron Complexes: Application to Fe^{2+/3+}-A β Model Systems Relevant to Alzheimer's Disease

Adrián L. Orjuela,^a Francisco Núñez-Zarur,^{b,*} Jorge Alí-Torres^{a,*}

^aDepartamento de Química, Universidad Nacional de Colombia-Sede Bogotá, 111321,
Colombia.

^bFacultad de Ciencias Básicas, Universidad de Medellín, Carrera 87 N° 30-65, 050026
Medellín, Colombia.

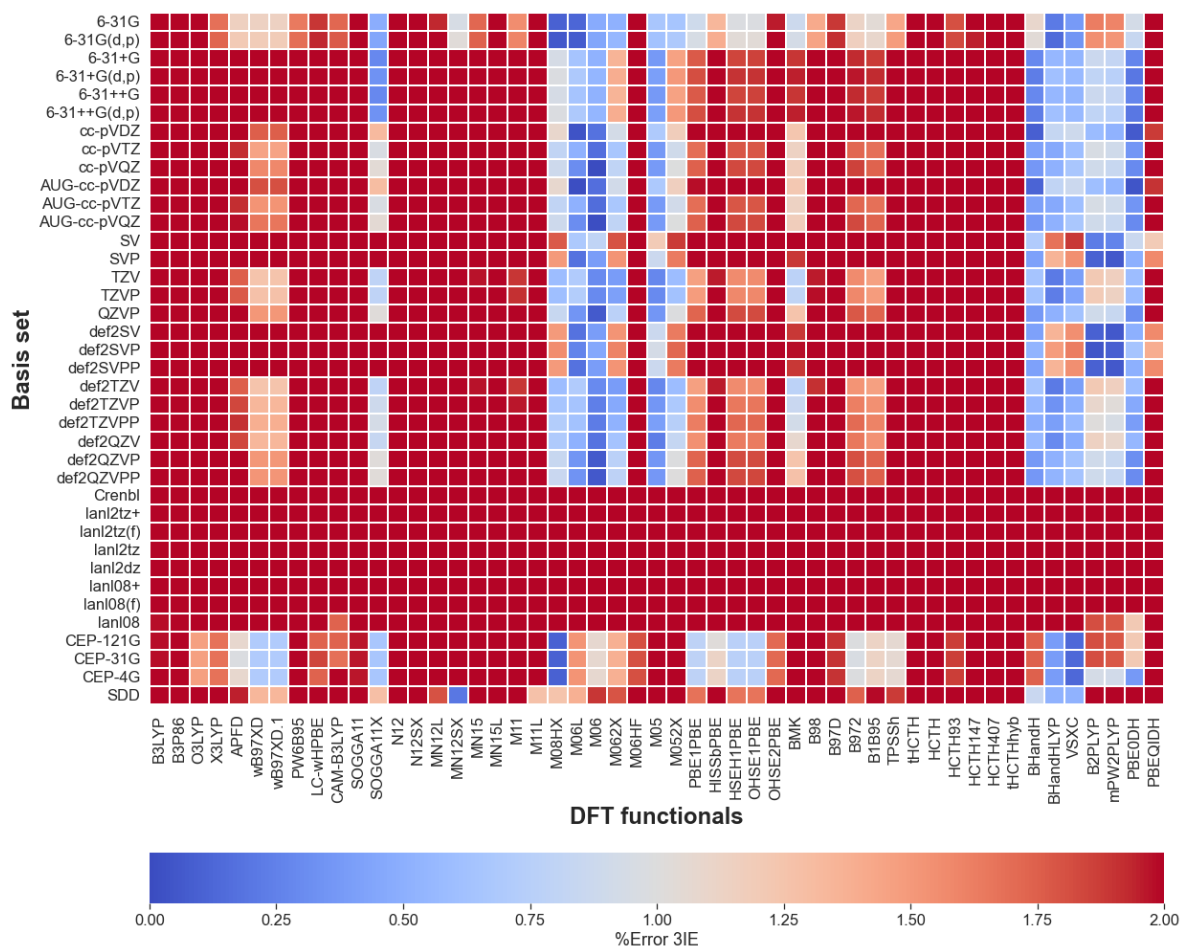


Figure S1. Heatmap for %Error Iron third ionization energy calculated with DFT functionals and basis sets. Iron third ionization energy experimental value is $707.42 \text{ kcal mol}^{-1}$.¹

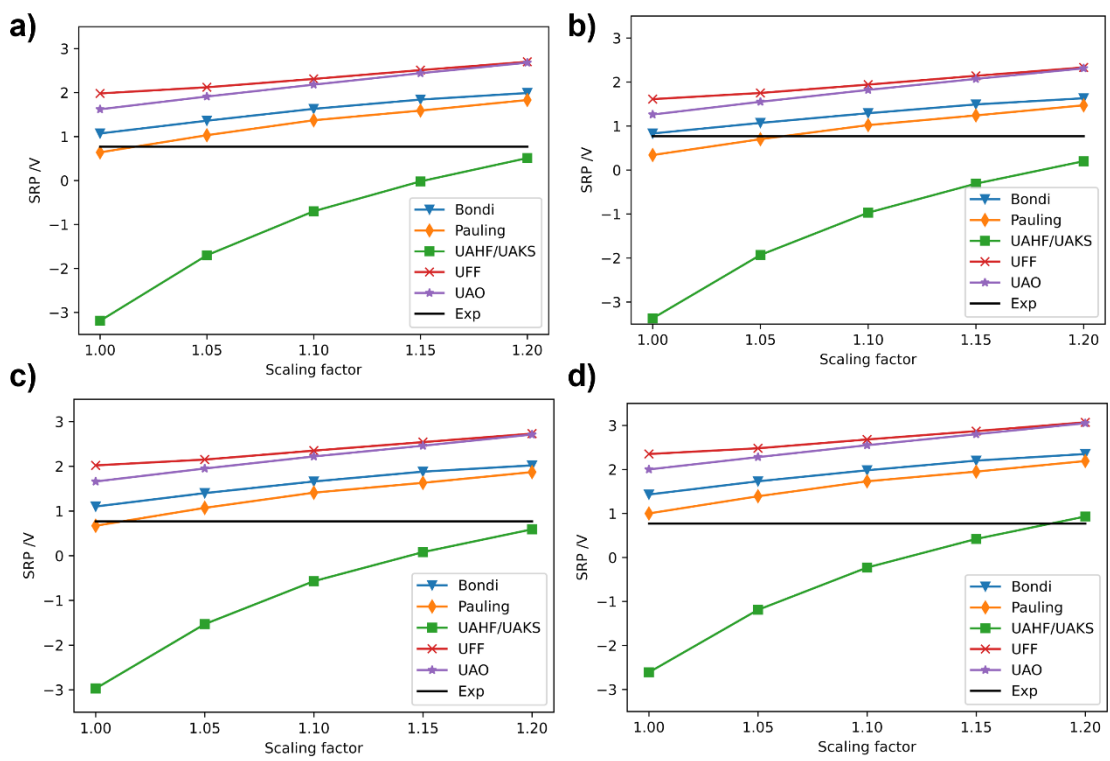


Figure S2. Calculated SRP of $[\text{Fe}(\text{H}_2\text{O})_6]^{3+}$ complex using C-PCM solvent model at a) M06/cc-pVQZ(Fe)-6-31+G(*d,p*)(O, H); b) M06L/cc-pVDZ(Fe)-6-31+G(*d,p*)(O, H); c) M06/6-31+G(*d,p*); d) B3LYP/6-31+G(*d,p*) levels of theory. Experimental SRP for $[\text{Fe}(\text{H}_2\text{O})_6]^{3+}$ is 0.77 V (solid black line).²

Table S1. Iron third ionization energy absolute errors calculated with different DFT functionals and basis sets. Only errors below 4 kcal mol⁻¹ are presented. Iron third ionization energy experimental value is 707.42 kcal mol⁻¹.¹

Basis set	M08HX	M06L	M06	M062X	M06HF	M05	M052X
6-31G	0.096	0.123	0.472	0.510	2.077	0.658	0.649
6-31G(d,p)	0.059	0.074	0.440	0.553	2.125	0.629	0.691
6-31+G	0.941	0.642	0.516	1.353	2.984	0.372	1.460
6-31+G(d,p)	0.977	0.689	0.546	1.393	3.030	0.399	1.500
6-31++G	0.941	0.642	0.516	1.353	2.984	0.372	1.460
6-31++G(d,p)	0.977	0.689	0.546	1.393	3.030	0.399	1.500
cc-pVDZ	1.090	0.034	0.174	0.927	3.028	0.699	1.174
cc-pVTZ	0.807	0.515	0.160	0.663	2.940	0.373	0.904
cc-pVQZ	0.883	0.306	0.005	0.801	3.214	0.375	0.999
AUG-cc-pVDZ	1.079	0.048	0.158	0.910	3.025	0.686	1.161
AUG-cc-pVTZ	0.809	0.508	0.156	0.667	2.949	0.378	0.907
AUG-cc-pVQZ	0.884	0.305	0.083	0.801	3.225	0.375	0.999
SV	1.770	0.680	0.803	1.802	3.822	1.196	1.878
SVP	1.497	0.173	0.393	1.531	3.734	0.869	1.637
TZV	0.587	0.706	0.290	0.383	2.788	0.280	0.593
TZVP	0.603	0.726	0.292	0.414	2.851	0.294	0.626
QZVP	0.846	0.350	0.068	0.771	3.032	0.356	0.991
def2SV	1.497	0.173	0.393	1.531	3.734	0.869	1.637
def2SVP	1.562	0.261	0.454	1.604	3.821	0.932	1.721
def2SVPP	1.497	0.173	0.393	1.531	3.734	0.869	1.637
def2TZV	0.587	0.706	0.290	0.383	2.788	0.280	0.593
def2TZVP	0.653	0.645	0.240	0.464	2.903	0.358	0.685
def2TZVPP	0.720	0.631	0.225	0.518	2.992	0.399	0.749
def2QZV	0.699	0.512	0.184	0.633	2.858	0.233	0.830
def2QZVP	0.846	0.350	0.068	0.771	3.032	0.356	0.991
def2QZVPP	0.857	0.340	0.060	0.782	3.043	0.363	1.002

Table S2. Training set information with solvent and standard reduction potential

Complex	Iron complex formula	SRP (V)	Solvent	Ref
1	[Fe(phen) ₃]	1.15	Water	3
2	[Fe(bpy) ₃]	1.03	Water	3
3	[Fe(Py ₂ Py) ₂]	1.30	Acetonitrile	4
4	[Fe(Py ₂ pep) ₂]	-0.04	Water	5
5	[Fe(Pr ₂ pep) ₂]	0.18	Water	6
6	[Fe(Py ₂ pepO) ₂]	-0.84	DMF	7
7	[Fe(PyIm ₂ H ₂) ₂]	-0.46	Acetonitrile	8
8	[Fe(sar)]	0.05	Water	9
9	[Fe(diammac)]	-0.15	Water	9
10	[Fe(tacn) ₂]	0.13	Water	10
11	[Fe(EDTA)]	0.1	Water	2
12	[Fe(PaPy ₂ O)(Cl)]	-0.27	DMF	7
13	[Fe(NTA)(H ₂ O) ₂]	0.37	Water	2
14	[Fe(Py ₃ tacn)]	0.97	Acetonitrile	11
15	[Fe(bpy)CN ₄]	0.54	Water	12
16	[Fe(DITim) ₂]	-0.44	Acetonitrile	13
17	[Fe(H ₂ O) ₆]	0.77	Water	2

Table S3. Relative energies (kcal/mol), charge and spin multiplicity of all Fe²⁺/Fe³⁺ complexes considered here (Figure 5 of main manuscript).

Complex	Designation	Iron charge	Multiplicity	ΔE_{SCF}	ΔG_{298}
1	[Fe(phen) ₃]	3	6	9.6	5.0
			2	0.0	0.0
		2	5	4.8	0.0
			1	0.0	1.6
2	[Fe(bpy) ₃]	3	6	11.4	6.8
			2	0.0	0.0
		2	5	6.3	0.0
			1	0.0	0.7
3	[Fe(Py _{r2} Py) ₂]	3	6	7.2	3.4
			2	0.0	0.0
		2	5	5.9	0.0
			1	0.0	0.6
4	[Fe(Py _{pep}) ₂]	3	6	8.0	2.8
			2	0.0	0.0
		2	5	0.0	0.0
			1	0.2	7.2
5	[Fe(Pr _{pep}) ₂]	3	6	5.0	0.0
			2	0.0	0.1
		2	5	0.0	0.0
			1	0.5	7.5
6	[Fe(Py _{pep} O) ₂]	3	6	0.0	0.0
			2	4.8	8.3
		2	5	0.0	0.0
			1	11.4	16.4
7	[Fe(PyIm ₂ H ₂) ₂]	3	6	5.1	1.5
			2	0.0	0.0
		2	5	0.0	0.0
			1	0.3	6.3
8	[Fe(sar)]	3	6	7.5	4.5
			2	0.0	0.0
		2	5	1.3	0.0
			1	0.0	3.7

Table S3. Continuation. Relative energies (kcal/mol), charge and spin multiplicity of all Fe²⁺/Fe³⁺ complexes considered here (Figure 5 of main manuscript).

Complex	Designation	Iron charge	Multiplicity	ΔE_{SCF}	ΔG_{298}
9	[Fe(diammac)]	3	6	20.3	15.1
			2	0.0	0.0
		2	5	8.2	2.4
			1	0.0	0.0
10	[Fe(tacn) ₂]	3	6	7.4	4.2
			2	0.0	0.0
		2	5	2.4	0.0
			1	0.0	2.5
11	[Fe(EDTA)]	3	6	0.0	0.0
			2	8.2	10.6
		2	5	0.0	0.0
			1	19.1	24.3
12	[Fe(PaPy ₂ O)(Cl)]	3	6	0.0	0.0
			2	6.4	10.3
		2	5	0.0	0.0
			1	10.3	15.3
13	[Fe(NTA)(H ₂ O) ₂]	3	6	0.0	0.0
			2	12.5	13.8
		2	5	0.0	0.0
			1	39.1	41.9
14	[Fe(Py ₃ tacn)]	3	6	6.4	2.2
			2	0.0	0.0
		2	5	1.7	0.0
			1	0.0	4.0
15	[Fe(bpy)CN ₄]	3	6	21.5	15.2
			2	0.0	0.0
		2	5	18.9	9.2
			1	0.0	0.0
16	[Fe(DITim) ₂]	3	6	7.5	3.4
			2	0.0	0.0
		2	5	0.0	0.0
			1	9.2	15.1
17	[Fe(H ₂ O) ₆]	3	6	0.0	0.0
			2	30.0	30.5
		2	5	0.0	0.0
			1	29.9	36.5

Table S4. Relative energies (kcal/mol), charge and spin multiplicity of the Fe²⁺/Fe³⁺-A β complexes considered here (Figure 7 of main manuscript).

Complex	Designation	Iron charge	Multiplicity	ΔE_{SCF}	ΔG_{298}
18²⁺	[Fe(Ohishis)(H ₂ O) ₃] ²⁺	2+	1	24.4	30.8
			3	18.5	19.9
			5	0.0	0.0
18³⁺	[Fe(Ohishis)(H ₂ O) ₃] ³⁺	3+	2	18.2	22.9
			4	10.1	11.2
			6	0.0	0.0
19²⁺	[Fe(Ohishis)(Im)(H ₂ O) ₂] ²⁺	2+	1	19.8	26.9
			3	15.6	17.0
			5	0.0	0.0
19³⁺	[Fe(Ohishis)(Im)(H ₂ O) ₂] ³⁺	3+	2	11.6	17.7
			4	5.7	7.7
			6	0.0	0.0
20²⁺	[Fe(Ohishis)(Ph)(H ₂ O)] ¹⁺	2+	1	29.6	44.3
			3	2.9	13.9
			5	0.0	0.0
20³⁺	[Fe(Nhishis)(Ph)(H ₂ O)] ¹⁺	3+	2	19.0	19.9
			4	5.6	6.6
			6	0.0	0.0

Table S5. RMSD (Å) of the optimized geometries at M06 and M06L level for representative iron complexes against B3LYP as a reference in gas phase. The ground spin states ($2S + 1$) for the iron complexes are shown in parenthesis.

Complex	Charge	M06L	M06
2 (2)	3+	0.042	0.138
2 (1)	2+	0.055	0.067
17(6)	3+	0.154	0.185
17(5)	2+	0.145	0.158
13 (6)	3+	0.095	0.341
13 (5)	2+	0.182	0.215
11 (6)	3+	0.152	0.156
11 (5)	2+	0.265	0.314

Table S6. Calculated SRP (V) of selected iron complexes using gas and solution phase optimized geometries, SMD solvent model and direct and isodesmic methods at M06L/cc-pVDZ(Fe)-6-31+G(*d,p*)(O, H) level of theory. The ground spin states ($2S + 1$) for the iron complexes are shown in parenthesis.

Complex	Exp	Optimization in gas phase		SMD Optimization	
		Direct	Isodesmic	Direct	Isodesmic
9 (2/1)	-0.15	-0.33	-0.05	-0.23	-0.04
8 (2/1)	0.05	-0.23	-0.05	-0.14	-0.06

References

- 1 A. Kramida, Yu.Ralchenko and J. Reader, NIST Atomic Spectra Database Ionization Energies Data, <https://physics.nist.gov/asd>, (accessed 5 June 2022).
- 2 S. G. Bratsch, *Standard Electrode Potentials and Temperature Coefficients in Water at 298.15 K*, 1989.
- 3 D. R. Lide, G. Baysinger, L. I. Berger, R. N. Goldberg, H. v Kehiaian, K. Kuchitsu, D. L. Roth and D. Zwillinger, *CRC Handbook of Chemistry and Physics*, CRC Press Inc., Florida, 1992.

- 4 A. Cabort, A. Michel, B. Therrien, H. Stoeckli-Evans, K. Bernauer, G. Süss-Fink, A. F. Williams and G. Stupka, *Inorganica Chim Acta*, 2003, **350**, 193–200.
- 5 Xiaolin Tao, Douglas W. Stephan and Pradip K. Mascharak, *J. Inorg. Chem.*, 1986, **26**, 755–759.
- 6 S. J. Brown, M. M. Olmstead and P. K. Mascharak, *Iron(II) and Iron(III) Complexes of N-(2-(4-Imidazolyl)ethyl)pyrimidine-4-carboxamide, a Ligand Resembling Part of the Metal-Binding Domain of Bleomycin*, 1990, vol. 29.
- 7 D. S. Marlin, M. M. Olmstead and P. K. Mascharak, *Eur J Inorg Chem*, 2002, 859–865.
- 8 R. F. Carina, L. Verzeognassi, G. Bernardinelli and A. F. Williams, *Chemical Communications*, 1998, 2681–2682.
- 9 Paul V. Bernhardt, Peter Comba, Trevor W. Hamble and Geoffrey A. Lawrance, *J inorg Chem*, 1991, **30**, 942–946.
- 10 Karl Wiegardt, Wilfried Schmidt, Willy Herrmann and Heinz-Josef Kuppers, *J Inorg Chem*.
- 11 K. Wiegardt, E. Schoffmann, B. Nuber and J. Weiss, *Inorg. Chem*, 1986, **25**, 4877–4883.
- 12 B. Philip George, G. I. H Hanania and D. H. Irvine, *Journal of chemical society*, 1959, 2548–2554.
- 13 J. Shearer, H. L. Jackson, D. Schweitzer, D. K. Rittenberg, T. M. Leavy, W. Kaminsky, R. C. Scarrow and J. A. Kovacs, *J Am Chem Soc*, 2002, **124**, 11417–11428.

Cartesian Coordinates of all complexes considered in this work

1 [Fe(phen)₃]³⁺ doublet

26	-0.000100000	0.000100000	0.000300000
6	3.005900000	-1.530600000	2.728100000
6	3.180700000	-2.816700000	2.243500000
6	2.424900000	-3.247200000	1.127000000
6	1.520600000	-2.315800000	0.565400000
6	2.082400000	-0.670700000	2.108500000
6	2.518700000	-4.556300000	0.539700000
6	0.731900000	-2.671900000	-0.564700000
6	0.833100000	-3.966100000	-1.126600000
6	1.753500000	-4.901800000	-0.539700000
6	0.010500000	-4.248400000	-2.243300000
1	0.048400000	-5.227700000	-2.713500000

6	-0.838900000	-3.267000000	-2.727700000
6	-0.873700000	-2.005800000	-2.107900000
1	3.211800000	-5.272500000	0.971500000
1	3.570100000	-1.171500000	3.582800000
1	3.890600000	-3.492400000	2.713400000
1	1.930700000	0.336600000	2.478700000
1	1.832900000	-5.895300000	-0.971800000
1	-1.481200000	-3.452700000	-3.582600000
1	-1.529200000	-1.226000000	-2.478000000
7	-0.105300000	-1.707100000	-1.054200000
7	1.350000000	-1.049800000	1.055000000
6	-0.177400000	3.369600000	2.726800000
6	0.849400000	4.163500000	2.242500000
6	1.600300000	3.723800000	1.126200000
6	1.245500000	2.474900000	0.564700000
6	-0.460600000	2.139900000	2.107500000
6	2.687600000	4.459000000	0.539100000
6	1.948300000	1.969600000	-0.565200000
6	3.019000000	2.703800000	-1.126900000
6	3.369500000	3.968700000	-0.539900000
6	3.674700000	2.132200000	-2.243400000
1	4.504200000	2.654300000	-2.713400000
6	3.249200000	0.905900000	-2.727600000
6	2.174100000	0.245600000	-2.107900000
1	2.961600000	5.417300000	0.971000000
1	-0.770700000	3.679000000	3.581300000
1	1.079900000	5.116200000	2.712300000
1	-1.257400000	1.505200000	2.477500000
1	4.190600000	4.533700000	-0.971900000
1	3.731300000	0.442200000	-3.582300000
1	1.826400000	-0.712000000	-2.477800000
7	1.531000000	0.762300000	-1.054600000
7	0.234100000	1.694700000	1.054300000
6	-2.828800000	-1.836700000	2.728800000
6	-4.030000000	-1.345400000	2.244000000
6	-4.025000000	-0.476100000	1.127000000
6	-2.766200000	-0.158800000	0.565300000
6	-1.622400000	-1.467000000	2.109100000
6	-5.205500000	0.096900000	0.539500000
6	-2.680300000	0.701900000	-0.565200000
6	-3.851700000	1.261000000	-1.127300000
6	-5.122300000	0.931900000	-0.540200000
6	-3.684900000	2.114200000	-2.244200000
1	-4.552000000	2.570900000	-2.714500000
6	-2.410300000	2.359300000	-2.728500000
6	-1.300600000	1.759200000	-2.108400000
1	-6.172400000	-0.145100000	0.971500000
1	-2.799800000	-2.504400000	3.583900000
1	-4.970100000	-1.622100000	2.714100000
1	-0.674100000	-1.839000000	2.479600000
1	-6.022300000	1.359700000	-0.972400000
1	-2.250000000	3.008400000	-3.583400000

1	-0.297500000	1.937000000	-2.478500000
7	-1.426100000	0.944300000	-1.054800000
7	-1.584500000	-0.643800000	1.055100000

1 [Fe(phen)₃]²⁺ Singlet

26	0.000700000	-0.000900000	-0.000400000
6	3.177300000	1.086000000	2.778300000
6	4.238900000	0.350700000	2.282600000
6	4.039300000	-0.467200000	1.146800000
6	2.743500000	-0.479100000	0.577700000
6	1.921800000	1.004700000	2.148100000
6	5.065700000	-1.277500000	0.549600000
6	2.474000000	-1.280600000	-0.575900000
6	3.498700000	-2.074200000	-1.144300000
6	4.805800000	-2.050000000	-0.546500000
6	3.163300000	-2.846500000	-2.280100000
1	3.914600000	-3.474000000	-2.752100000
6	1.873400000	-2.789900000	-2.776400000
6	0.922600000	-1.965400000	-2.146900000
1	6.058700000	-1.266100000	0.989900000
1	3.293600000	1.725000000	3.647600000
1	5.216500000	0.395800000	2.755100000
1	1.077800000	1.569400000	2.528300000
1	5.589900000	-2.659900000	-0.986200000
1	1.579900000	-3.369300000	-3.645700000
1	-0.090900000	-1.904400000	-2.527400000
7	1.203600000	-1.221700000	-1.074300000
7	1.696100000	0.242500000	1.075400000
6	-2.533600000	2.206600000	2.774300000
6	-2.426700000	3.493700000	2.279100000
6	-1.616400000	3.729900000	1.144800000
6	-0.957400000	2.613700000	0.576600000
6	-1.834400000	1.160000000	2.145200000
6	-1.426600000	5.024000000	0.548400000
6	-0.126500000	2.781200000	-0.575500000
6	0.049800000	4.065600000	-1.143100000
6	-0.625600000	5.185400000	-0.546200000
6	0.888600000	4.161700000	-2.277200000
1	1.057500000	5.126200000	-2.748400000
6	1.485000000	3.016300000	-2.773000000
6	1.244700000	1.780400000	-2.144500000
1	-1.933700000	5.878400000	0.987900000
1	-3.146700000	1.987800000	3.642600000
1	-2.955200000	4.317800000	2.750800000
1	-1.902300000	0.146700000	2.525100000
1	-0.488400000	6.169600000	-0.985300000
1	2.135100000	3.052000000	-3.641100000
1	1.698900000	0.872200000	-2.524900000
7	0.458300000	1.651700000	-1.073300000
7	-1.059700000	1.345700000	1.073900000
6	-0.650500000	-3.298200000	2.774100000

6	-1.819500000	-3.847100000	2.278600000
6	-2.427400000	-3.263000000	1.143600000
6	-1.787700000	-2.135700000	0.575100000
6	-0.091100000	-2.170800000	2.144800000
6	-3.643500000	-3.743700000	0.546600000
6	-2.346000000	-1.499700000	-0.577900000
6	-3.546800000	-1.987500000	-1.146400000
6	-4.181600000	-3.130600000	-0.549000000
6	-4.046600000	-1.309500000	-2.281800000
1	-4.966500000	-1.644200000	-2.753800000
6	-3.350200000	-0.222100000	-2.778000000
6	-2.159900000	0.186200000	-2.148500000
1	-4.132000000	-4.608700000	0.986500000
1	-0.155700000	-3.720400000	3.642800000
1	-2.270900000	-4.715600000	2.750700000
1	0.821000000	-1.724500000	2.525000000
1	-5.102800000	-3.502400000	-0.988600000
1	-3.704100000	0.322700000	-3.647100000
1	-1.598400000	1.032300000	-2.528900000
7	-1.657600000	-0.430200000	-1.076000000
7	-0.637800000	-1.592200000	1.072900000

2 [Fe(bpy)₃]³⁺ Doublet

26	-0.000300000	-0.000100000	0.000100000
6	-2.280100000	-2.425100000	2.729300000
6	-3.582500000	-2.220700000	2.270600000
6	-3.790300000	-1.372900000	1.182200000
6	-2.698100000	-0.747100000	0.576100000
6	-1.232300000	-1.777700000	2.081200000
6	-2.794700000	0.164300000	-0.576300000
6	-3.993800000	0.547000000	-1.182500000
6	-3.968400000	1.419500000	-2.271000000
1	-4.894500000	1.723400000	-2.750500000
6	-2.737800000	1.892400000	-2.729600000
6	-1.577500000	1.479200000	-2.081400000
1	-2.071000000	-3.074100000	3.573600000
1	-4.424300000	-2.712100000	2.750000000
1	-0.209700000	-1.911200000	2.411100000
1	-2.669400000	2.570800000	-3.574000000
1	-0.605700000	1.824200000	-2.411300000
7	-1.596800000	0.632400000	-1.031400000
7	-1.428700000	-0.953500000	1.031300000
6	3.240700000	-0.760100000	2.729100000
6	3.715500000	-1.989900000	2.270500000
6	3.085100000	-2.594300000	1.182300000
6	1.996500000	-1.962000000	0.576400000
6	2.155500000	-0.177000000	2.081300000
6	1.255400000	-2.502100000	-0.575400000
6	1.523900000	-3.732100000	-1.181200000
6	0.755000000	-4.147600000	-2.268800000
1	0.955200000	-5.101700000	-2.747900000

6	-0.271000000	-3.319400000	-2.726900000
6	-0.493600000	-2.107700000	-2.079300000
1	3.698100000	-0.254100000	3.573300000
1	4.562400000	-2.472700000	2.749700000
1	1.759400000	0.775100000	2.411300000
1	-0.893300000	-3.600400000	-3.570500000
1	-1.279100000	-1.439400000	-2.409000000
7	0.250200000	-1.699700000	-1.030300000
7	1.540100000	-0.759600000	1.031500000
6	-0.961900000	3.188700000	2.726900000
6	-0.132900000	4.213900000	2.268500000
6	0.706000000	3.969100000	1.180900000
6	0.701800000	2.710100000	0.575300000
6	-0.925100000	1.957200000	2.079400000
6	1.540100000	2.337400000	-0.576400000
6	2.471800000	3.184000000	-1.182200000
6	3.215200000	2.725300000	-2.270100000
1	3.941900000	3.375000000	-2.749400000
6	3.009300000	1.423000000	-2.728500000
6	2.070700000	0.625200000	-2.080700000
1	-1.629200000	3.332700000	3.570600000
1	-0.137600000	5.188800000	2.747500000
1	-1.552600000	1.138800000	2.409200000
1	3.563000000	1.024200000	-3.572500000
1	1.883500000	-0.389000000	-2.410500000
7	1.346400000	1.065800000	-1.031200000
7	-0.112400000	1.714400000	1.030300000
1	-4.942200000	0.173300000	-0.813500000
1	-4.795900000	-1.206400000	0.813100000
1	3.444100000	-3.548300000	0.813300000
1	2.322500000	-4.365700000	-0.812500000
1	2.622300000	4.192200000	-0.813500000
1	1.353600000	4.756300000	0.812000000

2 [Fe(bpy)₃]²⁺ Singlet

26	0.000400000	0.000300000	0.000200000
6	1.689200000	2.863900000	2.762900000
6	2.994200000	2.987400000	2.286200000
6	3.379000000	2.227300000	1.183700000
6	2.456400000	1.364000000	0.583200000
6	0.821800000	1.987800000	2.115900000
6	2.761800000	0.514400000	-0.584700000
6	4.022800000	0.436800000	-1.185600000
6	4.209900000	-0.393600000	-2.288600000
1	5.183600000	-0.463500000	-2.763900000
6	3.125100000	-1.129200000	-2.765500000
6	1.898600000	-1.006900000	-2.117900000
1	1.341400000	3.433200000	3.618800000
1	3.700200000	3.661800000	2.761200000
1	-0.198200000	1.864700000	2.459400000
1	3.219300000	-1.789000000	-3.621900000

1	1.033900000	-1.561700000	-2.461600000
7	1.706200000	-0.206900000	-1.051900000
7	1.183300000	1.247900000	1.050400000
6	-3.321700000	0.027700000	2.765800000
6	-4.083000000	1.094700000	2.289200000
6	-3.618900000	1.808500000	1.186300000
6	-2.409600000	1.443000000	0.585300000
6	-2.129100000	-0.283900000	2.118100000
6	-1.827700000	2.133700000	-0.582400000
6	-2.392400000	3.264300000	-1.182400000
6	-1.767200000	3.843600000	-2.284600000
1	-2.194500000	4.721600000	-2.759200000
6	-0.586500000	3.274200000	-2.761400000
6	-0.077900000	2.150900000	-2.114800000
1	-3.639300000	-0.558300000	3.622200000
1	-5.020200000	1.367600000	2.764600000
1	-1.510900000	-1.104600000	2.461400000
1	-0.062400000	3.687400000	-3.617000000
1	0.835700000	1.681000000	-2.458600000
7	-0.674200000	1.582400000	-1.049700000
7	-1.670900000	0.399500000	1.052100000
6	1.640200000	-2.895400000	2.759400000
6	1.094000000	-4.087000000	2.282800000
6	0.241400000	-4.039700000	1.181800000
6	-0.046200000	-2.808600000	0.582700000
6	1.314000000	-1.705800000	2.113600000
6	-0.936700000	-2.647800000	-0.583600000
6	-1.636000000	-3.700700000	-1.183300000
6	-2.450300000	-3.447200000	-2.285100000
1	-2.998900000	-4.255200000	-2.759500000
6	-2.544800000	-2.139900000	-2.762100000
6	-1.824000000	-1.139200000	-2.115500000
1	2.308500000	-2.879300000	3.614200000
1	1.326100000	-5.036000000	2.756700000
1	1.718000000	-0.761100000	2.457100000
1	-3.164200000	-1.891300000	-3.617600000
1	-1.871800000	-0.113000000	-2.459200000
7	-1.033700000	-1.373000000	-1.050600000
7	0.490800000	-1.648300000	1.049500000
1	4.854600000	1.013700000	-0.798400000
1	4.387800000	2.312100000	0.796800000
1	-4.198200000	2.638900000	0.799500000
1	-3.308800000	3.694400000	-0.795300000
1	-1.552300000	-4.709600000	-0.796200000
1	-0.190000000	-4.955600000	0.795000000

3 [Fe(Py₂Py)₂]³⁺ Doublet

26	-0.001800000	-0.011100000	-0.012400000
7	-0.455500000	-1.381100000	-1.380500000
7	-1.924000000	0.061500000	0.048800000
7	-0.246100000	1.397900000	1.383500000

7	0.362600000	1.337700000	-1.432600000
7	1.924400000	-0.051000000	-0.036200000
7	0.338500000	-1.430700000	1.344300000
6	0.351100000	-2.234600000	-2.289900000
6	-0.663500000	-3.233700000	-2.896200000
6	-2.047900000	-2.582000000	-2.639700000
6	-1.729500000	-1.569700000	-1.581400000
6	-2.632500000	-0.744900000	-0.762700000
6	-4.032500000	-0.715000000	-0.740100000
6	-4.662300000	0.169200000	0.144400000
6	-3.901500000	1.000100000	0.981700000
6	-2.508100000	0.919700000	0.906600000
6	-1.489500000	1.673700000	1.662100000
6	-1.670600000	2.703400000	2.735200000
6	-0.232600000	3.259700000	2.902900000
6	0.671200000	2.193800000	2.238600000
6	-0.494300000	2.152700000	-2.332100000
6	0.471800000	3.176400000	-2.974800000
6	1.881200000	2.568100000	-2.752200000
6	1.624400000	1.561600000	-1.672400000
6	2.579300000	0.769000000	-0.879000000
6	3.978200000	0.770900000	-0.916700000
6	4.667100000	-0.098000000	-0.059500000
6	3.963200000	-0.946500000	0.806400000
6	2.564900000	-0.896800000	0.792100000
6	1.596600000	-1.681300000	1.577600000
6	1.836200000	-2.766000000	2.583100000
6	0.420200000	-2.978400000	3.179400000
6	-0.531800000	-2.327600000	2.147800000
1	1.156000000	-2.715100000	-1.726900000
1	0.812900000	-1.584000000	-3.043100000
1	-0.599700000	-4.198200000	-2.384800000
1	-0.478200000	-3.411200000	-3.957200000
1	-2.449800000	-2.070800000	-3.527200000
1	-2.814400000	-3.296200000	-2.319100000
1	-4.615900000	-1.359600000	-1.390600000
1	-5.747000000	0.213000000	0.183300000
1	-4.386300000	1.686900000	1.668900000
1	-2.049300000	2.217200000	3.646900000
1	-2.407200000	3.467500000	2.462700000
1	0.029600000	3.423700000	3.949700000
1	-0.135900000	4.217700000	2.384500000
1	1.470000000	2.619200000	1.625000000
1	1.132700000	1.512600000	2.964300000
1	-1.300000000	2.614200000	-1.754900000
1	-0.952000000	1.478000000	-3.066300000
1	0.393600000	4.142500000	-2.468500000
1	0.251700000	3.339400000	-4.031400000
1	2.270600000	2.055900000	-3.644800000
1	2.636900000	3.307600000	-2.464600000
1	4.518100000	1.425700000	-1.594200000
1	5.753200000	-0.117200000	-0.069100000

1	4.491600000	-1.626200000	1.468100000
1	2.588700000	-2.487300000	3.329200000
1	2.221700000	-3.660300000	2.070900000
1	0.337800000	-2.472200000	4.145200000
1	0.190700000	-4.033400000	3.339700000
1	-0.985600000	-3.057300000	1.465600000
1	-1.339700000	-1.748200000	2.602700000

3 [Fe(Py_rPy)₂]²⁺ Singlet

26	0.000000000	-0.006000000	-0.006200000
7	-0.371900000	-1.409000000	-1.397900000
7	-1.922100000	-0.011400000	-0.012300000
7	-0.387600000	1.394700000	1.381900000
7	0.380900000	1.392700000	-1.399000000
7	1.922100000	-0.004200000	-0.002800000
7	0.378600000	-1.395200000	1.396700000
6	0.474100000	-2.238400000	-2.281900000
6	-0.484800000	-3.273000000	-2.917800000
6	-1.894300000	-2.664100000	-2.703300000
6	-1.627400000	-1.640800000	-1.634300000
6	-2.578800000	-0.846700000	-0.845700000
6	-3.976200000	-0.875100000	-0.875200000
6	-4.679500000	-0.019200000	-0.020000000
6	-3.985900000	0.840700000	0.839200000
6	-2.588100000	0.820200000	0.817600000
6	-1.645400000	1.619800000	1.611300000
6	-1.923200000	2.642000000	2.678700000
6	-0.518100000	3.258800000	2.899600000
6	0.449600000	2.228900000	2.269300000
6	-0.459900000	2.225700000	-2.284200000
6	0.503700000	3.259700000	-2.914100000
6	1.911000000	2.647000000	-2.695700000
6	1.637700000	1.622600000	-1.629300000
6	2.584200000	0.826400000	-0.836800000
6	3.981800000	0.846000000	-0.866100000
6	4.679500000	-0.013800000	-0.010100000
6	3.980400000	-0.867800000	0.850500000
6	2.582800000	-0.837400000	0.829600000
6	1.635100000	-1.628300000	1.626000000
6	1.906600000	-2.697500000	2.647900000
6	0.498700000	-2.916000000	3.259100000
6	-0.463500000	-2.283000000	2.225800000
1	1.281500000	-2.691300000	-1.698800000
1	0.939100000	-1.576600000	-3.024200000
1	-0.406200000	-4.232200000	-2.397300000
1	-0.262000000	-3.452100000	-3.971700000
1	-2.283300000	-2.169700000	-3.604800000
1	-2.644100000	-3.403300000	-2.401400000
1	-4.502700000	-1.546300000	-1.546200000
1	-5.765100000	-0.022200000	-0.023000000
1	-4.519900000	1.508900000	1.507300000

1	-2.313400000	2.145700000	3.578500000
1	-2.675600000	3.376900000	2.373100000
1	-0.301500000	3.439900000	3.954400000
1	-0.442200000	4.217900000	2.378400000
1	1.257000000	2.685700000	1.689500000
1	0.914200000	1.569600000	3.014100000
1	-1.268100000	2.679100000	-1.702500000
1	-0.923800000	1.566800000	-3.029700000
1	0.425400000	4.217700000	-2.391400000
1	0.285300000	3.441800000	-3.968400000
1	2.302000000	2.153300000	-3.596700000
1	2.661400000	3.384000000	-2.389800000
1	4.512600000	1.512900000	-1.538000000
1	5.765100000	-0.018200000	-0.013700000
1	4.510000000	-1.538900000	1.519100000
1	2.657000000	-2.394500000	3.386000000
1	2.296600000	-3.597700000	2.152000000
1	0.420200000	-2.395400000	4.218300000
1	0.279100000	-3.970500000	3.438700000
1	-0.925500000	-3.026300000	1.563100000
1	-1.272900000	-1.703600000	2.679700000

4 [Fe(Pyep)₂]¹⁺ Doublet

26	0.177000000	-0.000100000	0.000100000
6	-1.709200000	1.941300000	-0.809600000
7	-1.295600000	1.326100000	0.319500000
6	-1.914000000	1.599400000	1.481600000
6	-2.975300000	2.499500000	1.554000000
6	-3.414100000	3.129000000	0.387000000
6	-2.768700000	2.844500000	-0.816200000
7	0.102100000	0.764400000	-1.793100000
6	-0.933600000	1.602500000	-2.052800000
8	-1.234100000	2.102600000	-3.143000000
7	1.574300000	-1.319300000	-0.576700000
6	1.813700000	-2.518900000	-0.057800000
7	2.769400000	-3.147100000	-0.774400000
6	3.158300000	-2.314900000	-1.805600000
6	2.408700000	-1.173000000	-1.677700000
6	2.384400000	0.058200000	-2.524700000
6	0.964900000	0.465100000	-2.938600000
1	-1.547600000	1.080500000	2.359300000
1	-3.444900000	2.693300000	2.513000000
1	-4.243600000	3.829700000	0.416400000
1	-3.053100000	3.298100000	-1.759900000
1	3.131600000	-4.073000000	-0.585300000
1	3.913100000	-2.598600000	-2.523200000
1	1.328600000	-2.941800000	0.807900000
1	0.521400000	-0.339900000	-3.546400000
1	1.009800000	1.344700000	-3.590100000
1	2.975600000	-0.120000000	-3.429600000
1	2.866300000	0.888100000	-1.992700000

7	-1.296000000	-1.325700000	-0.319800000
7	0.101300000	-0.764600000	1.793100000
7	1.574900000	1.318600000	0.576800000
6	-1.710300000	-1.940700000	0.809200000
6	-2.770000000	-2.843600000	0.815400000
6	-3.414800000	-3.128200000	-0.388000000
6	-2.975400000	-2.498900000	-1.554900000
6	-1.914000000	-1.599000000	-1.482100000
1	-3.055000000	-3.297000000	1.759000000
1	-4.244500000	-3.828700000	-0.417700000
1	-3.444600000	-2.692800000	-2.514100000
1	-1.547000000	-1.080300000	-2.359700000
6	-0.935100000	-1.601800000	2.052700000
8	-1.236400000	-2.101300000	3.142900000
6	0.963600000	-0.465200000	2.938900000
6	2.383500000	-0.058900000	2.525400000
6	2.408500000	1.172200000	1.678400000
6	3.158300000	2.314000000	1.806500000
7	2.770300000	3.146100000	0.775000000
6	1.814800000	2.518000000	0.058000000
1	3.912800000	2.597500000	2.524600000
1	1.330200000	2.941100000	-0.807900000
1	3.132800000	4.071900000	0.586100000
1	0.520100000	0.340300000	3.546100000
1	1.007900000	-1.344600000	3.590800000
1	2.974400000	0.119100000	3.430500000
1	2.865200000	-0.889000000	1.993600000

4 [Fe(Pyep)₂] Quintet

26	-0.005800000	-0.138700000	0.005100000
6	2.230200000	1.611900000	-1.037800000
7	1.488800000	1.525700000	0.082700000
6	1.679300000	2.421900000	1.061600000
6	2.617800000	3.448800000	0.967000000
6	3.391900000	3.539900000	-0.193300000
6	3.199900000	2.604300000	-1.208700000
7	0.912200000	-0.201800000	-1.902600000
6	1.995300000	0.566300000	-2.112600000
8	2.811700000	0.502600000	-3.058200000
7	-1.402600000	-1.753700000	-0.731900000
6	-2.226100000	-2.494600000	-0.014100000
7	-2.892900000	-3.375700000	-0.804700000
6	-2.464900000	-3.177700000	-2.105000000
6	-1.541700000	-2.159800000	-2.049700000
6	-0.797600000	-1.504600000	-3.176100000
6	0.692700000	-1.234600000	-2.912500000
1	1.052500000	2.303300000	1.942100000
1	2.735100000	4.154300000	1.784400000
1	4.133800000	4.327300000	-0.301600000
1	3.773500000	2.611500000	-2.129200000
1	-3.578800000	-4.050400000	-0.496000000

1	-2.848800000	-3.758200000	-2.930800000
1	-2.371600000	-2.417300000	1.053600000
1	1.168800000	-0.935000000	-3.853800000
1	1.175200000	-2.179600000	-2.607000000
1	-1.280500000	-0.549700000	-3.428800000
1	-0.887700000	-2.142300000	-4.065100000
7	-1.659900000	1.332700000	-0.250900000
7	-0.772300000	0.066200000	1.966400000
7	1.483900000	-1.602900000	0.856800000
6	-2.315800000	1.577300000	0.899600000
6	-3.413000000	2.442200000	0.954100000
6	-3.838500000	3.067800000	-0.216600000
6	-3.148700000	2.818300000	-1.406300000
6	-2.064000000	1.943000000	-1.374100000
1	-3.892900000	2.602600000	1.913300000
1	-4.689100000	3.744700000	-0.202700000
1	-3.437800000	3.291800000	-2.340100000
1	-1.486900000	1.720400000	-2.268300000
6	-1.801200000	0.911000000	2.164600000
8	-2.351200000	1.212200000	3.245300000
6	-0.216700000	-0.508600000	3.191100000
6	0.255600000	-1.964900000	3.028800000
6	1.438500000	-2.152300000	2.127400000
6	2.603800000	-2.846500000	2.353600000
7	3.354300000	-2.714900000	1.198600000
6	2.640900000	-1.955700000	0.326400000
1	2.956500000	-3.405400000	3.207700000
1	2.994000000	-1.681300000	-0.657700000
1	4.273600000	-3.100600000	1.033700000
1	0.636700000	0.097900000	3.539600000
1	-0.968800000	-0.470400000	3.988100000
1	0.509800000	-2.359500000	4.021100000
1	-0.586800000	-2.568600000	2.662100000

5 [Fe(Prpep)₂]¹⁺ Doublet

26	0.175500000	-0.084500000	0.000600000
6	-2.165400000	-1.422100000	0.855100000
7	-1.600300000	-0.974900000	-0.287300000
6	-2.302600000	-1.106000000	-1.427700000
7	-3.516200000	-1.638600000	-1.517300000
6	-4.081800000	-2.069300000	-0.379700000
6	-3.433900000	-1.987000000	0.853100000
7	-0.122900000	-0.708300000	1.813700000
6	-1.304300000	-1.321800000	2.086400000
8	-1.675100000	-1.826100000	3.149800000
7	1.829900000	0.936000000	0.578800000
6	2.639100000	1.634300000	-0.213000000
7	3.584100000	2.257000000	0.520200000
6	3.370600000	1.956000000	1.848300000

6	2.267400000	1.141100000	1.886100000
6	1.558200000	0.601000000	3.091000000
6	0.899800000	-0.759100000	2.858300000
1	-1.836300000	-0.748500000	-2.338400000
1	-5.078300000	-2.494900000	-0.468700000
1	-3.867900000	-2.344200000	1.780700000
1	4.322600000	2.842600000	0.151100000
1	3.995900000	2.345200000	2.637500000
1	2.553900000	1.721500000	-1.283100000
1	0.436200000	-1.105700000	3.786300000
1	1.676200000	-1.489200000	2.582400000
1	0.794200000	1.316900000	3.424100000
1	2.275700000	0.513800000	3.914900000
7	-0.880700000	1.614800000	0.161800000
7	0.346500000	0.521000000	-1.855300000
7	1.183500000	-1.777100000	-0.414800000
6	-1.000500000	2.280700000	-1.006500000
6	-1.712800000	3.471100000	-1.079500000
6	-2.280300000	3.937800000	0.105900000
7	-2.158600000	3.278200000	1.268300000
6	-1.469300000	2.143200000	1.249700000
1	-1.804600000	3.986900000	-2.029200000
1	-2.850100000	4.863300000	0.135300000
1	-1.368700000	1.592100000	2.177900000
6	-0.332500000	1.645900000	-2.196600000
8	-0.425200000	2.164600000	-3.313200000
6	1.012500000	-0.161300000	-2.970400000
6	2.258400000	-0.948500000	-2.549900000
6	1.975400000	-2.007900000	-1.534500000
6	2.392800000	-3.314000000	-1.508700000
7	1.850500000	-3.868200000	-0.368000000
6	1.127900000	-2.920800000	0.263100000
1	3.012500000	-3.879200000	-2.188300000
1	0.586600000	-3.093700000	1.179400000
1	1.966700000	-4.823400000	-0.053600000
1	0.305100000	-0.849100000	-3.460400000
1	1.285400000	0.581600000	-3.727300000
1	2.684100000	-1.420400000	-3.442300000
1	3.028400000	-0.265500000	-2.170700000

5 [Fe(Prpep)₂] Singlet

26	-0.003400000	-0.136700000	0.005700000
6	2.252000000	1.594500000	-1.040000000
7	1.524100000	1.514400000	0.090000000
6	1.775800000	2.408000000	1.056100000
7	2.685100000	3.382500000	1.008100000
6	3.407300000	3.457300000	-0.121900000
6	3.233400000	2.575000000	-1.184900000
7	0.894700000	-0.177900000	-1.914300000
6	1.989700000	0.569500000	-2.127500000
8	2.799200000	0.509600000	-3.077200000

7	-1.421600000	-1.721800000	-0.729000000
6	-2.234600000	-2.475700000	-0.011500000
7	-2.922500000	-3.333200000	-0.808800000
6	-2.520800000	-3.107000000	-2.112500000
6	-1.590300000	-2.096400000	-2.053200000
6	-0.864000000	-1.422500000	-3.179900000
6	0.635800000	-1.182200000	-2.945200000
1	1.178500000	2.323600000	1.960300000
1	4.148700000	4.252900000	-0.165400000
1	3.819500000	2.620000000	-2.095900000
1	-3.607000000	-4.010400000	-0.502100000
1	-2.926000000	-3.664600000	-2.943700000
1	-2.357100000	-2.425200000	1.060600000
1	1.095200000	-0.865000000	-3.888700000
1	1.112400000	-2.140000000	-2.673900000
1	-1.338600000	-0.455500000	-3.398800000
1	-0.983400000	-2.036100000	-4.082000000
7	-1.654300000	1.361400000	-0.235400000
7	-0.748300000	0.087100000	1.973700000
7	1.468400000	-1.619300000	0.834900000
6	-2.301200000	1.590900000	0.923500000
6	-3.398200000	2.451700000	0.964200000
6	-3.782900000	3.045900000	-0.234700000
7	-3.137600000	2.826000000	-1.392100000
6	-2.099000000	1.992100000	-1.330300000
1	-3.902700000	2.633400000	1.906300000
1	-4.631400000	3.725800000	-0.280200000
1	-1.553300000	1.803600000	-2.251200000
6	-1.783500000	0.919100000	2.184100000
8	-2.342100000	1.209900000	3.261200000
6	-0.179500000	-0.492700000	3.191400000
6	0.265000000	-1.957000000	3.027000000
6	1.428800000	-2.168800000	2.106100000
6	2.580100000	-2.891200000	2.313700000
7	3.315500000	-2.777400000	1.147800000
6	2.608700000	-2.000600000	0.286800000
1	2.932000000	-3.458700000	3.162400000
1	2.953500000	-1.736200000	-0.702900000
1	4.222800000	-3.185200000	0.969200000
1	0.689400000	0.102700000	3.517700000
1	-0.916100000	-0.437700000	4.001200000
1	0.530000000	-2.351000000	4.016400000
1	-0.594200000	-2.548300000	2.679400000

6 [Fe(PyepO)₂]¹⁻ Sextet

26	0.000000000	0.000000000	0.520900000
7	0.000000000	2.080600000	0.196400000
7	1.535500000	0.379400000	-1.103200000
8	-1.406600000	0.545400000	1.744800000
6	-1.712900000	1.835200000	1.787300000
6	2.306800000	-0.540600000	-1.696300000

6	3.300300000	-0.198800000	-2.614400000
6	3.490900000	1.152200000	-2.917800000
6	2.689800000	2.107800000	-2.296400000
6	1.718000000	1.683000000	-1.384300000
1	2.116800000	-1.572900000	-1.416700000
1	3.905800000	-0.975900000	-3.071600000
1	4.257200000	1.454300000	-3.628500000
1	2.786500000	3.171300000	-2.485600000
6	-2.734800000	2.339300000	2.610700000
6	-3.016900000	3.708700000	2.626200000
6	-2.286500000	4.592200000	1.822400000
6	-1.263700000	4.113100000	0.992200000
6	-0.967500000	2.740700000	0.964300000
1	-3.288100000	1.638900000	3.231600000
1	-3.808800000	4.086500000	3.271300000
1	-2.506100000	5.657900000	1.840400000
1	-0.687000000	4.785200000	0.368600000
6	0.823100000	2.681100000	-0.679400000
8	0.928900000	3.890400000	-0.972500000
7	0.000000000	-2.080600000	0.196400000
7	-1.535500000	-0.379400000	-1.103200000
8	1.406600000	-0.545400000	1.744800000
6	1.712900000	-1.835200000	1.787300000
6	2.734800000	-2.339300000	2.610700000
6	3.016900000	-3.708700000	2.626200000
6	2.286500000	-4.592200000	1.822400000
6	1.263700000	-4.113100000	0.992200000
6	0.967500000	-2.740700000	0.964300000
1	3.288100000	-1.638900000	3.231600000
1	3.808800000	-4.086500000	3.271300000
1	2.506100000	-5.657900000	1.840400000
1	0.687000000	-4.785200000	0.368600000
6	-2.306800000	0.540600000	-1.696300000
6	-3.300300000	0.198800000	-2.614400000
6	-3.490900000	-1.152200000	-2.917800000
6	-2.689800000	-2.107800000	-2.296400000
6	-1.718000000	-1.683000000	-1.384300000
1	-2.116800000	1.572900000	-1.416700000
1	-3.905800000	0.975900000	-3.071600000
1	-4.257200000	-1.454300000	-3.628500000
1	-2.786500000	-3.171300000	-2.485600000
6	-0.823100000	-2.681100000	-0.679400000
8	-0.928900000	-3.890400000	-0.972500000

6 [Fe(PyepO)₂]²⁻ Quintet

26	0.000000000	0.000000000	0.533200000
7	0.000000000	2.164000000	0.154400000
7	1.544600000	0.394700000	-1.065700000
8	-1.450400000	0.719900000	1.823600000
6	-1.663200000	2.005800000	1.832100000
6	2.339100000	-0.531000000	-1.621800000
6	3.323600000	-0.217900000	-2.560900000
6	3.482100000	1.120200000	-2.939000000
6	2.659700000	2.084700000	-2.358700000

6	1.700800000	1.689700000	-1.415500000
1	2.169500000	-1.553100000	-1.293200000
1	3.944400000	-1.006900000	-2.979000000
1	4.237100000	1.403900000	-3.671300000
1	2.729000000	3.140600000	-2.598800000
6	-2.621000000	2.613400000	2.684300000
6	-2.838700000	3.995100000	2.669700000
6	-2.109400000	4.821000000	1.804300000
6	-1.150600000	4.254700000	0.945900000
6	-0.912500000	2.869800000	0.942500000
1	-3.181300000	1.962700000	3.354300000
1	-3.583800000	4.428700000	3.339900000
1	-2.278000000	5.898000000	1.792300000
1	-0.571900000	4.874000000	0.270100000
6	0.813900000	2.718600000	-0.746300000
8	0.943300000	3.924700000	-1.097000000
7	0.000000000	-2.164000000	0.154400000
7	-1.544600000	-0.394700000	-1.065700000
8	1.450400000	-0.719900000	1.823600000
6	1.663200000	-2.005800000	1.832100000
6	2.621000000	-2.613400000	2.684300000
6	2.838700000	-3.995100000	2.669700000
6	2.109400000	-4.821000000	1.804300000
6	1.150600000	-4.254700000	0.945900000
6	0.912500000	-2.869800000	0.942500000
1	3.181300000	-1.962700000	3.354300000
1	3.583800000	-4.428700000	3.339900000
1	2.278000000	-5.898000000	1.792300000
1	0.571900000	-4.874000000	0.270100000
6	-2.339100000	0.531000000	-1.621800000
6	-3.323600000	0.217900000	-2.560900000
6	-3.482100000	-1.120200000	-2.939000000
6	-2.659700000	-2.084700000	-2.358700000
6	-1.700800000	-1.689700000	-1.415500000
1	-2.169500000	1.553100000	-1.293200000
1	-3.944400000	1.006900000	-2.979000000
1	-4.237100000	-1.403900000	-3.671300000
1	-2.729000000	-3.140600000	-2.598800000
6	-0.813900000	-2.718600000	-0.746300000
8	-0.943300000	-3.924700000	-1.097000000

7 [Fe(PyIm₂H₂)₂]¹⁻ Doublet

26	0.000000000	0.000200000	0.000100000
7	-1.763100000	-2.553000000	-2.555100000
7	-0.316800000	-1.380700000	-1.382200000
7	-1.949400000	-0.000100000	-0.000200000
7	-0.317800000	1.380800000	1.382300000
7	-1.764700000	2.552600000	2.554900000
7	0.317200000	-1.382300000	1.380700000
7	1.763700000	-2.555600000	2.552300000
7	1.949400000	0.000200000	0.000200000

7	0.317400000	1.382500000	-1.380500000
7	1.764100000	2.555600000	-2.552200000
6	-1.630200000	-1.602900000	-1.604400000
6	0.386700000	-2.214600000	-2.217000000
6	-0.508000000	-2.952700000	-2.955500000
6	-2.602500000	-0.835700000	-0.836500000
6	-2.603100000	0.835300000	0.835700000
6	-4.000600000	0.860500000	0.860800000
6	-4.691200000	-0.000500000	-0.000800000
6	-4.000000000	-0.861300000	-0.862100000
6	-1.631300000	1.602700000	1.604000000
6	-0.509800000	2.952400000	2.955900000
6	0.385300000	2.214700000	2.217400000
6	1.630600000	-1.604500000	1.602500000
6	0.508700000	-2.955900000	2.952300000
6	-0.386100000	-2.217200000	2.214600000
6	2.602700000	-0.836300000	0.835400000
6	2.602900000	0.836700000	-0.834800000
6	4.000400000	0.862200000	-0.860000000
6	4.691200000	0.000300000	0.000600000
6	4.000200000	-0.861700000	0.860900000
6	1.630900000	1.604800000	-1.602200000
6	-0.385800000	2.217100000	-2.214800000
6	0.509100000	2.955700000	-2.952500000
1	-4.545500000	1.524100000	1.524800000
1	-5.777400000	-0.000700000	-0.001000000
1	-4.544400000	-1.525100000	-1.526400000
1	1.464400000	2.242200000	2.245200000
1	-0.361100000	3.709000000	3.713500000
1	1.465800000	-2.241800000	-2.244500000
1	-0.358900000	-3.709500000	-3.712800000
1	4.545100000	1.526700000	-1.523200000
1	5.777400000	0.000300000	0.000700000
1	4.544800000	-1.526100000	1.524300000
1	-1.464900000	2.244500000	-2.242500000
1	0.360200000	3.713100000	-3.709400000
1	-1.465200000	-2.244600000	2.242200000
1	0.359800000	-3.713500000	3.708900000
1	-2.633200000	-2.923700000	-2.925900000
1	-2.635100000	2.923000000	2.925500000
1	2.634000000	-2.926400000	2.922700000
1	2.634300000	2.926500000	-2.922500000

7 [Fe(PyIm₂H₂)₂]²⁻ Quintet

26	0.000000000	0.001700000	0.000500000
7	2.236100000	2.589800000	-2.556700000
7	0.608600000	1.548600000	-1.488400000
7	2.179100000	0.000300000	0.002400000
7	0.604300000	-1.545300000	1.491300000
7	2.228800000	-2.588700000	2.562000000
7	-0.610300000	1.556600000	1.481000000

7	-2.239600000	2.601800000	2.542600000
7	-2.178700000	-0.001300000	-0.002600000
7	-0.602200000	-1.554600000	-1.482500000
7	-2.226000000	-2.604300000	-2.548300000
6	1.935100000	1.656400000	-1.614600000
6	0.055800000	2.437000000	-2.376200000
6	1.056600000	3.095500000	-3.052100000
6	2.844900000	0.837900000	-0.813700000
6	2.842600000	-0.838100000	0.819500000
6	4.241600000	-0.870300000	0.847500000
6	4.938500000	-0.001400000	0.004500000
6	4.244100000	0.868300000	-0.839500000
6	1.930500000	-1.655200000	1.619300000
6	1.047800000	-3.092500000	3.056000000
6	0.049000000	-2.432600000	2.378600000
6	-1.937000000	1.663900000	1.605600000
6	-1.060900000	3.111200000	3.036300000
6	-0.059100000	2.450100000	2.364500000
6	-2.845700000	0.840300000	0.808500000
6	-2.841200000	-0.844600000	-0.815600000
6	-4.240200000	-0.877800000	-0.844200000
6	-4.938200000	-0.004800000	-0.006500000
6	-4.244800000	0.870000000	0.833300000
6	-1.928300000	-1.665600000	-1.610400000
6	-0.046400000	-2.446700000	-2.364700000
6	-1.044700000	-3.110500000	-3.039000000
1	4.782500000	-1.547200000	1.501100000
1	6.024300000	-0.002100000	0.005300000
1	4.786800000	1.544600000	-1.492300000
1	-1.020100000	-2.549300000	2.480600000
1	1.022100000	-3.853600000	3.821800000
1	-1.013000000	2.555300000	-2.479700000
1	1.033000000	3.856800000	-3.817700000
1	-4.780200000	-1.558600000	-1.494500000
1	-6.024000000	-0.006200000	-0.008000000
1	-4.788400000	1.549500000	1.481900000
1	1.022800000	-2.563600000	-2.465700000
1	-1.018400000	-3.875700000	-3.800600000
1	1.009600000	2.570000000	2.468100000
1	-1.038600000	3.876600000	3.797900000
1	3.161000000	2.873800000	-2.856400000
1	3.152900000	-2.873900000	2.863200000
1	-3.165000000	2.886400000	2.840300000
1	-3.149900000	-2.891400000	-2.848300000

8 [Fe(sar)]³⁺ Doublet

26	0.000000000	0.000000000	0.000000000
7	1.162400000	1.515600000	0.755600000
7	1.162400000	-1.411900000	0.934500000
7	-1.162300000	-0.103600000	1.689800000
7	-1.162400000	1.515600000	-0.755700000

7	-1.162400000	-1.412000000	-0.934300000
7	1.162300000	-0.103700000	-1.689800000
6	0.755000000	2.790100000	0.066000000
6	2.665700000	1.287200000	0.728200000
6	3.076600000	0.000400000	0.000000000
6	2.665700000	-1.273700000	0.750300000
6	0.754800000	-1.452800000	2.382900000
6	-0.755300000	-1.338200000	2.448700000
6	-2.665600000	-0.012500000	1.478400000
6	-3.076600000	0.000400000	0.000000000
6	-2.665700000	1.287200000	-0.728300000
6	-2.665700000	-1.273800000	-0.750300000
6	-0.755000000	2.790100000	-0.066200000
6	2.665600000	-0.012700000	-1.478400000
6	0.755300000	-1.338400000	-2.448600000
6	-0.754800000	-1.453000000	-2.382800000
1	-4.175800000	0.000400000	0.000000000
1	4.175800000	0.000400000	0.000000000
1	3.026900000	1.264600000	1.760600000
1	3.132800000	2.152500000	0.248800000
1	3.027000000	-2.156400000	0.214500000
1	3.132800000	-1.291200000	1.739500000
1	3.026500000	0.892800000	-1.975300000
1	3.132900000	-0.860500000	-1.988000000
1	-3.026900000	1.264400000	-1.760700000
1	-3.132800000	2.152500000	-0.249000000
1	-3.026500000	0.892900000	1.975200000
1	-3.132900000	-0.860300000	1.988100000
1	-3.132800000	-1.291400000	-1.739400000
1	-3.027000000	-2.156400000	-0.214300000
1	-1.109600000	-2.375400000	-2.856300000
1	-1.239100000	-0.616800000	-2.898100000
1	1.110500000	-1.288200000	-3.484100000
1	1.239600000	-2.202200000	-1.980900000
1	-1.110100000	3.661700000	-0.627600000
1	-1.239300000	2.817300000	0.915700000
1	1.110100000	3.661800000	0.627300000
1	1.239300000	2.817200000	-0.915900000
1	-1.110500000	-1.287900000	3.484200000
1	-1.239600000	-2.202100000	1.981100000
1	1.109600000	-2.375200000	2.856500000
1	1.239100000	-0.616600000	2.898200000
1	-0.920200000	1.645400000	-1.740500000
1	0.919600000	0.684000000	-2.294800000
1	0.920200000	1.645600000	1.740300000
1	-0.919600000	0.684200000	2.294700000
1	0.920200000	-2.329500000	0.554200000
1	-0.920200000	-2.329600000	-0.554100000

8 [Fe(sar)]²⁺ Singlet

26	0.000200000	0.000100000	0.000000000
----	-------------	-------------	-------------

7	1.184000000	1.693700000	0.172300000
7	1.184300000	-0.996200000	1.380400000
7	-1.183700000	0.479900000	1.632900000
7	-1.183900000	1.174300000	-1.232100000
7	-1.184000000	-1.654400000	-0.400700000
7	1.184100000	-0.697700000	-1.553000000
6	0.757400000	2.629500000	-0.913100000
6	2.674600000	1.468000000	0.200600000
6	3.080700000	0.000200000	-0.000200000
6	2.674900000	-0.907600000	1.170800000
6	0.757800000	-0.523900000	2.733400000
6	-0.758200000	-0.416600000	2.751200000
6	-2.674300000	0.467800000	1.405800000
6	-3.080800000	0.000100000	0.000100000
6	-2.674600000	0.983400000	-1.108000000
6	-2.674700000	-1.451300000	-0.297700000
6	-0.758500000	2.591100000	-1.014800000
6	2.674800000	-0.560200000	-1.371700000
6	0.757600000	-2.105700000	-1.820000000
6	-0.758400000	-2.174700000	-1.736200000
1	-4.180600000	0.000200000	0.000300000
1	4.180500000	0.000300000	-0.000200000
1	3.065700000	1.824700000	1.159200000
1	3.142400000	2.086300000	-0.573100000
1	3.066100000	-1.916100000	1.000400000
1	3.142700000	-0.546600000	2.093100000
1	3.065700000	0.091600000	-2.160000000
1	3.142800000	-1.539400000	-1.520200000
1	-3.064300000	0.629200000	-2.068100000
1	-3.143400000	1.956200000	-0.924400000
1	-3.064200000	1.476300000	1.579400000
1	-3.143100000	-0.177900000	2.156200000
1	-3.143600000	-1.778300000	-1.232000000
1	-3.064800000	-2.105800000	0.489000000
1	-1.117400000	-3.197500000	-1.904100000
1	-1.213300000	-1.542400000	-2.507000000
1	1.116000000	-2.458200000	-2.795000000
1	1.212600000	-2.748100000	-1.057700000
1	-1.117700000	3.247800000	-1.816800000
1	-1.213700000	2.942300000	-0.082000000
1	1.115500000	3.650100000	-0.730000000
1	1.212500000	2.291300000	-1.850800000
1	-1.117100000	-0.050500000	3.721000000
1	-1.213200000	-1.400200000	2.589100000
1	1.116100000	-1.192400000	3.525900000
1	1.212800000	0.457400000	2.908800000
1	-0.952300000	0.966400000	-2.205200000
1	0.953600000	-0.177600000	-2.401600000
1	0.953300000	2.168000000	1.047300000
1	-0.952200000	1.426500000	1.939500000
1	0.953600000	-1.991000000	1.353600000
1	-0.952600000	-2.393200000	0.266000000

9 [Fe(diammac)]³⁺ Doublet

26	0.000000000	0.000000000	0.054000000
6	-1.607300000	-3.915800000	-0.071300000
6	-0.711800000	-2.673700000	-0.058700000
6	0.235700000	-2.666000000	1.168600000
7	0.614900000	-1.243700000	1.529800000
6	0.000000000	-0.759700000	2.823400000
6	0.000000000	0.759700000	2.823400000
7	-0.614900000	1.243700000	1.529800000
6	-0.235700000	2.666000000	1.168600000
6	0.711800000	2.673700000	-0.058700000
6	1.607300000	3.915800000	-0.071300000
7	1.497200000	1.377000000	0.052500000
7	0.737300000	-1.171200000	-1.422300000
6	0.635400000	-0.419800000	-2.730000000
6	-0.635400000	0.419800000	-2.730000000
7	-0.737300000	1.171200000	-1.422300000
6	-0.040300000	2.511700000	-1.391000000
7	-1.497200000	-1.377000000	0.052500000
6	0.040300000	-2.511700000	-1.391000000
1	1.733400000	-1.346000000	-1.263600000
1	1.631000000	-1.210300000	1.652700000
1	-1.631000000	1.210300000	1.652700000
1	-1.733400000	1.346000000	-1.263600000
1	-2.089700000	-1.403200000	0.888900000
1	-2.166000000	-1.327500000	-0.723500000
1	2.089700000	1.403200000	0.888900000
1	2.166000000	1.327500000	-0.723500000
1	-0.671000000	-2.552000000	-2.222100000
1	0.763000000	-3.318200000	-1.546000000
1	-0.250600000	-3.131400000	2.031200000
1	1.139900000	-3.246300000	0.964300000
1	-1.019800000	-1.151600000	2.883400000
1	0.547900000	-1.159500000	3.683900000
1	1.019800000	1.151600000	2.883400000
1	-0.547900000	1.159500000	3.683900000
1	-1.139900000	3.246300000	0.964300000
1	0.250600000	3.131400000	2.031200000
1	0.671000000	2.552000000	-2.222100000
1	-0.763000000	3.318200000	-1.546000000
1	-0.650300000	1.113500000	-3.577700000
1	-1.527000000	-0.208900000	-2.820200000
1	0.650300000	-1.113500000	-3.577700000
1	1.527000000	0.208900000	-2.820200000
1	-2.218800000	-3.976400000	0.835800000
1	-0.998900000	-4.826300000	-0.116500000
1	-2.275000000	-3.924200000	-0.939800000
1	0.998900000	4.826300000	-0.116500000
1	2.218800000	3.976400000	0.835800000
1	2.275000000	3.924200000	-0.939800000

9 [Fe(diammac)]²⁺ Singlet

26	0.000000000	0.000000000	0.055600000
6	0.495200000	4.208300000	-0.068600000
6	0.000000000	2.758200000	-0.055200000
6	-0.923600000	2.504000000	1.168700000
7	-0.939800000	1.047000000	1.541300000
6	-0.198800000	0.735700000	2.808300000
6	0.198800000	-0.735700000	2.808300000
7	0.939800000	-1.047000000	1.541300000
6	0.923600000	-2.504000000	1.168700000
6	0.000000000	-2.758200000	-0.055200000
6	-0.495200000	-4.208300000	-0.068600000
7	-1.108400000	-1.747700000	0.059600000
7	-1.028900000	0.948600000	-1.434400000
6	-0.721600000	0.250800000	-2.724900000
6	0.721600000	-0.250800000	-2.724900000
7	1.028900000	-0.948600000	-1.434400000
6	0.681600000	-2.406600000	-1.393300000
7	1.108400000	1.747700000	0.059600000
6	-0.681600000	2.406600000	-1.393300000
1	-2.035700000	0.870100000	-1.290500000
1	-1.912000000	0.770600000	1.685200000
1	1.912000000	-0.770600000	1.685200000
1	2.035700000	-0.870100000	-1.290500000
1	1.664500000	1.942600000	0.896600000
1	1.765200000	1.891000000	-0.712500000
1	-1.664500000	-1.942600000	0.896600000
1	-1.765200000	-1.891000000	-0.712500000
1	0.010300000	2.627800000	-2.213900000
1	-1.571300000	3.024200000	-1.554200000
1	-0.584800000	3.099400000	2.023700000
1	-1.941800000	2.834900000	0.942800000
1	0.694700000	1.367300000	2.845400000
1	-0.796800000	0.979600000	3.694700000
1	-0.694700000	-1.367300000	2.845400000
1	0.796800000	-0.979600000	3.694700000
1	1.941800000	-2.834900000	0.942800000
1	0.584800000	-3.099400000	2.023700000
1	-0.010300000	-2.627800000	-2.213900000
1	1.571300000	-3.024200000	-1.554200000
1	0.899800000	-0.899800000	-3.590900000
1	1.417800000	0.590000000	-2.812100000
1	-0.899800000	0.899800000	-3.590900000
1	-1.417800000	-0.590000000	-2.812100000
1	1.067000000	4.438700000	0.837400000
1	-0.345300000	4.910000000	-0.114300000
1	1.136400000	4.404500000	-0.935400000
1	0.345300000	-4.910000000	-0.114300000
1	-1.067000000	-4.438700000	0.837400000
1	-1.136400000	-4.404500000	-0.935400000

10 [Fe(tacn)₂]³⁺ Doublet

26	0.000000000	0.076800000	0.000000000
7	1.354600000	0.042300000	1.534000000
7	1.337000000	-1.290700000	-0.746700000
7	1.251000000	1.434700000	-0.845600000
7	-1.337000000	-1.290600000	0.746900000
7	-1.354600000	0.042000000	-1.534000000
7	-1.251000000	1.434900000	0.845300000
6	1.847600000	-1.374400000	1.725900000
6	1.826800000	-2.159700000	0.388000000
6	2.473000000	-0.620200000	-1.496100000
6	2.042600000	0.768500000	-1.940300000
6	2.062100000	2.070100000	0.257000000
6	2.489800000	1.020100000	1.273900000
6	-1.847600000	-1.374700000	-1.725700000
6	-1.826800000	-2.159700000	-0.387600000
6	-2.473000000	-0.619900000	1.496200000
6	-2.042600000	0.768900000	1.940200000
6	-2.062100000	2.070100000	-0.257300000
6	-2.489800000	1.019800000	-1.274000000
1	1.392100000	0.714900000	-2.819600000
1	2.907100000	1.380800000	-2.221300000
1	2.933400000	2.590200000	-0.157100000
1	1.430400000	2.834400000	0.721400000
1	3.352200000	0.453600000	0.923900000
1	2.788700000	1.493300000	2.214600000
1	2.848000000	-1.349300000	2.167800000
1	1.201600000	-1.858200000	2.463600000
1	2.813800000	-2.560300000	0.139100000
1	1.158100000	-3.020700000	0.466100000
1	3.341400000	-0.580000000	-0.838900000
1	2.762600000	-1.231600000	-2.356700000
1	-2.813900000	-2.560200000	-0.138700000
1	-1.158200000	-3.020800000	-0.465500000
1	-3.341500000	-0.579700000	0.839000000
1	-2.762600000	-1.231100000	2.356900000
1	-2.907000000	1.381200000	2.221100000
1	-1.392000000	0.715400000	2.819500000
1	-2.933400000	2.590200000	0.156700000
1	-1.430400000	2.834300000	-0.721900000
1	-3.352200000	0.453400000	-0.923800000
1	-2.788800000	1.492900000	-2.214800000
1	-2.847900000	-1.349700000	-2.167700000
1	-1.201500000	-1.858600000	-2.463300000
1	0.922000000	0.318900000	2.417900000
1	0.745900000	2.203200000	-1.294300000
1	0.882500000	-1.918200000	-1.412700000
1	-0.745900000	2.203400000	1.293900000
1	-0.882500000	-1.918000000	1.413000000
1	-0.922000000	0.318500000	-2.417900000

10 [Fe(tacn)₂]²⁺ Singlet

26	0.000000000	0.000000000	0.000000000
7	0.786900000	1.375300000	1.341800000
7	-1.584400000	-0.006200000	1.341800000
7	0.797600000	-1.369100000	1.341800000
7	-0.786900000	1.375300000	-1.341800000
7	-0.797600000	-1.369100000	-1.341800000
7	1.584400000	-0.006200000	-1.341800000
6	-0.231300000	1.779800000	2.376900000
6	-1.635500000	1.361000000	1.942600000
6	-1.425700000	-1.090200000	2.376900000
6	-0.360900000	-2.096900000	1.942600000
6	1.657000000	-0.689600000	2.376900000
6	1.996500000	0.735900000	1.942600000
6	-1.657000000	-0.689600000	-2.376900000
6	-1.996500000	0.735900000	-1.942600000
6	0.231300000	1.779800000	-2.376900000
6	1.635500000	1.361000000	-1.942600000
6	1.425700000	-1.090200000	-2.376900000
6	0.360900000	-2.096900000	-1.942600000
1	-0.753400000	-2.774400000	1.177600000
1	-0.054500000	-2.718200000	2.794000000
1	1.117800000	-0.682400000	3.327300000
1	2.574400000	-1.260600000	2.550700000
1	2.381300000	1.311900000	2.794000000
1	2.779400000	0.734700000	1.177600000
1	0.032000000	1.309200000	3.327300000
1	-0.195400000	2.859800000	2.550700000
1	-2.326800000	1.406300000	2.794000000
1	-2.026000000	2.039600000	1.177600000
1	-1.149900000	-0.626900000	3.327300000
1	-2.378900000	-1.599200000	2.550700000
1	-2.381300000	1.311900000	-2.794000000
1	-2.779400000	0.734700000	-1.177600000
1	-0.032000000	1.309200000	-3.327300000
1	0.195400000	2.859800000	-2.550700000
1	2.326800000	1.406300000	-2.794000000
1	2.026000000	2.039600000	-1.177600000
1	1.149900000	-0.626900000	-3.327300000
1	2.378900000	-1.599200000	-2.550700000
1	0.054500000	-2.718200000	-2.794000000
1	0.753400000	-2.774400000	-1.177600000
1	-1.117800000	-0.682400000	-3.327300000
1	-2.574400000	-1.260600000	-2.550700000
1	1.102600000	2.228500000	0.880500000
1	1.378600000	-2.069200000	0.880500000
1	-2.481300000	-0.159300000	0.880500000
1	2.481300000	-0.159300000	-0.880500000
1	-1.102600000	2.228500000	-0.880500000
1	-1.378600000	-2.069200000	-0.880500000

11 [Fe(EDTA)(H₂O)]¹⁻ Sextet

7	-1.472900000	-0.143200000	1.102300000
6	-0.727700000	0.140200000	2.340300000
1	-0.642300000	1.225800000	2.443300000
1	-1.272200000	-0.228900000	3.226500000
6	0.668000000	-0.487500000	2.306100000
1	1.191000000	-0.257600000	3.250800000
1	0.592500000	-1.575800000	2.235800000
7	1.428200000	-0.002900000	1.144400000
6	-2.532100000	0.836700000	0.802800000
1	-3.453000000	0.640600000	1.369900000
1	-2.172400000	1.836500000	1.063000000
6	-2.844700000	0.854300000	-0.706900000
6	-1.967200000	-1.533400000	1.037400000
1	-2.873000000	-1.554000000	0.422600000
1	-2.237900000	-1.911600000	2.032900000
6	-0.972600000	-2.504600000	0.372600000
6	1.860200000	1.403800000	1.285600000
1	2.846100000	1.521700000	0.824400000
1	1.967000000	1.683500000	2.342300000
6	0.933900000	2.420000000	0.588300000
6	2.537600000	-0.882600000	0.736200000
1	3.421200000	-0.766100000	1.379600000
1	2.199500000	-1.922000000	0.788000000
6	2.918500000	-0.596100000	-0.730600000
8	0.135100000	1.925200000	-0.305500000
8	1.022700000	3.606600000	0.900800000
8	1.949100000	-0.107400000	-1.441900000
8	4.056200000	-0.845700000	-1.124800000
8	-0.124800000	-1.946400000	-0.438000000
8	-1.052400000	-3.706300000	0.618700000
8	-1.891600000	0.399600000	-1.460400000
8	-3.926600000	1.294800000	-1.091500000
26	0.001700000	-0.006000000	-0.768400000
8	-0.006400000	-0.138400000	-3.013000000
1	-0.703000000	0.500500000	-3.245100000
1	0.871800000	0.222600000	-3.227500000

11 [Fe(EDTA)(H₂O)]²⁻ Quintet

7	-1.484700000	0.028100000	1.129200000
6	-0.678500000	0.361200000	2.311300000
1	-0.511900000	1.441700000	2.318400000
1	-1.211400000	0.102200000	3.247100000
6	0.680100000	-0.370500000	2.309500000
1	1.213600000	-0.115200000	3.245900000
1	0.513500000	-1.451000000	2.312400000
7	1.485600000	-0.032800000	1.128200000
6	-2.440900000	1.060900000	0.693700000
1	-3.391300000	1.014900000	1.248900000

1	-1.986400000	2.044100000	0.852500000
6	-2.734200000	0.958000000	-0.831300000
6	-2.099700000	-1.312100000	1.207300000
1	-3.007400000	-1.305900000	0.593600000
1	-2.405600000	-1.545600000	2.239600000
6	-1.219200000	-2.469200000	0.656100000
6	2.100600000	1.307200000	1.211100000
1	3.007900000	1.303400000	0.597000000
1	2.406900000	1.536600000	2.244200000
6	1.219700000	2.466400000	0.665000000
6	2.441500000	-1.063800000	0.688000000
1	3.392200000	-1.020000000	1.242800000
1	1.987000000	-2.047600000	0.843000000
6	2.734000000	-0.954800000	-0.836700000
8	0.378100000	2.145000000	-0.233700000
8	1.446900000	3.602800000	1.133800000
8	1.786900000	-0.439200000	-1.541200000
8	3.820500000	-1.387200000	-1.249700000
8	-0.378300000	-2.144100000	-0.242000000
8	-1.445900000	-3.607400000	1.120500000
8	-1.787500000	0.445100000	-1.538100000
8	-3.820800000	1.392200000	-1.242000000
26	0.000000000	0.000800000	-0.617300000
8	-0.003400000	0.010300000	-4.004400000
1	-0.745400000	0.210800000	-3.402000000
1	0.740200000	-0.193800000	-3.405200000

12 [Fe(PaPy₂O)(Cl)] Sextet

26	-0.231000000	0.114100000	-0.558900000
17	-1.437000000	0.720200000	-2.510600000
8	1.786300000	-1.581300000	2.753400000
8	1.422700000	-0.335800000	-1.281300000
7	-1.513300000	-1.684400000	-0.500200000
7	-2.040500000	0.764800000	0.734500000
7	0.404700000	-0.489700000	1.282900000
7	0.055200000	2.267700000	-0.165000000
6	-1.100800000	-2.899600000	-0.889600000
1	-0.104800000	-2.947500000	-1.320400000
6	-1.895500000	-4.034500000	-0.751300000
1	-1.526400000	-4.999700000	-1.082900000
6	-3.157700000	-3.895100000	-0.171200000
1	-3.802900000	-4.758800000	-0.035800000
6	-3.578300000	-2.631000000	0.241100000
1	-4.551900000	-2.488800000	0.702000000
6	-2.728400000	-1.538200000	0.053500000
6	-3.164600000	-0.120800000	0.374100000
1	-3.619700000	0.281900000	-0.537500000
1	-3.934400000	-0.131300000	1.161400000
6	-1.587900000	0.611500000	2.145200000
1	-2.458800000	0.512200000	2.813000000
1	-1.067100000	1.534200000	2.416200000

6	-0.617700000	-0.552800000	2.322100000
1	-0.164500000	-0.494900000	3.318200000
1	-1.149800000	-1.517400000	2.291900000
6	1.593900000	-1.070800000	1.633500000
6	2.714300000	-1.078600000	0.627700000
6	3.975700000	-1.493800000	1.087600000
1	4.053100000	-1.771000000	2.134200000
6	5.083600000	-1.555200000	0.246200000
1	6.047000000	-1.874800000	0.634500000
6	4.941300000	-1.207500000	-1.104700000
1	5.795400000	-1.256500000	-1.776800000
6	3.704000000	-0.803200000	-1.592300000
1	3.564000000	-0.538600000	-2.637000000
6	2.579000000	-0.728600000	-0.741000000
6	-2.306600000	2.179200000	0.406800000
1	-2.962100000	2.654200000	1.153800000
1	-2.811100000	2.210500000	-0.564600000
6	-1.012600000	2.958000000	0.273200000
6	-0.936000000	4.327300000	0.532900000
1	-1.809700000	4.860400000	0.897400000
6	0.271400000	4.991900000	0.314600000
1	0.352500000	6.058300000	0.507200000
6	1.371100000	4.267600000	-0.147100000
1	2.329600000	4.743600000	-0.327300000
6	1.219400000	2.900900000	-0.370400000
1	2.038600000	2.283000000	-0.725200000

12 [Fe(PaPy₂O)(Cl)]¹⁻ Quintet

26	-0.255800000	0.110200000	-0.596300000
17	-1.918100000	0.495300000	-2.554500000
8	2.180500000	-1.363700000	2.683500000
8	1.532600000	0.062800000	-1.332400000
7	-1.135300000	-1.936300000	-0.573200000
7	-2.135500000	0.292700000	0.816100000
7	0.597200000	-0.425300000	1.297700000
7	-0.494600000	2.258300000	-0.205200000
6	-0.477000000	-3.020800000	-1.002900000
1	0.465700000	-2.827500000	-1.508400000
6	-0.957000000	-4.316200000	-0.814800000
1	-0.388100000	-5.166000000	-1.180700000
6	-2.167800000	-4.484000000	-0.139900000
1	-2.572100000	-5.477900000	0.037500000
6	-2.846100000	-3.353700000	0.316700000
1	-3.784400000	-3.445200000	0.858700000
6	-2.299200000	-2.089200000	0.078200000
6	-3.032200000	-0.816000000	0.465400000
1	-3.596500000	-0.506300000	-0.421600000
1	-3.750400000	-1.031900000	1.276800000
6	-1.580600000	0.217500000	2.190200000
1	-2.380800000	-0.056500000	2.903900000
1	-1.239700000	1.225200000	2.448400000

6	-0.384600000	-0.728500000	2.321300000
1	0.037200000	-0.613000000	3.330300000
1	-0.720600000	-1.780500000	2.267300000
6	1.852200000	-0.808400000	1.598000000
6	2.934300000	-0.534600000	0.574700000
6	4.257800000	-0.723100000	1.011300000
1	4.380900000	-1.048400000	2.040600000
6	5.364800000	-0.516000000	0.189800000
1	6.372500000	-0.667500000	0.572600000
6	5.152500000	-0.115300000	-1.138300000
1	5.998200000	0.049100000	-1.806500000
6	3.858500000	0.068200000	-1.608900000
1	3.670900000	0.367500000	-2.638100000
6	2.716000000	-0.129900000	-0.782000000
6	-2.719400000	1.611700000	0.528500000
1	-3.440300000	1.925900000	1.305000000
1	-3.242500000	1.536800000	-0.431200000
6	-1.643100000	2.668900000	0.363000000
6	-1.844500000	4.002000000	0.728200000
1	-2.779600000	4.299300000	1.197000000
6	-0.833900000	4.934500000	0.485400000
1	-0.969200000	5.977900000	0.760600000
6	0.353900000	4.500000000	-0.106700000
1	1.171000000	5.186400000	-0.309700000
6	0.481400000	3.149900000	-0.430600000
1	1.382100000	2.747100000	-0.886100000

13 [Fe(NTA)(H₂O)₂] Sextet

7	0.859200000	-1.076500000	0.035500000
6	1.003100000	-1.365500000	1.478200000
1	1.190500000	-2.428500000	1.667900000
1	1.860800000	-0.804800000	1.866300000
6	0.132400000	-2.115500000	-0.721500000
1	0.810900000	-2.851800000	-1.167500000
1	-0.532200000	-2.654000000	-0.036000000
6	-0.230900000	-0.902200000	2.271300000
6	-0.757600000	-1.493300000	-1.814300000
8	-0.921900000	0.061000000	1.676300000
8	-0.501500000	-1.375300000	3.356200000
8	-1.153800000	-2.152400000	-2.753700000
8	-1.079200000	-0.226900000	-1.589400000
6	2.116900000	-0.643200000	-0.606500000
1	2.977100000	-1.229400000	-0.262900000
1	2.027600000	-0.784900000	-1.689600000
6	2.366000000	0.855500000	-0.363800000
8	3.482700000	1.330300000	-0.423900000
8	1.260300000	1.544600000	-0.137500000
26	-0.501600000	0.749000000	-0.061300000
8	-2.828700000	1.106600000	0.161700000
1	-3.230300000	0.620600000	-0.579200000
1	-2.983500000	0.578000000	0.965700000

8	-0.898400000	2.837000000	-0.380700000
1	-1.660400000	3.252000000	0.055100000
1	-0.089700000	3.351200000	-0.207000000

13 [Fe(NTA)] Quintet

7	1.091300000	-0.066700000	0.883000000
6	0.250100000	-0.160700000	2.089300000
1	0.755900000	-0.691200000	2.907600000
1	0.040800000	0.855600000	2.444300000
6	1.893400000	-1.274800000	0.612600000
1	2.912600000	-1.192700000	1.014600000
1	1.415500000	-2.124900000	1.114400000
6	-1.131800000	-0.814800000	1.838900000
6	1.967000000	-1.650800000	-0.892900000
8	-1.565600000	-0.751000000	0.612700000
8	-1.742500000	-1.289900000	2.796000000
8	2.889600000	-2.375100000	-1.264800000
8	0.996900000	-1.205300000	-1.636600000
6	1.838400000	1.199000000	0.776100000
1	2.291900000	1.498100000	1.732000000
1	2.654400000	1.054200000	0.057600000
6	0.969200000	2.368900000	0.232900000
8	1.314100000	3.521500000	0.498500000
8	-0.039800000	2.016400000	-0.503800000
26	-0.305500000	0.032600000	-0.840300000
8	-3.926800000	-0.394200000	-0.558800000
1	-4.281800000	-1.242200000	-0.863400000
1	-3.188000000	-0.627500000	0.071400000
8	-1.965600000	0.727100000	-2.090700000
1	-2.802400000	0.411800000	-1.658200000
1	-1.896400000	1.682100000	-1.916500000

14 [Fe(Py₃tacn)]³⁺ Doublet

26	-0.009400000	-0.009100000	0.308800000
7	1.240700000	-1.172600000	-0.777100000
7	1.574500000	0.020500000	1.577100000
7	-1.646000000	-0.441300000	-0.793300000
7	0.454000000	1.666900000	-0.732300000
7	-0.756400000	-1.438300000	1.532900000
7	-0.883700000	1.325700000	1.558200000
6	0.920600000	-1.942400000	-1.844500000
6	1.854100000	-2.743900000	-2.493100000
6	3.170900000	-2.762500000	-2.027600000
6	3.510300000	-1.962000000	-0.932800000
6	2.530000000	-1.174600000	-0.336200000
6	2.819300000	-0.195500000	0.770400000
6	1.553300000	1.382500000	2.217500000

6	1.410100000	-1.072800000	2.627100000
6	0.123700000	1.719600000	2.634200000
6	0.414800000	-2.131000000	2.165800000
6	-2.161200000	0.257900000	-1.833100000
6	-2.280300000	-1.580500000	-0.392500000
6	1.345800000	1.806200000	-1.742200000
6	-0.240300000	2.766700000	-0.321200000
6	-1.564900000	-2.368100000	0.675500000
6	-1.637400000	-0.780200000	2.588300000
6	-1.285800000	2.511400000	0.736100000
6	-2.064500000	0.622500000	2.164000000
6	-3.323100000	-0.131600000	-2.489300000
6	-3.452600000	-2.019800000	-1.000800000
6	1.583800000	3.025500000	-2.366400000
6	-0.039500000	4.019400000	-0.893900000
6	-3.987100000	-1.285500000	-2.063600000
6	0.885800000	4.155700000	-1.932900000
1	-0.107900000	-1.904500000	-2.182100000
1	1.547200000	-3.341600000	-3.345700000
1	3.921100000	-3.384800000	-2.507700000
1	4.527200000	-1.944400000	-0.551100000
1	3.112200000	0.765900000	0.334600000
1	3.648100000	-0.521500000	1.407500000
1	1.925800000	2.099500000	1.484800000
1	2.224800000	1.414300000	3.084300000
1	1.083900000	-0.602700000	3.555900000
1	2.380600000	-1.530300000	2.839000000
1	-0.149800000	1.202700000	3.554700000
1	0.036700000	2.789500000	2.844800000
1	0.859500000	-2.785800000	1.414800000
1	0.094700000	-2.757800000	3.007300000
1	-1.619500000	1.145000000	-2.138400000
1	1.867500000	0.910800000	-2.056900000
1	-0.875200000	-3.074900000	0.200900000
1	-2.256100000	-2.959000000	1.285800000
1	-1.076800000	-0.753500000	3.523400000
1	-2.517700000	-1.402000000	2.776000000
1	-2.242200000	2.280200000	0.254300000
1	-1.452400000	3.389300000	1.369400000
1	-2.850900000	0.583000000	1.409100000
1	-2.454900000	1.183200000	3.022200000
1	-3.697500000	0.462900000	-3.316800000
1	-3.937300000	-2.928100000	-0.653800000
1	2.305500000	3.082800000	-3.175300000
1	-0.601900000	4.876900000	-0.535100000
1	-4.901700000	-1.611100000	-2.551500000
1	1.056900000	5.124700000	-2.393400000

14 [Fe(Py₃tacn)]²⁺ Singlet

26	-0.000600000	0.000000000	0.286300000
7	-1.724800000	0.142300000	-0.777900000

7	-1.189600000	-1.083300000	1.555900000
7	0.987300000	1.422100000	-0.776200000
7	0.739600000	-1.565900000	-0.775400000
7	-0.346300000	1.571400000	1.555000000
7	1.531400000	-0.486700000	1.557800000
6	-2.015900000	0.966300000	-1.807400000
6	-3.257700000	0.985500000	-2.436300000
6	-4.255300000	0.121400000	-1.983000000
6	-3.963300000	-0.740600000	-0.924000000
6	-2.691800000	-0.713600000	-0.353600000
6	-2.265000000	-1.685200000	0.722800000
6	-0.300300000	-2.107900000	2.175800000
6	-1.765700000	-0.154300000	2.600300000
6	1.013700000	-1.448100000	2.603500000
6	-1.679400000	1.313600000	2.172700000
6	1.848700000	1.262400000	-1.803700000
6	0.728500000	2.687400000	-0.352500000
6	0.172900000	-2.230900000	-1.805000000
6	1.964000000	-1.974600000	-0.349700000
6	-0.328300000	2.803800000	0.722000000
6	0.744300000	1.605700000	2.601400000
6	2.591000000	-1.118500000	0.726800000
6	1.973200000	0.797000000	2.176100000
6	2.487600000	2.328200000	-2.431300000
6	1.341800000	3.802200000	-0.921700000
6	0.778100000	-3.316000000	-2.432700000
6	2.624300000	-3.062200000	-0.919000000
6	2.236700000	3.624300000	-1.978600000
6	2.025200000	-3.747000000	-1.978100000
1	-1.217200000	1.622800000	-2.134200000
1	-3.433100000	1.668200000	-3.261600000
1	-5.238800000	0.116100000	-2.443500000
1	-4.711500000	-1.431800000	-0.547100000
1	-1.854600000	-2.581300000	0.244200000
1	-3.118400000	-2.010600000	1.331100000
1	-0.113700000	-2.878500000	1.426000000
1	-0.776100000	-2.593200000	3.039200000
1	-1.221900000	-0.312600000	3.533700000
1	-2.808300000	-0.418200000	2.808400000
1	0.878000000	-0.896200000	3.535600000
1	1.763300000	-2.218800000	2.813800000
1	-2.438700000	1.537200000	1.421600000
1	-1.863300000	1.968400000	3.035800000
1	2.019000000	0.242500000	-2.130100000
1	-0.795000000	-1.868300000	-2.132900000
1	-1.308700000	2.896800000	0.241700000
1	-0.184200000	3.705400000	1.330600000
1	0.333300000	1.213700000	3.533900000
1	1.036700000	2.640600000	2.810200000
1	3.163300000	-0.316100000	0.248100000
1	3.298200000	-1.694900000	1.336500000
1	2.547900000	1.342700000	1.426100000

1	2.630600000	0.629000000	3.040500000
1	3.168400000	2.138900000	-3.254900000
1	1.116300000	4.795800000	-0.545300000
1	0.275600000	-3.810000000	-3.258100000
1	3.596800000	-3.363900000	-0.541000000
1	2.724700000	4.478700000	-2.438200000
1	2.522300000	-4.596000000	-2.437700000

15 [Fe(bpy)CN₄]¹⁻ Doublet

26	-0.001300000	-1.134300000	0.000000000
7	-1.303400000	0.431900000	0.000000000
7	1.304600000	0.429500000	0.000000000
7	-0.001400000	-0.892700000	3.130200000
7	-2.302800000	-3.191600000	0.000000000
7	2.297900000	-3.194400000	0.000000000
7	-0.001400000	-0.892700000	-3.130200000
6	-1.380200000	-2.470100000	0.000000000
6	1.376100000	-2.472000000	0.000000000
6	-0.001400000	-1.066100000	-1.971500000
6	-0.001400000	-1.066100000	1.971500000
6	-0.736000000	1.660200000	0.000000000
6	-1.519000000	2.819700000	0.000000000
6	-2.906100000	2.705400000	0.000000000
6	-3.476700000	1.433400000	0.000000000
6	-2.640000000	0.319700000	0.000000000
6	0.739300000	1.658900000	0.000000000
6	2.641000000	0.315100000	0.000000000
6	3.479600000	1.427300000	0.000000000
6	2.911300000	2.700300000	0.000000000
6	1.524300000	2.817000000	0.000000000
1	1.059100000	3.796300000	0.000000000
1	3.535400000	3.590000000	0.000000000
1	4.555400000	1.284100000	0.000000000
1	3.025100000	-0.698800000	0.000000000
1	-1.052100000	3.798200000	0.000000000
1	-3.528700000	3.596200000	0.000000000
1	-4.552800000	1.292100000	0.000000000
1	-3.025800000	-0.693500000	0.000000000

15 [Fe(bpy)CN₄]²⁻ Singlet

26	-0.000700000	-1.097600000	0.000000000
7	-1.280900000	0.414500000	0.000000000
7	1.281500000	0.412700000	0.000000000
7	-0.000700000	-0.966100000	3.156500000
7	-2.356100000	-3.157400000	0.000000000
7	2.351900000	-3.160500000	0.000000000
7	-0.000700000	-0.966100000	-3.156500000
6	-1.423700000	-2.438700000	0.000000000
6	1.420400000	-2.440600000	0.000000000

6	-0.000700000	-1.093500000	-1.986500000
6	-0.000700000	-1.093500000	1.986500000
6	-0.730500000	1.661800000	0.000000000
6	-1.522900000	2.820000000	0.000000000
6	-2.908100000	2.706300000	0.000000000
6	-3.467200000	1.421000000	0.000000000
6	-2.627300000	0.313900000	0.000000000
6	0.732800000	1.660800000	0.000000000
6	2.627800000	0.310400000	0.000000000
6	3.469100000	1.416300000	0.000000000
6	2.911800000	2.702400000	0.000000000
6	1.526800000	2.817900000	0.000000000
1	1.059600000	3.798300000	0.000000000
1	3.541800000	3.589800000	0.000000000
1	4.545800000	1.265200000	0.000000000
1	3.007000000	-0.706500000	0.000000000
1	-1.054400000	3.799700000	0.000000000
1	-3.536900000	3.594700000	0.000000000
1	-4.544000000	1.271300000	0.000000000
1	-3.007900000	-0.702400000	0.000000000

16 [Fe(DITim)₂]¹⁺ Doublet

26	0.000000000	0.006200000	0.000000000
16	0.894900000	1.460000000	-1.416800000
16	-0.895000000	1.459900000	1.416700000
7	-1.760000000	0.152700000	-1.015400000
7	1.760000000	0.152900000	1.015300000
7	0.691700000	-1.555600000	-1.222800000
7	-0.691500000	-1.555600000	1.222900000
6	-0.114000000	-2.336100000	-2.031500000
6	0.678400000	-3.173500000	-2.777000000
7	1.977200000	-2.889300000	-2.405900000
6	1.942300000	-1.906300000	-1.476800000
6	-1.593900000	-2.146200000	-2.062400000
6	-2.009600000	-0.674900000	-2.216300000
6	-2.583000000	1.121200000	-0.757900000
6	-2.351800000	2.042500000	0.429800000
6	-3.789500000	1.422800000	-1.627100000
6	-2.078000000	3.481500000	-0.076300000
6	-3.588800000	2.044300000	1.359800000
6	0.114300000	-2.336000000	2.031600000
6	-0.678100000	-3.173400000	2.777200000
7	-1.976900000	-2.889200000	2.406100000
6	-1.942100000	-1.906300000	1.476800000
6	1.594200000	-2.146000000	2.062400000
6	2.009800000	-0.674700000	2.216200000
6	2.582900000	1.121600000	0.757900000
6	3.789300000	1.423300000	1.627100000
6	2.351600000	2.042800000	-0.429900000
6	2.077500000	3.481800000	0.076200000
6	3.588600000	2.044800000	-1.359800000

1	2.812400000	-3.318300000	-2.782500000
1	2.824300000	-1.458200000	-1.047500000
1	0.440300000	-3.918400000	-3.521300000
1	-2.062300000	-2.570100000	-1.165900000
1	-2.003100000	-2.697000000	-2.916700000
1	-1.457000000	-0.224200000	-3.051300000
1	-3.069400000	-0.660300000	-2.478000000
1	-4.301300000	2.325400000	-1.296400000
1	-3.495900000	1.568700000	-2.672500000
1	-4.520400000	0.604900000	-1.599600000
1	-1.894200000	4.129900000	0.785900000
1	-1.196800000	3.505800000	-0.722200000
1	-2.933600000	3.892900000	-0.626000000
1	-3.369300000	2.650800000	2.244000000
1	-4.471300000	2.476500000	0.873600000
1	-3.835500000	1.034600000	1.704900000
1	-2.812100000	-3.318300000	2.782800000
1	-0.439900000	-3.918100000	3.521600000
1	-2.824100000	-1.458300000	1.047500000
1	2.003400000	-2.696800000	2.916600000
1	2.062500000	-2.569900000	1.165900000
1	3.069700000	-0.660100000	2.477700000
1	1.457400000	-0.224100000	3.051400000
1	4.300800000	2.326100000	1.296600000
1	3.495700000	1.569000000	2.672500000
1	4.520400000	0.605600000	1.599400000
1	1.893600000	4.130100000	-0.786100000
1	1.196300000	3.506000000	0.722100000
1	2.933000000	3.893300000	0.625900000
1	3.369000000	2.651300000	-2.244000000
1	4.471000000	2.477100000	-0.873500000
1	3.835500000	1.035100000	-1.704900000

16 [Fe(DITim)₂]²⁻ Singlet

26	0.000000000	0.063200000	0.000000000
16	0.959000000	1.476600000	-1.692500000
16	-0.959800000	1.476000000	1.692600000
7	-2.306100000	0.045600000	-0.550700000
7	2.306100000	0.046500000	0.550600000
7	0.105300000	-1.662300000	-1.523600000
7	-0.104500000	-1.662300000	1.523600000
6	-0.943400000	-2.438500000	-1.977900000
6	-0.519500000	-3.193100000	-3.046600000
7	0.811300000	-2.861200000	-3.232300000
6	1.137800000	-1.927500000	-2.299600000
6	-2.312100000	-2.317100000	-1.388500000
6	-2.905600000	-0.899000000	-1.502200000

6	-2.948200000	1.128700000	-0.276600000
6	-2.418200000	2.131600000	0.756700000
6	-4.259400000	1.479200000	-0.965100000
6	-2.029400000	3.441500000	0.025900000
6	-3.536700000	2.430800000	1.786500000
6	0.944600000	-2.438100000	1.977800000
6	0.521100000	-3.193000000	3.046500000
7	-0.809800000	-2.861600000	3.232400000
6	-1.136700000	-1.927900000	2.299800000
6	2.313100000	-2.316200000	1.388200000
6	2.906100000	-0.898000000	1.501900000
6	2.947700000	1.129900000	0.276500000
6	4.258800000	1.481000000	0.964900000
6	2.417200000	2.132800000	-0.756600000
6	2.027800000	3.442400000	-0.025600000
6	3.535400000	2.432700000	-1.786500000
1	1.419800000	-3.212200000	-3.958500000
1	2.097300000	-1.435600000	-2.246800000
1	-1.029200000	-3.906000000	-3.677800000
1	-2.302200000	-2.612100000	-0.331900000
1	-2.983400000	-3.010800000	-1.909900000
1	-2.764900000	-0.530300000	-2.529100000
1	-3.988100000	-0.979800000	-1.333900000
1	-4.555100000	2.511900000	-0.781600000
1	-4.183600000	1.336500000	-2.049000000
1	-5.074000000	0.834500000	-0.606900000
1	-1.677700000	4.167000000	0.766700000
1	-1.220400000	3.259100000	-0.687300000
1	-2.880900000	3.889500000	-0.507500000
1	-3.138500000	3.106700000	2.549400000
1	-4.414000000	2.913500000	1.334400000
1	-3.861000000	1.514700000	2.293300000
1	-1.418000000	-3.212900000	3.958700000
1	1.031200000	-3.905800000	3.677600000
1	-2.096400000	-1.436400000	2.247200000
1	2.984800000	-3.009700000	1.909500000
1	2.303300000	-2.611300000	0.331600000
1	3.988600000	-0.978300000	1.333500000
1	2.765400000	-0.529400000	2.528800000
1	4.554100000	2.513800000	0.781600000
1	4.183100000	1.338100000	2.048800000
1	5.073700000	0.836700000	0.606700000
1	1.675700000	4.167800000	-0.766200000
1	1.218900000	3.259500000	0.687600000
1	2.879100000	3.890600000	0.507800000
1	3.136800000	3.108400000	-2.549200000
1	4.412500000	2.915700000	-1.334400000
1	3.860100000	1.516700000	-2.293400000

17 [Fe(H₂O)₆]³⁺ Sextet

26	0.000000000	0.000100000	0.000000000
----	-------------	-------------	-------------

8	-1.606400000	0.254200000	-1.246500000
1	-1.795100000	1.041400000	-1.805300000
8	0.701700000	1.851900000	-0.526500000
1	1.311800000	2.056800000	-1.270400000
8	1.606500000	-0.254300000	1.246600000
1	1.794600000	-1.041100000	1.806000000
8	1.061500000	-0.839500000	-1.538500000
1	0.745200000	-0.980800000	-2.459100000
8	-0.701800000	-1.852000000	0.526200000
1	-1.311400000	-2.057100000	1.270400000
8	-1.061400000	0.839600000	1.538600000
1	-1.984400000	1.177300000	1.497200000
1	-2.335500000	-0.388100000	-1.399600000
1	0.492200000	2.704800000	-0.083500000
1	-0.492800000	-2.704700000	0.082700000
1	2.336200000	0.387500000	1.399000000
1	1.984200000	-1.177900000	-1.496700000
1	-0.744900000	0.981000000	2.459200000

17 [Fe(H₂O)₆]²⁺ Quintet

26	0.000000000	0.000000000	0.000000000
8	-1.853500000	-0.006000000	-1.113800000
1	-1.941900000	-0.004900000	-2.083900000
8	1.151300000	0.008100000	-1.792800000
1	1.482900000	-0.773700000	-2.270800000
8	1.853500000	0.006100000	1.113800000
1	1.941900000	0.005100000	2.083900000
8	0.009500000	-2.170200000	-0.003600000
1	-0.556700000	-2.753100000	-0.540600000
8	-1.151300000	-0.008100000	1.792800000
1	-1.482900000	0.773800000	2.270800000
8	-0.009400000	2.170200000	0.003500000
1	-0.581000000	2.749800000	-0.531400000
1	-2.755600000	-0.010700000	-0.746300000
1	1.476100000	0.794500000	-2.267900000
1	-1.476200000	-0.794400000	2.268000000
1	2.755600000	0.010400000	0.746300000
1	0.580900000	-2.749800000	0.531500000
1	0.556900000	2.753100000	0.540400000

18²⁺ [Fe(Ohishis)(H₂O)₃]²⁺ Quintet

6	4.320700000	0.220200000	0.142000000
6	3.094600000	-1.586200000	-0.178200000
6	2.995600000	0.539600000	0.313300000
6	-4.281300000	-0.096700000	0.205200000
6	-2.905600000	-1.780700000	-0.169500000
6	-2.986400000	0.345600000	0.325100000
7	4.360900000	-1.120000000	-0.168400000
7	2.232600000	-0.613900000	0.108600000

7	-4.208400000	-1.434800000	-0.109300000
7	-2.126500000	-0.732000000	0.085600000
6	2.458600000	1.883700000	0.726700000
6	1.709100000	2.724200000	-0.347500000
6	0.286800000	2.265400000	-0.536800000
6	-2.547100000	1.736300000	0.693400000
7	-0.725400000	3.114800000	-0.387400000
8	0.028500000	1.060700000	-0.817700000
6	-2.122400000	2.664400000	-0.490600000
1	5.215100000	0.818900000	0.224500000
1	2.842800000	-2.615700000	-0.381900000
1	-5.223900000	0.415600000	0.324900000
1	-2.566500000	-2.783300000	-0.380800000
1	1.817800000	1.777800000	1.610800000
1	3.314900000	2.480200000	1.053200000
1	-3.378500000	2.210800000	1.222400000
1	-1.726300000	1.687100000	1.416300000
1	2.222500000	2.644000000	-1.312400000
1	1.731600000	3.777700000	-0.054000000
1	-0.532400000	4.089600000	-0.192500000
1	-2.248200000	2.153400000	-1.447900000
1	-2.737500000	3.564700000	-0.509500000
1	-4.994500000	-2.055500000	-0.257000000
1	5.195400000	-1.665200000	-0.345700000
26	0.059500000	-0.754900000	0.019900000
8	0.044600000	-0.647500000	2.226600000
1	-0.740200000	-0.723700000	2.788600000
1	0.823400000	-0.688600000	2.800400000
8	0.081100000	-1.604700000	-2.096900000
1	0.836900000	-1.359200000	-2.651400000
1	-0.704900000	-1.431900000	-2.636700000
8	0.111900000	-3.000100000	0.291000000
1	0.157800000	-3.569900000	-0.490300000
1	0.151900000	-3.560300000	1.078700000

18³⁺ [Fe(Ohishis)(H₂O)₃]³⁺ Sextet

6	4.264900000	0.189800000	0.139600000
6	3.029400000	-1.606400000	-0.203800000
6	2.948600000	0.542900000	0.293700000
6	-4.205000000	-0.216900000	0.206800000
6	-2.783500000	-1.876500000	-0.089100000
6	-2.933900000	0.293100000	0.295000000
7	4.286200000	-1.152200000	-0.175100000
7	2.167400000	-0.608200000	0.070200000
7	-4.082700000	-1.566800000	-0.039900000
7	-2.031800000	-0.774400000	0.101300000
6	2.457900000	1.895600000	0.745000000
6	1.666000000	2.768200000	-0.267000000
6	0.238800000	2.326700000	-0.395100000
6	-2.601200000	1.723100000	0.640500000

7	-0.784900000	3.146500000	-0.419700000
8	-0.022600000	1.067900000	-0.474200000
6	-2.184300000	2.673100000	-0.528100000
1	5.171200000	0.769900000	0.240400000
1	2.770300000	-2.632400000	-0.414700000
1	-5.168400000	0.261800000	0.311300000
1	-2.413900000	-2.877100000	-0.250800000
1	1.878800000	1.800600000	1.671900000
1	3.346700000	2.469200000	1.021100000
1	-3.504400000	2.141700000	1.093100000
1	-1.845000000	1.762600000	1.431000000
1	2.125800000	2.717600000	-1.262900000
1	1.704300000	3.815800000	0.046000000
1	-0.611700000	4.147900000	-0.373500000
1	-2.308700000	2.191700000	-1.502000000
1	-2.802300000	3.570900000	-0.523700000
1	-4.851700000	-2.222500000	-0.150000000
1	5.120000000	-1.708600000	-0.344600000
26	0.071000000	-0.736900000	-0.032100000
8	0.090300000	-0.761900000	2.106000000
1	-0.692500000	-0.775800000	2.681000000
1	0.880100000	-0.734400000	2.670700000
8	0.082600000	-1.359600000	-2.098400000
1	0.838500000	-1.171300000	-2.680100000
1	-0.713200000	-1.300800000	-2.653800000
8	0.166800000	-2.909800000	0.167800000
1	0.211100000	-3.542500000	-0.567500000
1	0.218200000	-3.409100000	0.999300000

19²⁺ [Fe(Ohishis)(Im)(H₂O)₂]²⁺ Quintet

6	-3.818300000	-2.094000000	0.082300000
6	-3.211900000	-0.035500000	-0.397500000
6	-2.476400000	-1.950700000	0.313400000
6	4.216800000	0.913700000	0.136100000
6	2.404300000	2.024500000	-0.426000000
6	3.123200000	0.105900000	0.294700000
7	-4.264300000	-0.875800000	-0.369100000
7	-2.109200000	-0.645500000	0.006600000
7	3.743700000	2.119100000	-0.322700000
7	1.985100000	0.821400000	-0.064500000
6	-1.560300000	-3.001900000	0.856600000
6	-0.573800000	-3.649800000	-0.135400000
6	0.621600000	-2.780000000	-0.375900000
6	3.121300000	-1.305600000	0.786000000
7	1.845200000	-3.252700000	-0.142000000
8	0.489600000	-1.601200000	-0.774700000
6	3.016100000	-2.394200000	-0.309400000
1	-4.478500000	-2.940900000	0.210200000
1	-3.282600000	1.000700000	-0.705100000
1	5.268100000	0.734700000	0.315900000
1	1.771500000	2.842600000	-0.748700000

1	-0.999100000	-2.612700000	1.718700000
1	-2.193300000	-3.802000000	1.256600000
1	4.046100000	-1.458100000	1.354100000
1	2.304800000	-1.452000000	1.505400000
1	-1.069300000	-3.818600000	-1.100600000
1	-0.265400000	-4.630300000	0.244700000
1	1.963700000	-4.214500000	0.152500000
1	2.963400000	-1.934800000	-1.303000000
1	3.893000000	-3.045300000	-0.297600000
1	4.301300000	2.937100000	-0.534600000
1	-5.217800000	-0.645700000	-0.619900000
1	-1.150100000	2.872400000	-1.873800000
6	-1.189000000	3.089400000	-0.813700000
7	-0.849200000	2.249600000	0.155800000
7	-1.591800000	4.267500000	-0.295400000
6	-1.046300000	2.933000000	1.339800000
6	-1.508100000	4.189700000	1.074000000
1	-1.901300000	5.072200000	-0.827100000
1	-1.777800000	5.012400000	1.720000000
1	-0.847300000	2.482800000	2.302200000
26	-0.119300000	0.237900000	-0.080400000
8	0.036000000	-0.073200000	2.114500000
1	0.760600000	0.254300000	2.662900000
1	-0.710200000	-0.258700000	2.699100000
8	-0.280100000	0.647000000	-2.319900000
1	0.574100000	0.581200000	-2.767400000
1	-0.849200000	0.003900000	-2.763200000

19³⁺ [Fe(Ohishis)(Im)(H₂O)₂]³⁺ Sextet

6	-2.984600000	-3.119100000	0.180900000
6	-3.051900000	-0.947400000	-0.202800000
6	-1.714900000	-2.619300000	0.318400000
6	3.655400000	2.199800000	0.251500000
6	1.548400000	2.723800000	-0.134600000
6	2.907500000	1.052200000	0.331900000
7	-3.798200000	-2.057200000	-0.149500000
7	-1.767400000	-1.234800000	0.068700000
7	2.786300000	3.225700000	-0.047300000
7	1.563700000	1.397200000	0.080400000
6	-0.516300000	-3.414800000	0.765700000
6	0.628500000	-3.642600000	-0.256500000
6	1.513500000	-2.436800000	-0.384600000
6	3.446400000	-0.303400000	0.709300000
7	2.827100000	-2.514700000	-0.358200000
8	0.991000000	-1.274600000	-0.510100000
6	3.694300000	-1.322000000	-0.447900000
1	-3.368800000	-4.121700000	0.301400000
1	-3.448000000	0.029700000	-0.428800000
1	4.713600000	2.366400000	0.392300000
1	0.674600000	3.321100000	-0.340700000
1	-0.098300000	-2.992600000	1.687700000

1	-0.889100000	-4.403500000	1.046100000
1	4.406000000	-0.123500000	1.201800000
1	2.815900000	-0.770100000	1.472500000
1	0.217900000	-3.871700000	-1.248100000
1	1.220900000	-4.509800000	0.048800000
1	3.262600000	-3.429000000	-0.276700000
1	3.546400000	-0.858200000	-1.426900000
1	4.718900000	-1.692600000	-0.412600000
1	3.039300000	4.202100000	-0.165900000
1	-4.799600000	-2.105700000	-0.312100000
1	-1.875300000	2.331400000	-2.064400000
6	-2.042000000	2.512100000	-1.013900000
7	-1.502600000	1.817200000	0.003700000
7	-2.833500000	3.484400000	-0.532800000
6	-1.994100000	2.398700000	1.172700000
6	-2.821800000	3.435700000	0.846300000
1	-3.356300000	4.148700000	-1.096700000
1	-3.386700000	4.123500000	1.458400000
1	-1.725100000	2.041700000	2.152900000
26	-0.178100000	0.175100000	-0.085600000
8	-0.056400000	0.023700000	2.059600000
1	0.575000000	0.499200000	2.622500000
1	-0.667300000	-0.467900000	2.631000000
8	-0.335400000	0.426900000	-2.268300000
1	0.467800000	0.679900000	-2.753300000
1	-0.747700000	-0.284600000	-2.786000000

20²⁺ [Fe(Nhishis)(Ph)(H₂O)] Quintet

6	-1.690000000	4.009300000	-0.431500000
6	-2.461600000	1.931700000	-0.531400000
6	-0.641100000	3.130200000	-0.547200000
6	3.996100000	-2.328800000	-0.535000000
6	2.430900000	-1.581400000	-1.907100000
6	3.007800000	-1.707400000	0.190800000
7	-2.836800000	3.232200000	-0.425100000
7	-1.145000000	1.840500000	-0.611100000
7	3.612200000	-2.242600000	-1.860000000
7	2.036500000	-1.244600000	-0.687400000
6	0.838500000	3.356700000	-0.567200000
6	1.566200000	2.787300000	0.665100000
6	2.928500000	-1.569300000	1.690300000
6	1.809400000	-0.650700000	2.203600000
1	-1.723500000	5.084600000	-0.352200000
1	-3.153300000	1.101900000	-0.524500000
1	4.910700000	-2.813300000	-0.230700000
1	1.896900000	-1.353600000	-2.817200000
1	1.257700000	2.903500000	-1.477100000
1	1.043100000	4.431100000	-0.629400000
1	2.786200000	-2.567400000	2.125200000
1	3.887800000	-1.198200000	2.069400000

1	1.228600000	3.324000000	1.563500000
1	2.637900000	3.008700000	0.571400000
1	0.841800000	-1.003300000	1.826800000
1	1.779000000	-0.732100000	3.294100000
1	4.122400000	-2.597400000	-2.654800000
1	-3.784900000	3.567300000	-0.339400000
7	1.359500000	1.346800000	0.838400000
6	2.047700000	0.831600000	1.886900000
8	2.840000000	1.471200000	2.603000000
26	0.293000000	0.140900000	-0.385100000
8	-0.073100000	-0.172800000	-2.829200000
1	-0.724800000	-0.751200000	-2.362700000
1	-0.572400000	0.599500000	-3.123900000
8	-1.119300000	-1.195200000	-0.665200000
6	-2.217200000	-1.610500000	-0.032100000
6	-2.471700000	-1.282300000	1.318900000
6	-3.172500000	-2.400400000	-0.711000000
6	-3.632000000	-1.726300000	1.956200000
1	-1.745900000	-0.679000000	1.858400000
6	-4.329200000	-2.836800000	-0.064700000
1	-2.980300000	-2.668800000	-1.746500000
6	-4.572600000	-2.504800000	1.273400000
1	-3.798900000	-1.462300000	2.997700000
1	-5.045400000	-3.446300000	-0.610600000
1	-5.472000000	-2.850400000	1.774000000

20³⁺ [Fe(Nhishis)(Ph)(H₂O)]¹⁺ Sextet

6	-1.438000000	4.134500000	-0.543800000
6	-1.223000000	2.472800000	-1.990100000
6	-0.672100000	3.145500000	0.021100000
6	3.253800000	-2.915300000	-0.794400000
6	1.088900000	-2.715000000	-1.227100000
6	2.854300000	-1.633500000	-0.509300000
7	-1.768900000	3.693400000	-1.810900000
7	-0.544100000	2.112800000	-0.904500000
7	2.125900000	-3.577500000	-1.245200000
7	1.499600000	-1.527800000	-0.792900000
6	-0.079500000	3.060800000	1.396500000
6	-0.070600000	1.621200000	1.943000000
6	3.624900000	-0.497000000	0.086900000
6	3.289900000	-0.197700000	1.568700000
1	-1.771700000	5.085800000	-0.160200000
1	-1.350000000	1.880200000	-2.883700000
1	4.211600000	-3.403900000	-0.706400000
1	0.079600000	-2.963300000	-1.518400000
1	0.946800000	3.445400000	1.410800000
1	-0.661800000	3.700000000	2.068800000
1	4.688500000	-0.747500000	0.028800000
1	3.495000000	0.410100000	-0.517200000
1	-1.056600000	1.165100000	1.795900000
1	0.134000000	1.648300000	3.014900000

1	3.079400000	-1.140200000	2.090500000
1	4.176400000	0.223900000	2.046900000
1	2.079000000	-4.546500000	-1.530100000
1	-2.343200000	4.186300000	-2.481100000
7	0.949200000	0.767600000	1.284900000
6	2.169500000	0.778200000	1.946800000
8	2.376000000	1.519400000	2.908500000
26	0.310800000	0.183800000	-0.449000000
8	1.368400000	0.760000000	-2.391700000
1	1.569000000	1.686300000	-2.586300000
1	2.062900000	0.212400000	-2.783500000
8	-1.262900000	-0.745300000	-0.616600000
6	-2.285000000	-1.336500000	0.017900000
6	-2.202900000	-1.670300000	1.386200000
6	-3.457000000	-1.640600000	-0.704800000
6	-3.280100000	-2.293000000	2.013200000
1	-1.293500000	-1.442500000	1.934500000
6	-4.525900000	-2.262500000	-0.063800000
1	-3.506300000	-1.378700000	-1.757200000
6	-4.444900000	-2.590800000	1.295200000
1	-3.211500000	-2.548600000	3.066400000
1	-5.426900000	-2.492700000	-0.624600000
1	-5.280500000	-3.075500000	1.789600000