Electronic supplementary information (ESI) for

What Factors Tune the Chemical Equilibrium between the Metal-Iodosylarene Oxidants and the High-Valent Metal-Oxo Ones?

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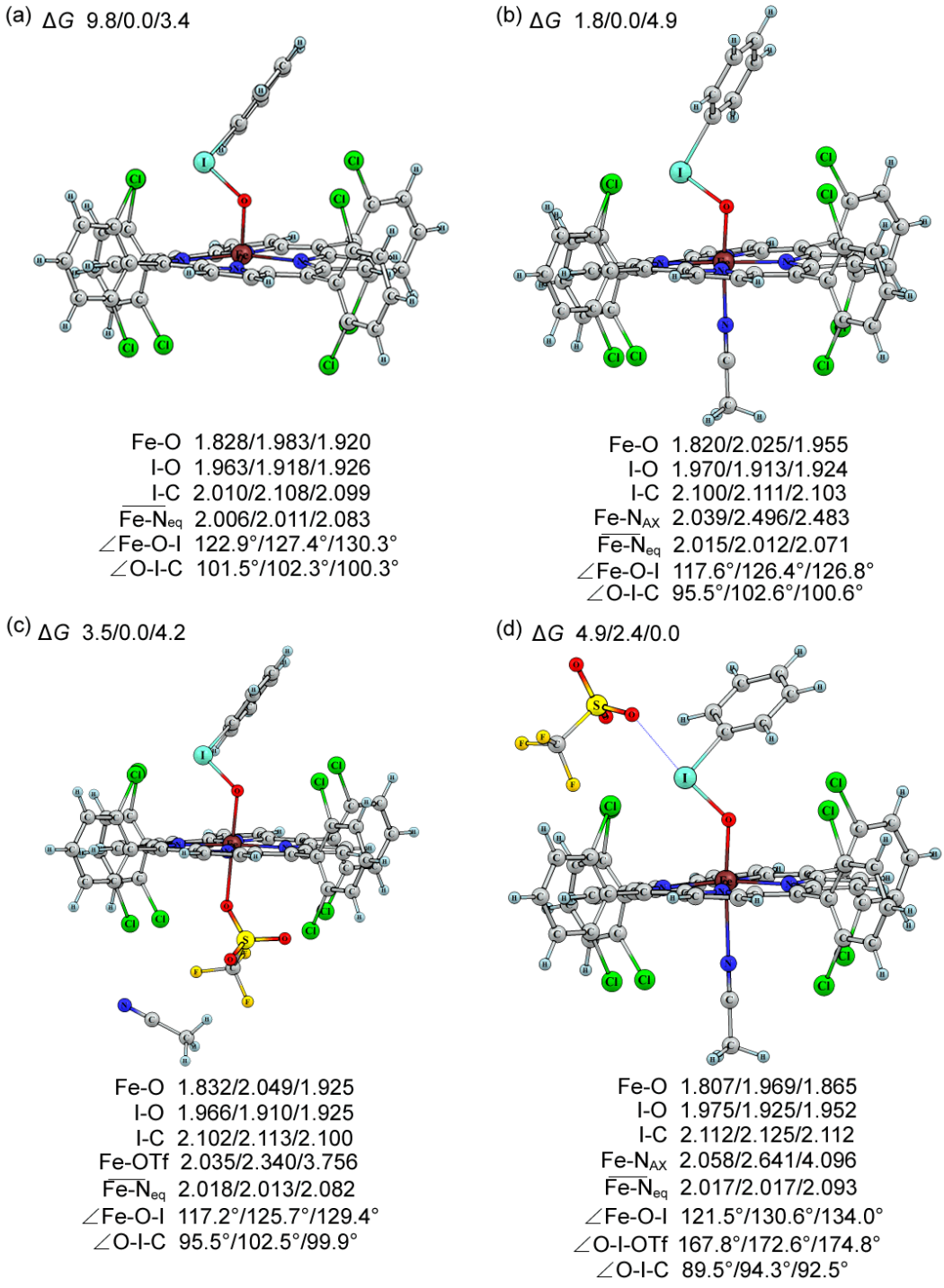


Fig. S1 The structures and energies calculated at UB3LYP/LANL2DZdp for I, LANL2DZ for Fe, 6-31G** for N,O, 6-31G* for S, 6-31G for H, C, F, Cl of four models of the reaction system: (a) the model system without acetonitrile and triflate (**1a**); (b) the model system with acetonitrile (**1b**); (c) the model system acetonitrile and with triflate at the axial position (**1c**) and (d) the model system with acetonitrile at the axial position and the triflate has a halogen bond with the iodine (**1d**) respectively. Relative Gibbs free energies ΔG are in kcal mol^{-1} units, the bond lengths are in Å units. Values were presented with the sequence of doublet/quartet/sextet.

Table S1. The energies calculated at UB3LYP/LANL2DZdp for I, LANL2DZ for Fe, 6-31G** for N,O, 6-31G* for S, 6-31G for H, C, F, Cl of four models of the reaction system: (a) the model system without acetonitrile and triflate (**1a**); (b) the model system with acetonitrile (**1b**); (c) the model system acetonitrile and with triflate at the axial position (**1c**) and (d) the model system with acetonitrile at the axial position and the triflate has a halogen bond with the iodine (**1d**) respectively. Absolute SCF energies and free energies are in a.u. and the relative ones are in kcal mol^{-1}.

		SCF	ΔE	SCF+ZPE	ΔE	G	ΔG
(a)	^{2}**1a**	-6030.212090	8.2	-6029.592586	8.5	-6029.661023	9.8
	^{4}**1a**	-6030.225090	0.0	-6029.606057	0.0	-6029.676577	0.0
	^{6}**1a**	-6030.217833	4.6	-6029.600406	3.6	-6029.671268	3.4
(b)	^{2}**1b**	-6162.974116	0.0	-6162.306479	0.0	-6162.379507	1.8
	^{4}**1b**	-6162.972250	1.2	-6162.306357	0.1	-6162.382368	0.0
	^{6}**1b**	-6162.961729	7.8	-6162.297734	5.5	-6162.374502	4.9
(c)	^{2}**1c**	-7124.480560	0.9	-7123.786738	1.6	-7123.868153	3.5
	^{4}**1c**	-7124.482051	0.0	-7123.789349	0.0	-7123.873790	0.0
	^{6}**1c**	-7124.470894	7.0	-7123.779664	6.1	-7123.867903	4.2
(d)	^{2}**1d**	-7124.489905	0.0	-7123.795274	0.3	-7123.877664	4.9
	^{4}**1d**	-7124.488435	0.9	-7123.795781	0.0	-7123.881581	2.4
	^{6}**1d**	-7124.486343	2.2	-7123.795373	0.2	-7123.885396	0.0

Table S2. DFT functional and basis set benchmark on **1d**. Absolute energies are in a.u. and the relative ones are in kcal mol^{-1}. The basis set employs LANL2DZdp for I, LANL2DZ for Fe, 6-31G** for N,O, 6-31G* for S, 6-31G for H, C, F, Cl, and the basis set of single-point energies employs LANL2DZdp for I, LANL2DZ for Fe, 6-31+G** for the others, the functions employ UB3LYP, UPBE0, UM06, UOPBE and UBP86 respectively.

		SCF	ΔE	SCF+ZPE	ΔE	SPE	ΔE	SPE+ZPE	ΔE	G	ΔG
UB3LYP	^{2}**1d**	-7124.489905	0.0	-7123.795274	0.3	-7125.323982	2.3	-7124.62935	4.6	-7123.877664	4.9
	^{4}**1d**	-7124.488435	0.9	-7123.795781	0.0	-7125.324083	2.3	-7124.631429	3.3	-7123.881581	2.4
	^{6}**1d**	-7124.486343	2.2	-7123.795373	0.2	-7125.327672	0.0	-7124.636702	0.0	-7123.885396	0.0
UPBE0	^{2}**1d**	-7119.767131	2.9	-7119.063158	5.2	-7120.606752	7.6	-7119.91212	9.9	-7119.145585	7.1
	^{4}**1d**	-7119.769487	1.4	-7119.067507	2.5	-7120.610939	4.9	-7119.918285	6.0	-7119.151996	3.0
	^{6}**1d**	-7119.771709	0.0	-7119.071495	0.0	-7120.618814	0.0	-7119.927844	0.0	-7119.156831	0.0
UM06	^{2}**1d**	-7122.395379	17.1	-7121.695815	18.5	-7123.159967	22.4	-7122.468755	22.6	-7121.767809	18.7
	^{4}**1d**	-7122.419033	2.2	-7121.721125	2.7	-7123.187659	5.0	-7122.495005	6.1	-7121.794151	2.2
	^{6}**1d**	-7122.422596	0.0	-7121.725370	0.0	-7123.195675	0.0	-7122.504705	0.0	-7121.797677	0.0
UOPBE	^{2}**1d**	-7123.303886	4.4	-7122.617506	6.7	-7124.088040	6.1	-7123.401660	8.4	-7122.704758	6.2
	^{4}**1d**	-7123.308606	1.5	-7122.624209	1.9	-7124.091493	3.9	-7123.407096	5.0	-7122.711552	1.9
	^{6}**1d**	-7123.310964	0.0	-7122.628179	0.0	-7124.097778	0.0	-7123.414993	0.0	-7122.714607	0.0
UBP86	^{2}**1d**	-7125.007496	0.0	-7124.334998	0.0	-7125.764854	0.0	-7125.073642	0.0	-7124.420290	0.0
	^{4}**1d**	-7124.987042	12.8	-7124.316352	11.7	-7125.745639	12.1	-7125.052985	13.0	-7124.404653	8.6
	^{6}**1d**	-7124.971058	22.9	-7124.302336	20.5	-7125.733210	19.9	-7125.04224	19.7	-7124.394056	16.5

Table S3. The annihilation of the first spin contaminant calculated at UB3LYP/LANL2DZdp for I, LANL2DZ for Fe, 6-31G** for N,O, 6-31G* for S, 6-31G for H, C, F, Cl of different computing models (1) of the reaction, the structure without acetonitrile and trifluoromethanesulfonate (**1a**), with acetonitrile (**1b**), with trifluoromethanesulfonate at the axial coordination of the porphyrin (**1c**) and with trifluoro-methanesulfonate at the distal site of the porphyrin (**1d**) respectively, and of the intermediates (2) in the chemical equilibrium between **1b** and **2** in the absence or the presence of counterion OTf.

(1)

	1a	**1b**	**1c**	**1d**
Doublet	0.7559	0.7505	0.7506	0.7503
Quartet	3.7507	3.7507	3.7507	3.7506
Sextet	8.7501	8.7500	8.7501	8.7501

(2)

	2+PhI	**TS_{1b}**	**1b**	**2+PhI+OTf^-**	**TS_{1d}**	**1d**
Doublet	0.9879	0.7893	0.7505	0.9879	0.7988	0.7503
Quartet	3.7527	3.7600	3.7507	3.7527	3.7515	3.7506
Sextet	8.7548	8.7687	8.7500	8.7548	8.7738	8.7501

Note. The expectation values of s(s+1) and the calculated values of the great majority of intermediates were very close, so the spin contaminant had no influence on the computing results.

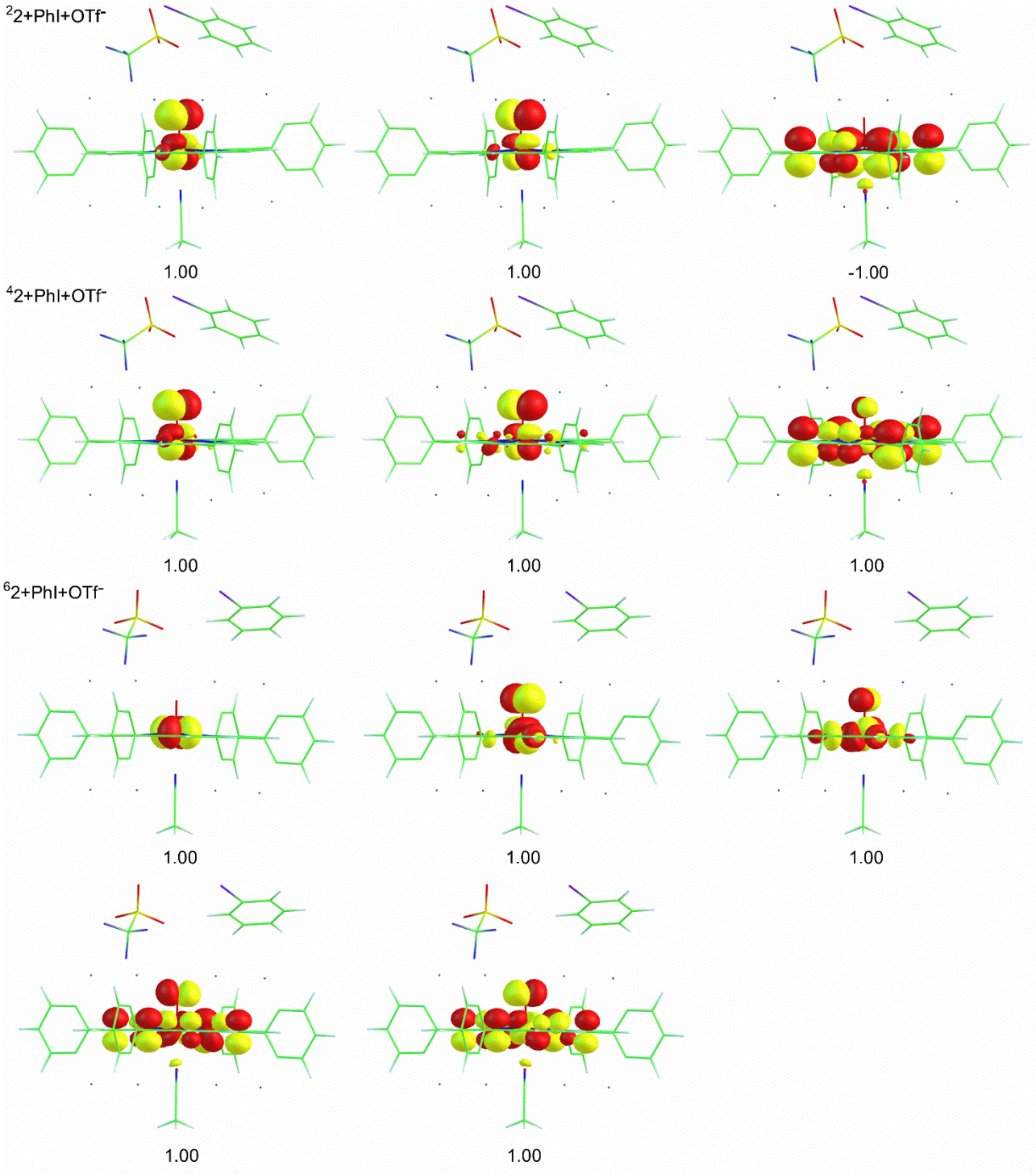
Table S4. Various calculated energies for the chemical equilibrium between **1d** and **2** in the presence of counterion OTf. Calculations are at the UB3LYP/LANL2DZdp(I),LANL2DZ(Fe), 6-31G**(N,O),6-31G*(S),6-31G(H,C,F,Cl) level. Absolute SCF energies and Gibbs free energies are in a.u. and the relative ones are in kcal mol^{-1}.

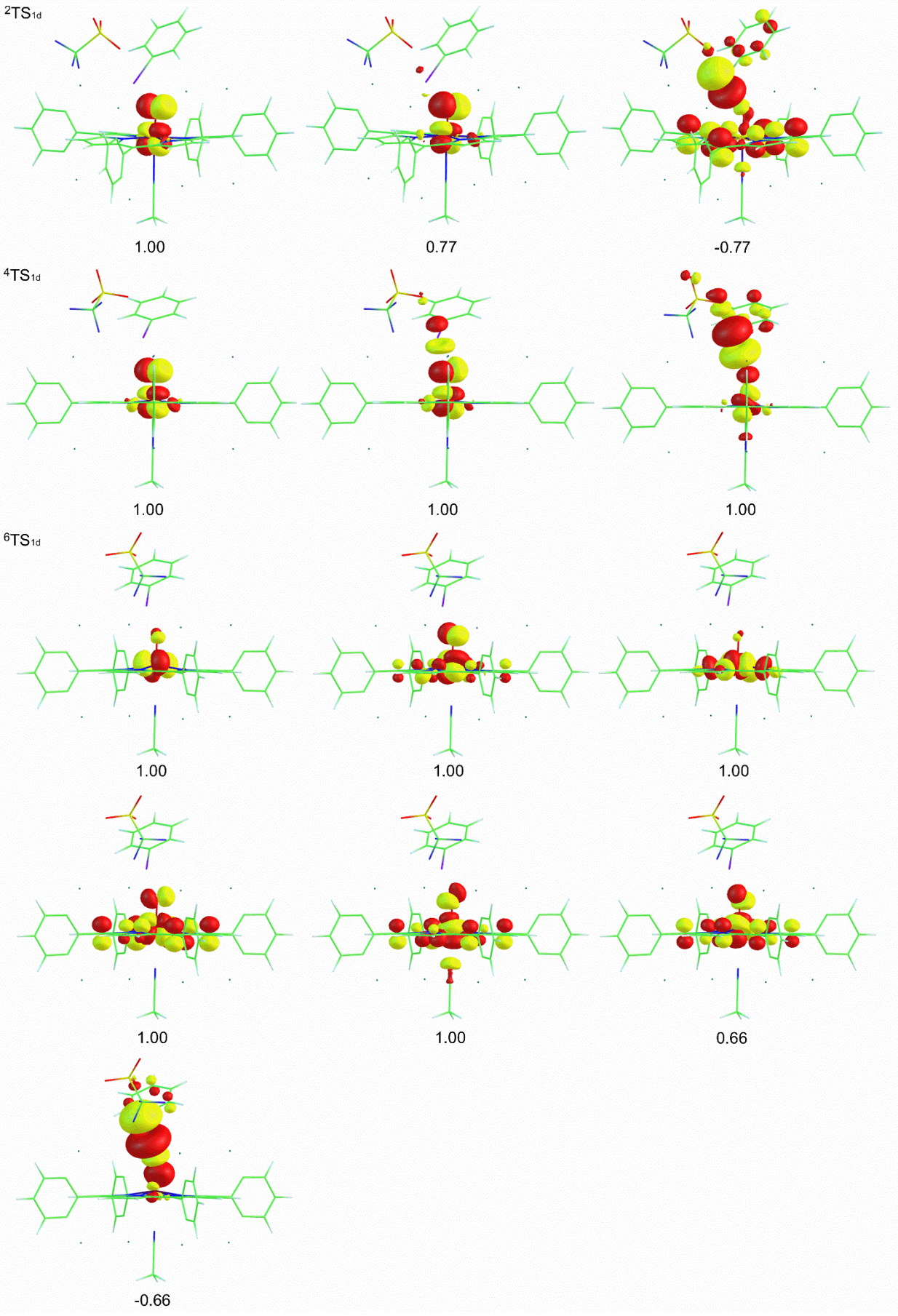
	SCF	ΔE	SCF+ZPE	ΔE	G	ΔG
^{2}**2+PhI+OTf^{-}**	-7124.486566	0.4	-7123.795354	0.0	-7123.884923	0.1
^{4}**2+PhI+OTf^{-}**	-7124.486873	0.0	-7123.795316	0.0	-7123.885151	0.0
^{6}**2+PhI+OTf^{-}**	-7124.463899	14.4	-7123.77406	13.4	-7123.863423	13.6
^{2} **TS_{1d}**	-7124.464027	14.3	-7123.772307	14.5	-7123.858939	16.4
^{4} **TS_{1d}**	-7124.456331	19.2	-7123.76416	19.6	-7123.850991	21.4
^{6} **TS_{1d}**	-7124.450677	22.7	-7123.763499	20.0	-7123.852788	20.3
^{2}**1d**	-7124.489906	-1.9	-7123.795274	0.1	-7123.877664	4.7
^{4}**1d**	-7124.488435	-1.0	-7123.795781	-0.3	-7123.881581	2.2
^{6}**1d**	-7124.486343	0.3	-7123.795373	0.0	-7123.885396	-0.2

Table S5. Mulliken spin density and charge of the key intermediates in the chemical equilibrium between **1d** and **2** in the presence of counterion OTf. Calculations are at the UB3LYP/LANL2DZdp(I),LANL2DZ(Fe),6-31G**(N,O),6-31G*(S),6-31G(H,C,F,Cl) level.

	Spin densities						Charges					
	Fe	O	I	Por+An	Ph	OTf	Fe	O	I	Por+An	Ph	OTf
^{2}**2+PhI+OTf^{-}**	1.12	0.94	0.00	-1.06	-0.00	-0.00	0.56	-0.36	-0.06	0.74	0.02	-0.90
^{4}**2+PhI+OTf^{-}**	1.09	0.94	0.00	0.98	0.00	0.00	0.56	-0.36	-0.06	0.74	0.02	0.90
^{6}**2+PhI+OTf^{-}**	2.97	0.68	-0.00	1.34	-0.00	-0.00	0.79	-0.37	-0.06	0.54	0.02	-0.92
^{2}**TS$_{1d}$**	1.05	0.69	-0.20	-0.47	-0.05	-0.01	0.63	-0.41	0.21	0.33	0.13	-0.89
^{4}**TS$_{1d}$**	1.73	0.57	0.61	-0.07	0.09	0.08	0.72	-0.52	0.43	-0.02	0.18	-0.79
^{6}**TS$_{1d}$**	3.87	0.23	-0.35	1.26	-0.01	-0.01	0.90	-0.63	0.32	0.18	0.11	-0.89
^{2}**1d**	2.80	0.16	0.03	0.00	0.01	0.00	0.79	-0.68	0.78	-0.05	0.15	-1.00
^{4}**1d**	0.89	0.13	-0.00	-0.02	-0.00	-0.00	0.63	-0.65	0.72	-0.04	0.13	-0.79
^{6}**1d**	4.04	0.28	0.05	0.61	0.01	0.01	0.97	-0.70	0.73	-0.35	0.13	-0.79

Fig. S2 Spin natural orbitals (SNO) and their occupation values of the key intermediates in the chemical equilibrium between **1d** and **2** in the presence of counterion OTf. Calculations are at the UB3LYP/LANL2DZdp(I),LANL2DZ(Fe),6-31G**(N,O),6-31G*(S),6-31G(H,C,F,Cl) level.

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-0.77
^{4}TS$_{1d}$
1.00
1.00
1.00
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1.00
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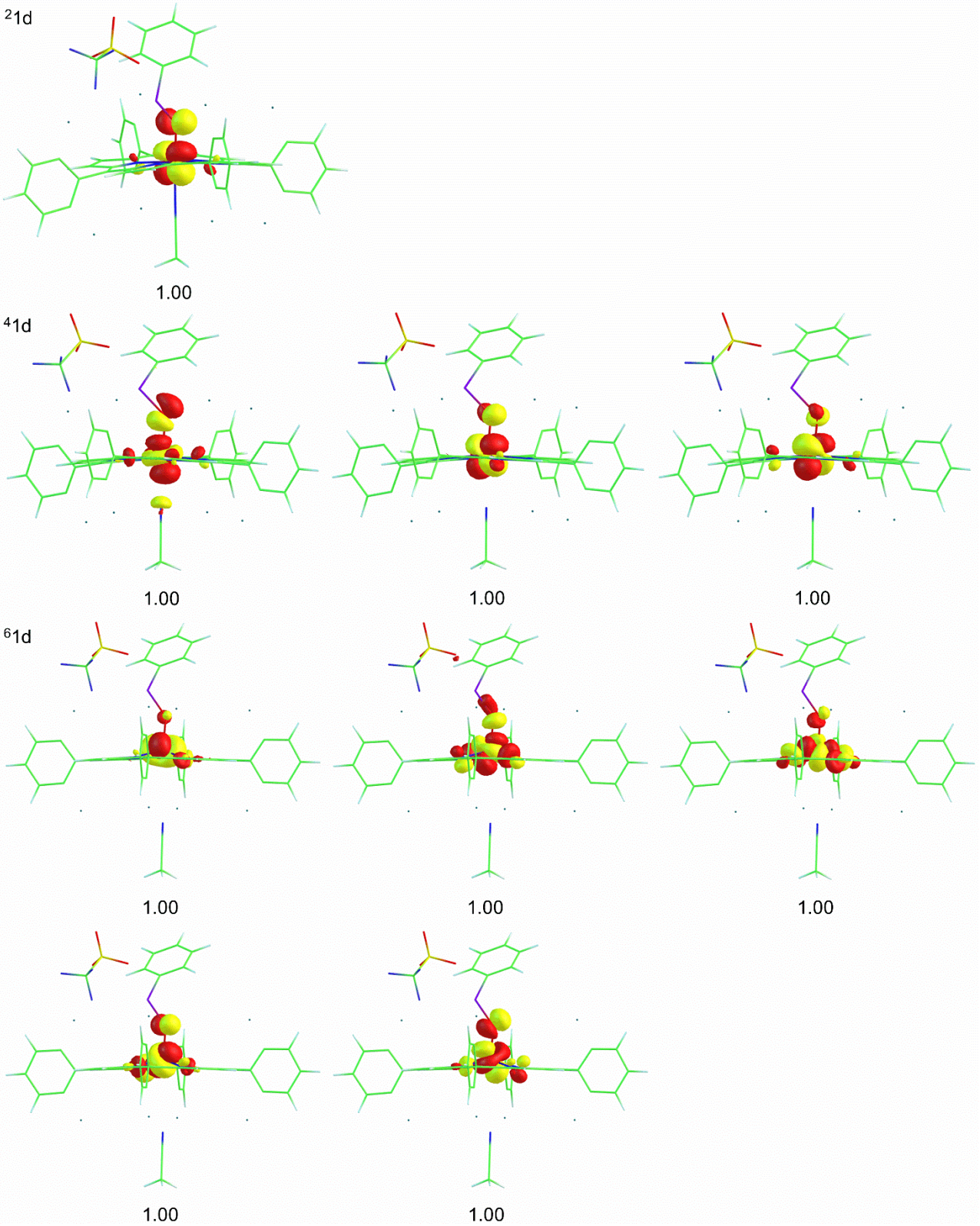
1.00
1.00
0.66
-0.66


^{2}1d
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^{4}1d
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1.00
1.00
^{6}1d
1.00
1.00
1.00
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1.00

Table S6. Various calculated energies for the chemical equilibrium between **1b** and **2** in the absence of counterion OTf. Calculations are at the UB3LYP/LANL2DZdp(I),LANL2DZ(Fe), 6-31G**(N,O),6-31G*(S),6-31G(H,C,F,Cl) level. Absolute SCF energies and Gibbs free energies are in a.u. and the relative ones are in kcal mol^{-1}.

	SCF	ΔE	SCF+ZPE	ΔE	G	ΔG
^{2}**2+PhI**	-6162.979392	0.1	-6162.314859	0.1	-6162.393342	0.9
^{4}**2+PhI**	-6162.979514	0.0	-6162.314948	0.0	-6162.394802	0.0
^{6}**2+PhI**	-6162.956665	14.4	-6162.293632	13.4	-6162.37288	13.7
^{2}**TS$_{1b}$**	-6162.958117	13.5	-6162.292582	14.1	-6162.366743	17.6
^{4}**TS$_{1b}$**	-6162.935091	27.9	-6162.274107	25.7	-6162.347353	29.8
^{6}**TS$_{1b}$**	-6162.943645	22.5	-6162.283032	20.1	-6162.361581	20.8
^{2}**1b**	-6162.974116	3.4	-6162.306479	5.4	-6162.379507	9.6
^{4}**1b**	-6162.972223	4.6	-6162.306423	5.4	-6162.380797	8.8
^{6}**1b**	-6162.961728	11.2	-6162.297734	10.8	-6162.374502	12.7

Fig. S3 Geometric information of the key intermediates in the chemical equilibrium between **1b** and **2** in the absence of counterion OTf. Lengthes are in Å units. Calculations are at the UB3LYP/LANL2DZdp(I),LANL2DZ(Fe),6-31G**(N,O),6-31G*(S),6-31G(H,C,F,Cl) level.

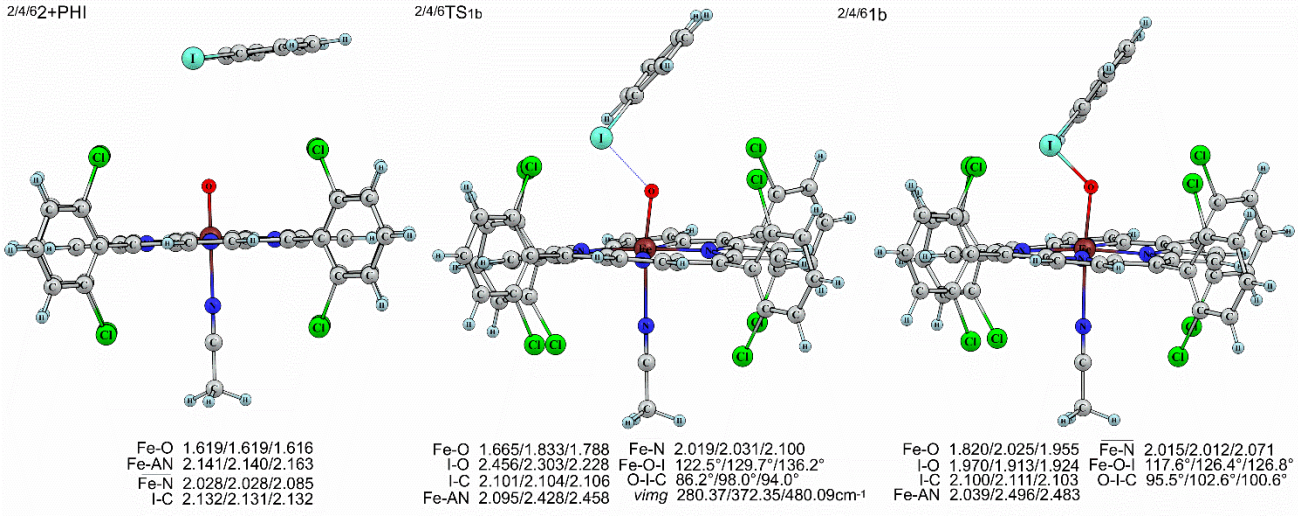
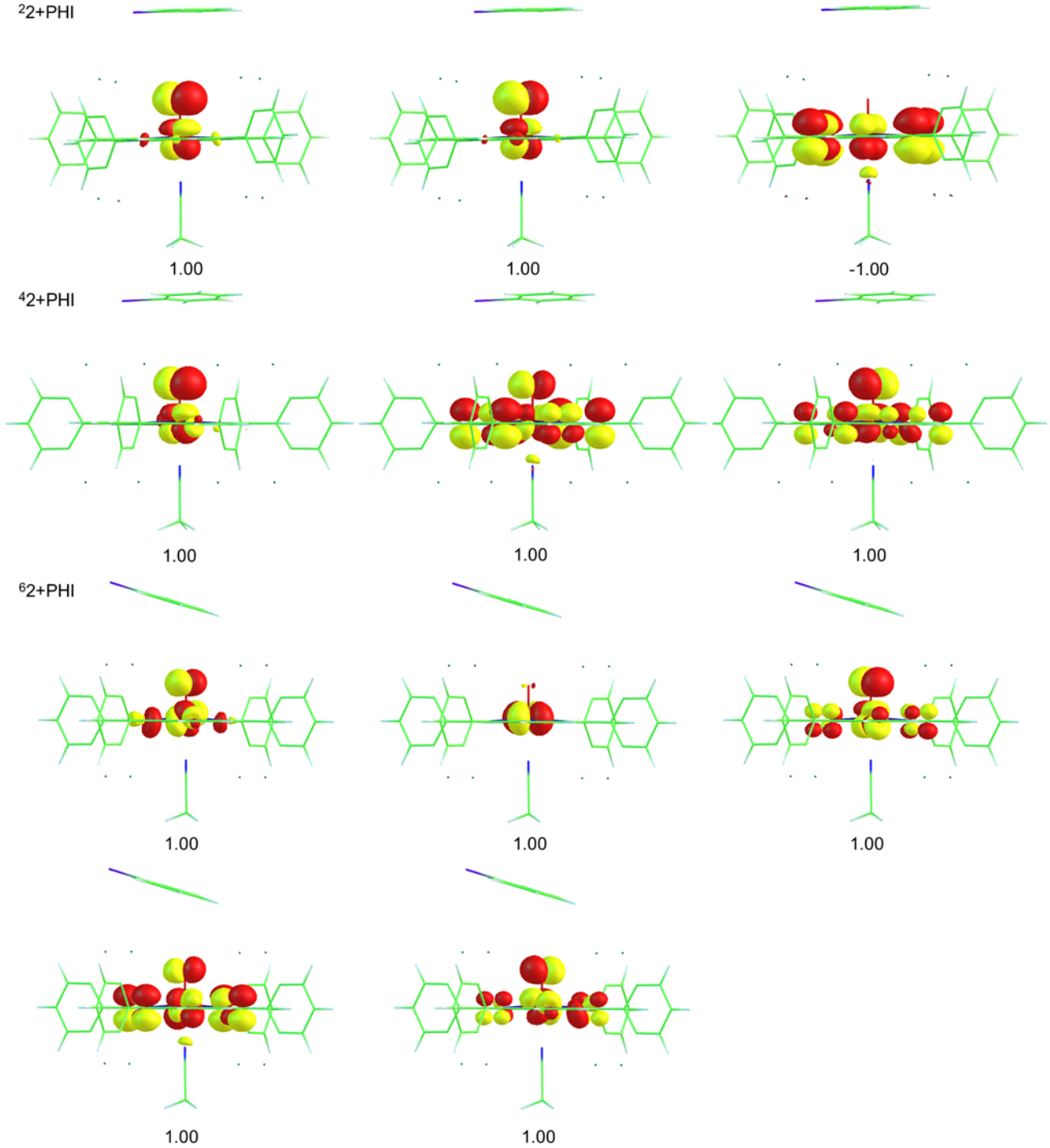


Table S7. Mulliken spin density and charge of the key intermediates in the chemical equilibrium between **1b** and **2** in the absence of counterion OTf. Calculations are at the UB3LYP/LANL2DZdp(I),LANL2DZ(Fe),6-31G**(N,O),6-31G*(S),6-31G(H,C,F,Cl) level.

	Spin densities					Charges				
	Fe	O	I	Por+Acn	Ph	Fe	O	I	Por+Acn	Ph
^{2}**2+PhI**	1.12	0.94	0.00	-1.06	-0.00	0.59	-0.36	-0.04	0.77	0.04
^{4}**2+PhI**	1.09	0.93	-0.00	0.97	0.00	0.58	-0.37	-0.04	0.78	0.04
^{6}**2+PhI**	2.97	0.68	-0.00	1.34	-0.00	0.80	-0.37	-0.04	0.57	0.04
^{2}**TS$_{1b}$**	0.91	0.79	0.07	-0.77	-0.01	0.62	-0.43	0.20	0.51	0.09
^{4}**TS$_{1b}$**	1.18	0.57	0.29	0.93	0.03	0.65	-0.53	0.25	0.56	0.07
^{6}**TS$_{1b}$**	3.89	0.21	-0.32	1.23	-0.01	0.91	-0.63	0.42	0.18	0.12
^{2}**1b**	1.02	0.04	-0.03	-0.04	-0.00	0.73	-0.65	0.79	-0.07	0.20
^{4}**1b**	2.78	0.17	0.04	-0.01	0.01	0.81	-0.69	0.80	-0.08	0.16
^{6}**1b**	4.10	0.18	0.03	0.68	0.01	1.00	-0.68	0.80	-0.28	0.16

Fig. S4 Spin natural orbitals (SNO) and their occupation values of the key intermediates in the chemical equilibrium between **1b** and **2** in the absence of counterion OTf. Calculations are at the UB3LYP/LANL2DZdp(I),LANL2DZ(Fe),6-31G**(N,O),6-31G*(S),6-31G(H,C,F,Cl) level.



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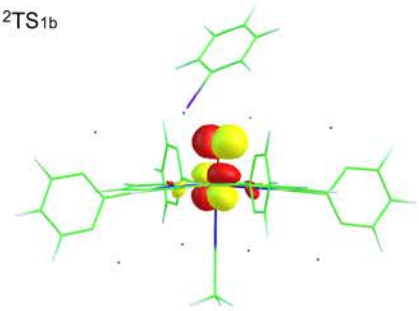

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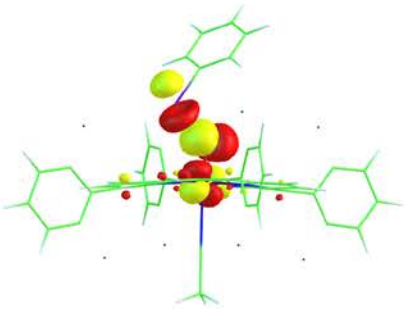

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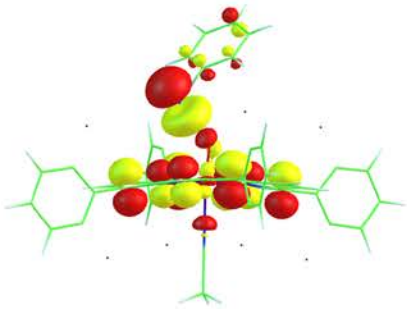

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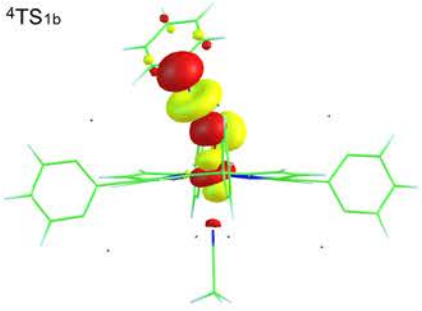

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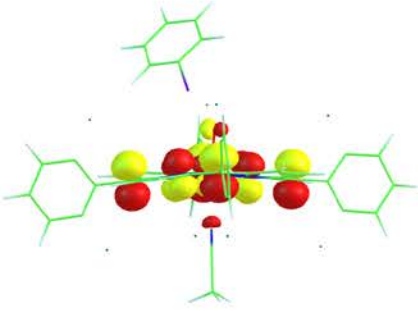

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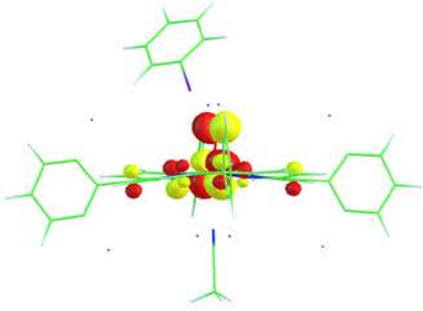

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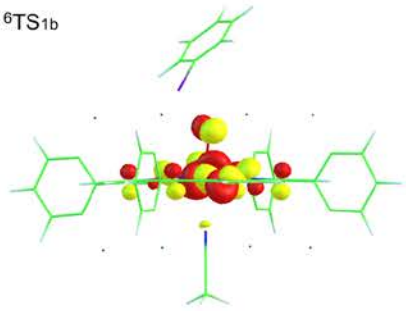
^{6}TS$_{1b}$



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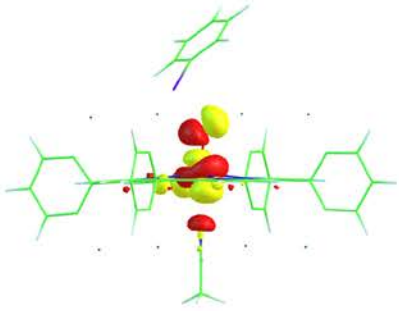

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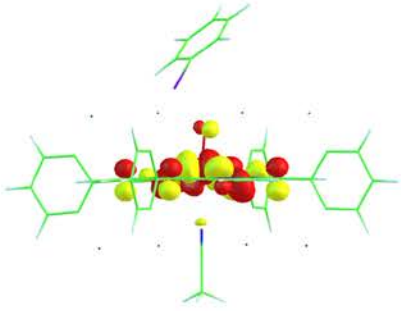

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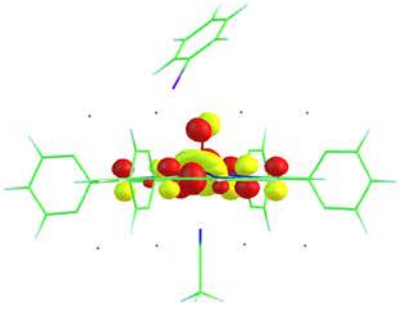

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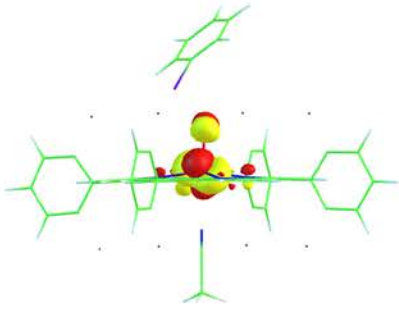

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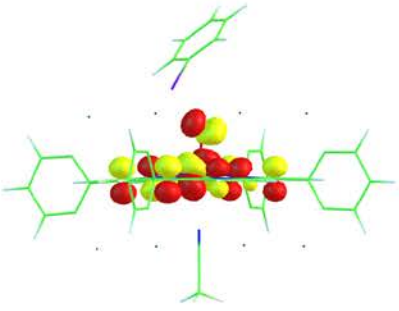

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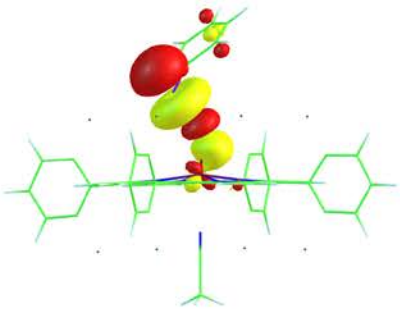

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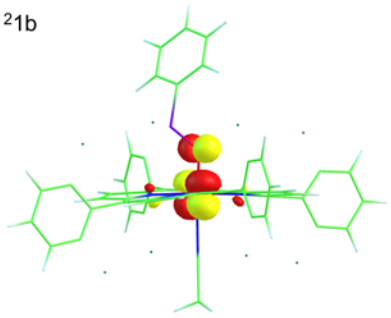

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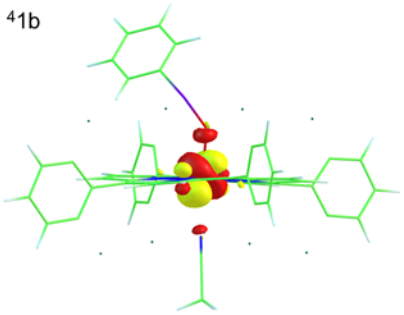

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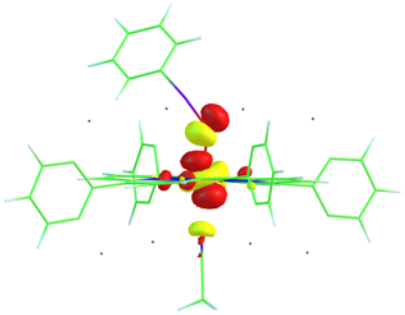

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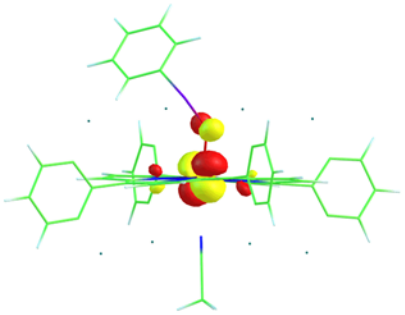

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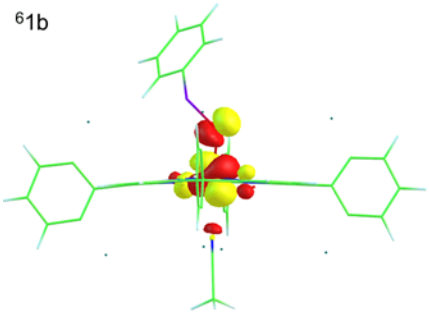
^{6}1b



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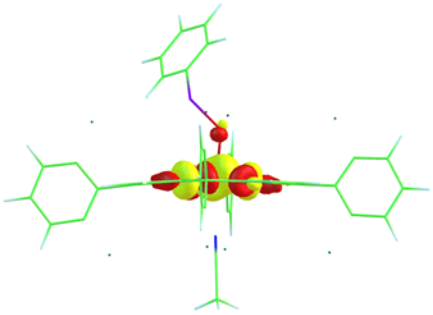

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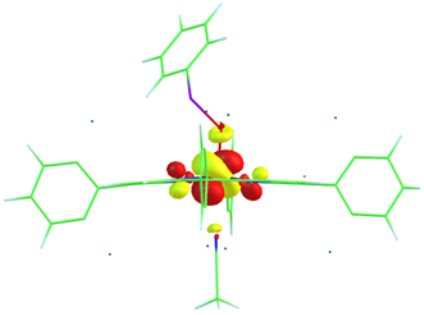

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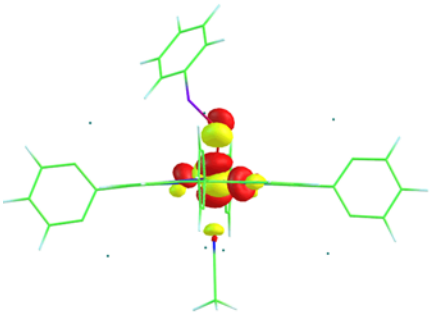

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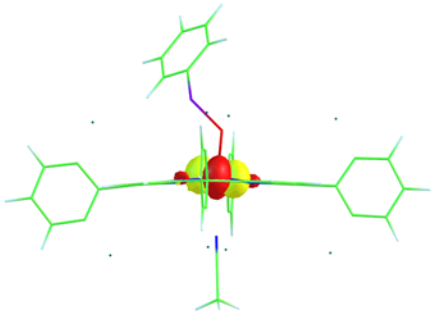


1.00

Fig. S5 The displacement vectors of the transition states in the chemical equilibrium (a) between **1d** and **2** in the presence of OTf and (b) between **1b** and **2** in the absence of OTf.

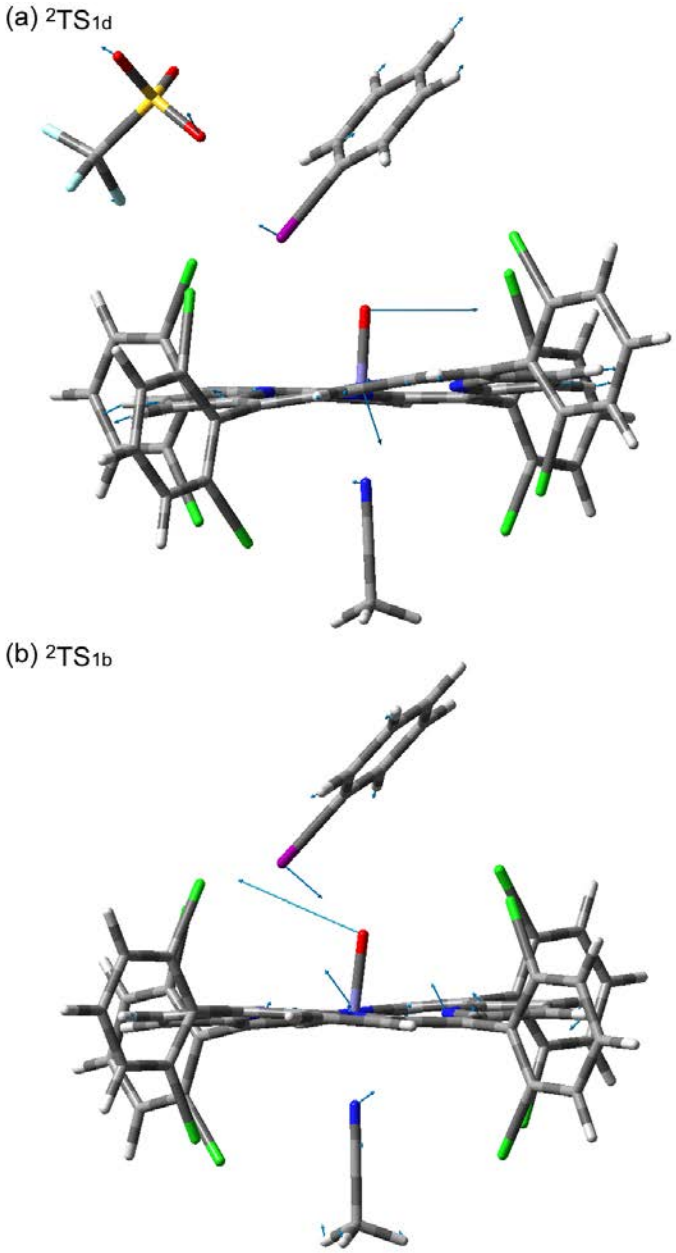


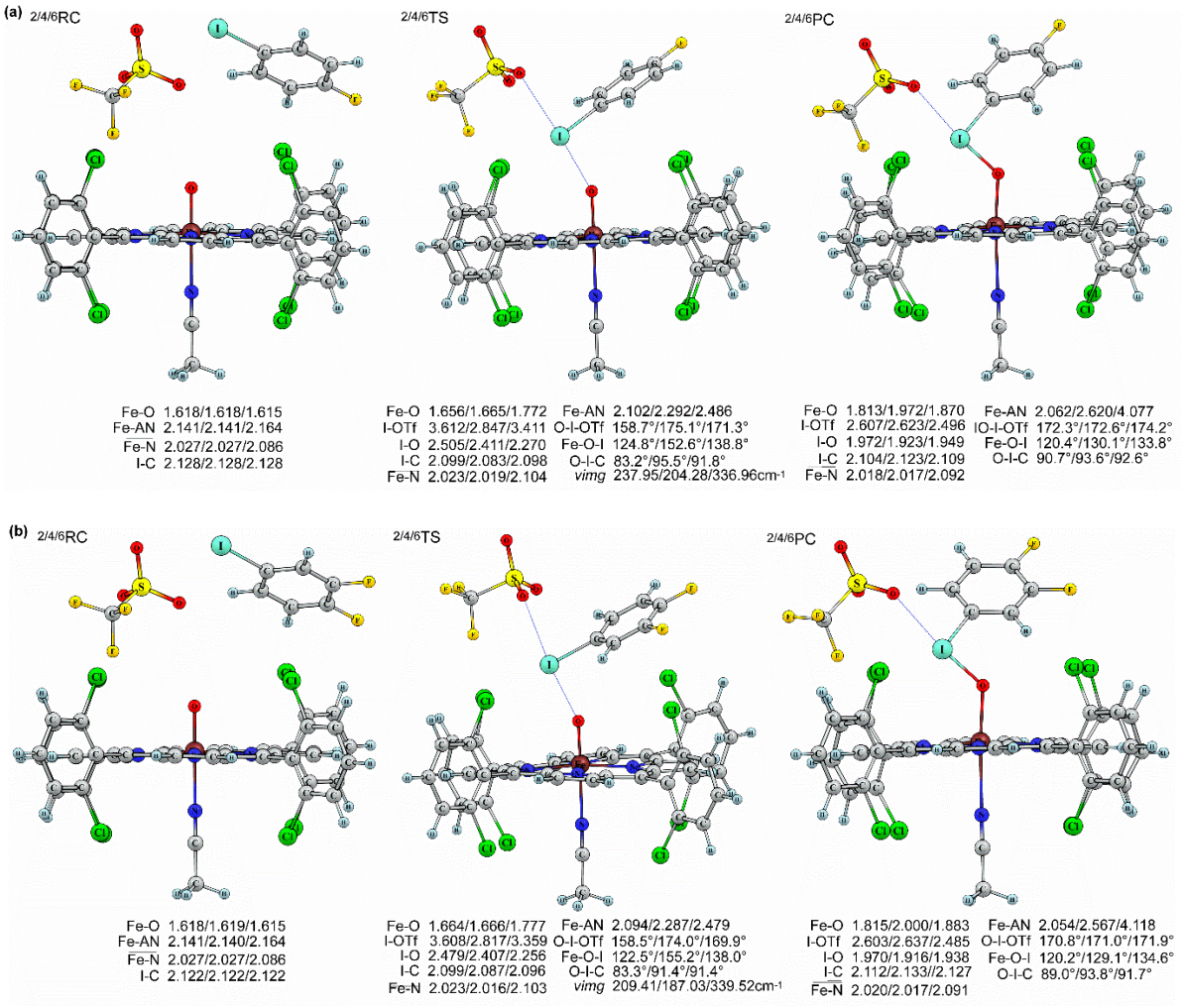
Table S8. Data on the substituent effects. The Gibbs free energy barriers $\Delta G^{\neq}$ and chemical reaction heats ΔG are at the UB3LYP/LANL2DZdp(I),LANL2DZ(Fe),6-31G**(N,O),6-31G*(S),6-31G(H,C,F,Cl) level. Energies are in kcal mol^{-1}.

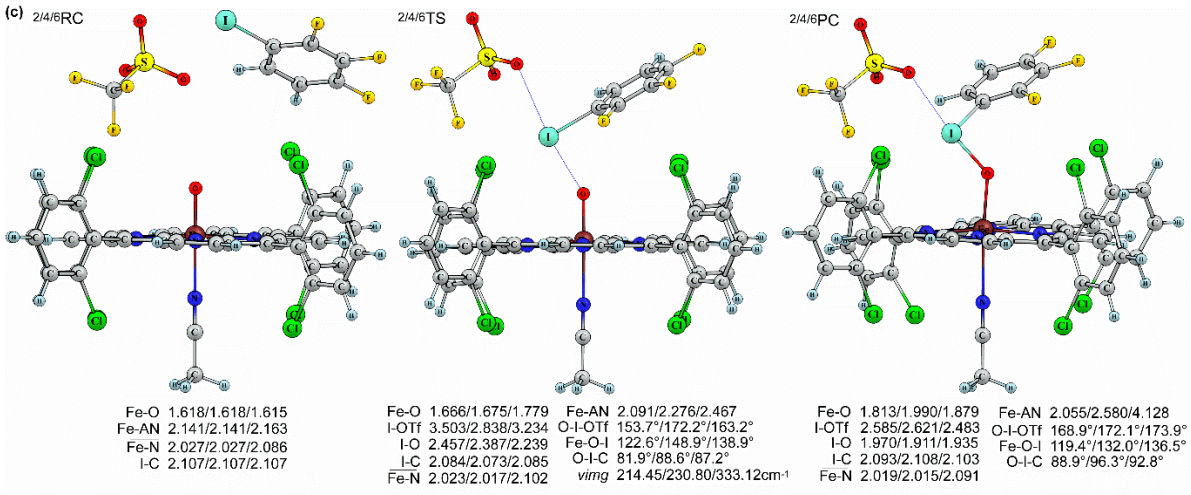
	PhI	FC_6H_4I	$F_2C_6H_3I$	$F_3C_6H_2I$	F_4C_6HI	F_5C_6I
$\Delta G^{\neq}$	16.4	17.6	18.3	18.5	21.1	21.1
ΔG	-0.2	1.6	2.7	5.1	8.3	8.8

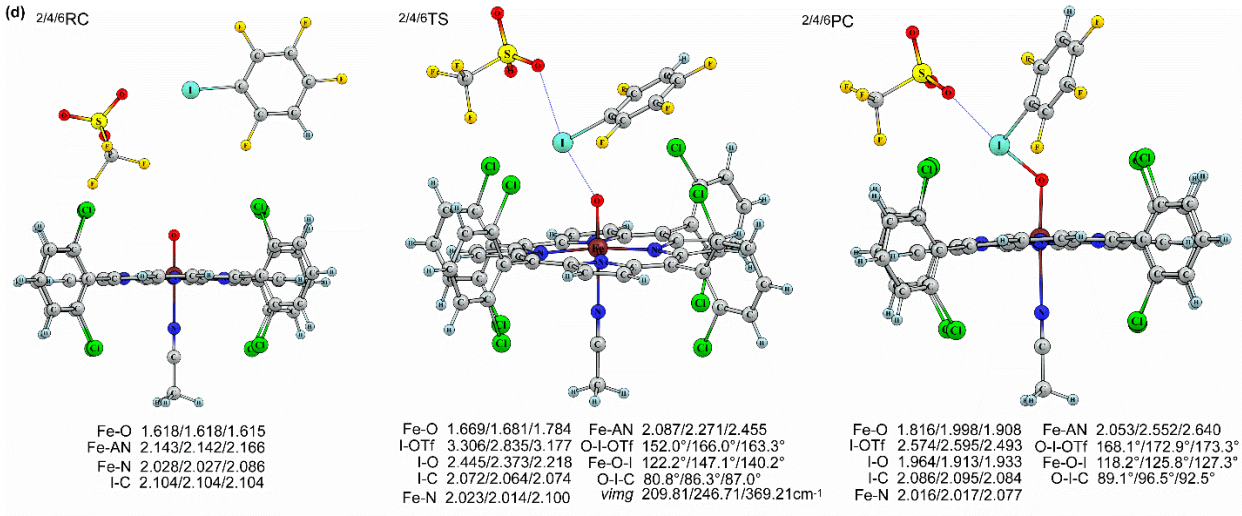
Table S9. Data on the substituent effects. The ionization potentials(IPs) (in kcal mol^{-1}) of substituent iodobenzenes. Calculations are at the UB3LYP/LANL2DZdp(I),6-31G**(N,O),6-31G(H, C, F) level.

	PhI	FC_6H_4I	$F_2C_6H_3I$	$F_3C_6H_2I$	F_4C_6HI	F_5C_6I
IP	150.4	151.3	155.1	159.2	162.6	166.8

Fig. S6 Data on the substituent effects. Geometric information of the key intermediates in the chemical equilibrium between various florine-substituted (a-1F, b-2F, c-3F, d-4F and e-5F substituted PhIOs) **1d** and **2** in the presence of counterion OTf. Lengthes are in Å units. Calculations are at the UB3LYP/LANL2DZdp(I),LANL2DZ(Fe),6-31G**(N,O),6-31G*(S),6-31G(H,C,F,Cl) level.




(c)
2/4/6RC
Fe-O 1.618/1.618/1.615
Fe-AN 2.141/2.141/2.163
Fe-N 2.027/2.027/2.086
I-C 2.107/2.107/2.107
2/4/6TS
Fe-O 1.666/1.675/1.779
I-OTf 3.503/2.838/3.234
I-O 2.457/2.387/2.239
I-C 2.084/2.073/2.085
Fe-N 2.023/2.017/2.102
Fe-AN 2.091/2.276/2.467
O-I-OTf 153.7°/172.2°/163.2°
Fe-O-I 122.6°/148.9°/138.9°
O-I-C 81.9°/88.6°/87.2°
vimg 214.45/230.80/333.12cm-1
2/4/6PC
Fe-O 1.813/1.990/1.879
I-OTf 2.585/2.621/2.483
I-O 1.970/1.911/1.935
I-C 2.093/2.108/2.103
Fe-N 2.019/2.015/2.091
Fe-AN 2.055/2.580/4.128
O-I-OTf 168.9°/172.1°/173.9°
Fe-O-I 119.4°/132.0°/136.5°
O-I-C 88.9°/96.3°/92.8°


(d)
2/4/6RC
Fe-O 1.618/1.618/1.615
Fe-AN 2.143/2.142/2.166
Fe-N 2.028/2.027/2.086
I-C 2.104/2.104/2.104
2/4/6TS
Fe-O 1.669/1.681/1.784
I-OTf 3.306/2.835/3.177
I-O 2.445/2.373/2.218
I-C 2.072/2.064/2.074
Fe-N 2.023/2.014/2.100
Fe-AN 2.087/2.271/2.455
O-I-OTf 152.0°/166.0°/163.3°
Fe-O-I 122.2°/147.1°/140.2°
O-I-C 80.8°/86.3°/87.0°
vimg 209.81/246.71/369.21cm-1
2/4/6PC
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I-OTf 2.574/2.595/2.493
I-O 1.964/1.913/1.933
I-C 2.086/2.095/2.084
Fe-N 2.016/2.017/2.077
Fe-AN 2.053/2.552/2.640
O-I-OTf 168.1°/172.9°/173.3°
Fe-O-I 118.2°/125.8°/127.3°
O-I-C 89.1°/96.5°/92.5°

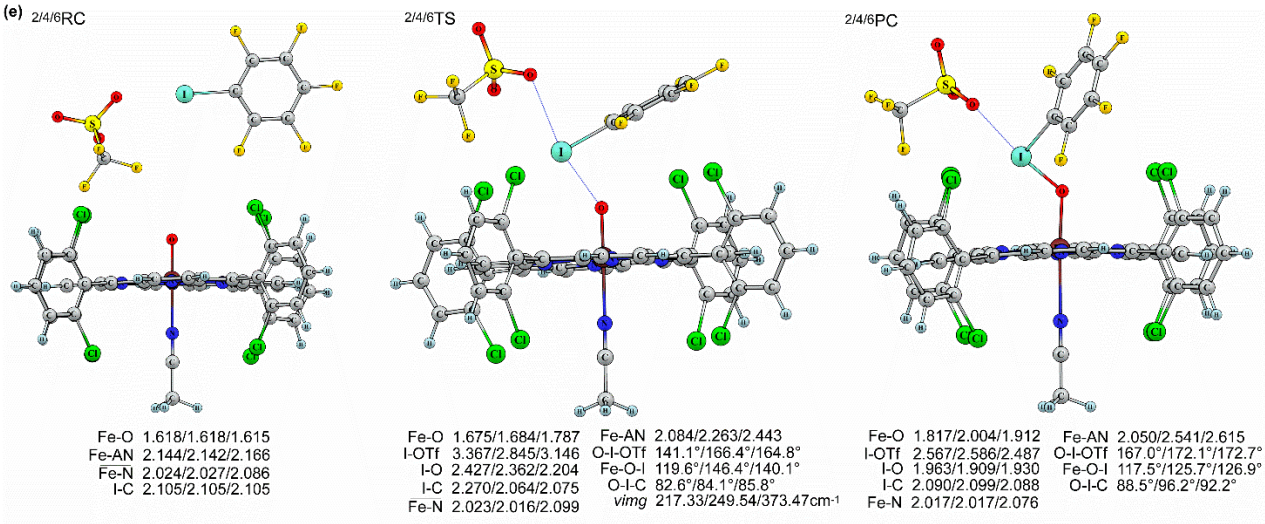
(e)
2/4/6RC
Fe-O 1.618/1.618/1.615
Fe-AN 2.144/2.142/2.166
Fe-N 2.024/2.027/2.086
I-C 2.105/2.105/2.105
2/4/6TS
Fe-O 1.675/1.684/1.787
I-OTf 3.367/2.845/3.146
I-O 2.427/2.362/2.204
I-C 2.270/2.064/2.075
Fe-N 2.023/2.016/2.099
Fe-AN 2.084/2.263/2.443
O-I-OTf 141.1°/166.4°/164.8°
Fe-O-I 119.6°/146.4°/140.1°
O-I-C 82.6°/84.1°/85.8°
vimg 217.33/249.54/373.47cm-1
2/4/6PC
Fe-O 1.817/2.004/1.912
I-OTf 2.567/2.586/2.487
I-O 1.963/1.909/1.930
I-C 2.090/2.099/2.088
Fe-N 2.017/2.017/2.076
Fe-AN 2.050/2.541/2.615
O-I-OTf 167.0°/172.1°/172.7°
Fe-O-I 117.5°/125.7°/126.9°
O-I-C 88.5°/96.2°/92.2°

Table S10. Data on the substituent effects. Various calculated energies of the key intermediates in the chemical equilibrium between various florine-substituted (a-1F, b-2F, c-3F, d-4F and e-5F substituted PhIOs) **1d** and **2** in the presence of counterion OTf. Lengthes are in Å units. Calculations are at the UB3LYP/LANL2DZdp(I),LANL2DZ(Fe),6-31G**(N,O),6-31G*(S),6-31G(H,C,F,Cl) level. Absolute SCF energies and Gibbs free energies are in a.u. and the relative ones are in kcal mol^{-1}.

(a) For the one-fluorine substituent case

	SCF	ΔE	SCF+ZPE	ΔE	G	ΔG
^{2}RC	-7223.699473	0.2	-7223.016803	0.0	-7223.10732	0.0
^{4}RC	-7223.699783	0.0	-7223.016702	0.1	-7223.106235	0.7
^{6}RC	-7223.676792	14.4	-7222.995466	13.4	-7223.08604	13.4
^{2}TS	-7223.676278	14.8	-7222.992801	15.1	-7223.079328	17.6
^{4}TS	-7223.667962	20.0	-7222.984366	20.4	-7223.07211	22.1
^{6}TS	-7223.662671	23.3	-7222.98413	20.5	-7223.073033	21.5
^{2}PC	-7223.703343	-2.2	-7223.017365	-0.4	-7223.100872	4.0
^{4}PC	-7223.700311	-0.3	-7223.016223	0.4	-7223.102666	2.9
^{6}PC	-7223.697863	1.2	-7223.015395	0.9	-7223.104816	1.6

(b) For the two-fluorine substituent case

	SCF	ΔE	SCF+ZPE	ΔE	G	ΔG
^{2}RC	-7322.90384	0.2	-7322.229671	0.0	-7322.32009	0.1
^{4}RC	-7322.904146	0.0	-7322.229602	0.0	-7322.320174	0.0
^{6}RC	-7322.881166	14.4	-7322.208294	13.4	-7322.29859	13.6
^{2}TS	-7322.88069	14.7	-7322.205427	15.2	-7322.291073	18.3
^{4}TS	-7322.870567	21.1	-7322.195364	21.5	-7322.282591	23.6
^{6}TS	-7322.865664	24.2	-7322.195539	21.4	-7322.286403	21.2
^{2}PC	-7322.90689	-1.7	-7322.22912	0.3	-7322.311114	5.7
^{4}PC	-7322.904054	0.1	-7322.228127	1.0	-7322.313825	4.0
^{6}PC	-7322.900439	2.3	-7322.226356	2.1	-7322.316024	2.7

(c) For the three-fluorine substituent case

	SCF	ΔE	SCF+ZPE	ΔE	G	ΔG
^{2}RC	-7422.10654	0.2	-7421.440681	0.0	-7421.530896	0.0
^{4}RC	-7422.106849	0.0	-7421.440612	0.0	-7421.530893	0.0
^{6}RC	-7422.083854	14.4	-7421.419384	13.4	-7421.510358	12.9
^{2}TS	-7422.083181	14.9	-7421.416123	15.4	-7421.501381	18.5
^{4}TS	-7422.071881	21.9	-7421.40517	22.3	-7421.492956	23.8
^{6}TS	-7422.068417	24.1	-7421.406433	21.5	-7421.496013	21.9
^{2}PC	-7422.107531	-0.4	-7421.438224	1.5	-7421.521231	6.1
^{4}PC	-7422.103332	2.2	-7421.435877	3.0	-7421.52273	5.1
^{6}PC	-7422.099594	4.6	-7421.433783	4.3	-7421.521331	6.0

(d) For the four-fluorine substituent case

	SCF	ΔE	SCF+ZPE	ΔE	G	ΔG
^{2}RC	-7521.317387	0.2	-7520.660097	0.0	-7520.750243	0.1
^{4}RC	-7521.317694	0.0	-7520.660043	0.0	-7520.750365	0.0
^{6}RC	-7521.294827	14.4	-7520.63884	13.3	-7520.729119	13.4
^{2}TS	-7521.28894	18.1	-7520.630488	18.6	-7520.716721	21.1
^{4}TS	-7521.276978	25.6	-7520.618791	25.9	-7520.706307	27.7
^{6}TS	-7521.274175	27.3	-7520.620652	24.8	-7520.709493	25.7
^{2}PC	-7521.312581	3.2	-7520.652037	5.1	-7520.735296	9.5
^{4}PC	-7521.309425	5.2	-7520.650631	5.9	-7520.737169	8.3
^{6}PC	-7521.301529	10.2	-7520.644515	9.8	-7520.733104	10.9

(e) For the five-fluorine substituent case

	SCF	ΔE	SCF+ZPE	ΔE	G	ΔG
^{2}RC	-7620.511609	0.3	-7619.862216	0.3	-7619.950701	1.1
^{4}RC	-7620.51212	0.0	-7619.862724	0.0	-7619.952404	0.0
^{6}RC	-7620.489212	14.4	-7619.841572	13.3	-7619.932182	12.7
^{2}TS	-7620.480815	19.6	-7619.830802	20.0	-7619.918869	21.1
^{4}TS	-7620.468887	27.1	-7619.81904	27.1	-7619.906804	28.6
^{6}TS	-7620.466875	28.4	-7619.821559	25.8	-7619.910539	26.3
^{2}PC	-7620.504551	4.7	-7619.852359	6.5	-7619.936362	10.1
^{4}PC	-7620.501457	6.7	-7619.851033	7.3	-7619.938448	8.8
^{6}PC	-7620.493174	11.9	-7619.844453	11.4	-7619.932679	12.4

Table S12. Data on the substituent effects. Mulliken spin density and charge of the key intermediates in the chemical equilibrium between various florine-substituted (a-1F, b-2F, c-3F, d-4F and e-5F substituted PhIOs) **1d** and **2** in the presence of counterion OTf. Lengthes are in Å units. Calculations are at the UB3LYP/LANL2DZdp(I),LANL2DZ(Fe),6-31G**(N,O),6-31G*(S),6-31G(H,C,F,Cl) level.

(a) For the one-fluorine substituent case

	Spin densities						Charges					
	Fe	O	I	Por+An	Ph	OTf	Fe	O	I	Por+An	Ph	OTf
^{2}RC	1.12	0.94	-0.00	-1.05	-0.00	0.00	0.56	-0.36	-0.04	0.74	-0.01	-0.89
^{4}RC	1.08	0.94	0.00	0.97	0.00	0.00	0.56	-0.36	-0.04	0.74	-0.01	-0.89
^{6}RC	3.01	0.65	0.00	1.33	-0.00	-0.00	0.76	-0.37	-0.04	0.55	-0.01	-0.89
^{2}TS	0.99	0.67	-0.12	-0.51	-0.03	-0.00	0.63	-0.42	0.25	0.35	0.08	-0.88
^{4}TS	1.78	0.54	0.59	-0.08	0.09	0.08	0.73	-0.52	0.45	-0.02	0.16	-0.79
^{6}TS	3.87	0.23	-0.35	1.26	-0.01	-0.01	0.90	-0.63	0.34	0.18	0.09	-0.89
^{4}PC	0.95	0.10	-0.00	-0.04	-0.00	-0.00	0.64	-0.65	0.73	-0.06	0.12	-0.77
^{2}PC	2.77	0.20	0.03	-0.01	0.01	0.00	0.79	-0.73	0.78	-0.13	0.08	-0.78
^{6}PC	4.02	0.27	0.04	0.65	0.01	0.01	1.05	-0.77	0.82	-0.50	0.14	-0.74

(b) For the two-fluorine substituent case

	Spin densities						Charges					
	Fe	O	I	Por+An	Ph	OTf	Fe	O	I	Por+An	Ph	OTf
^{2}RC	1.12	0.94	0.00	-1.06	0.00	0.00	0.56	-0.36	-0.01	0.75	-0.04	-0.89
^{4}RC	1.09	0.94	0.00	0.97	0.00	0.00	0.56	-0.36	-0.01	0.74	-0.04	-0.89
^{6}RC	3.01	0.65	0.00	1.33	-0.00	-0.00	0.76	-0.37	-0.01	0.55	-0.03	-0.89
^{2}TS	0.95	0.67	-0.06	-0.54	-0.02	-0.00	0.63	-0.43	0.27	0.37	0.04	-0.88
^{4}TS	1.78	0.55	0.60	-0.07	0.06	0.09	0.73	-0.53	0.47	-0.02	0.12	-0.78
^{6}TS	3.88	0.22	-0.34	1.26	-0.01	-0.01	0.90	-0.63	0.36	0.19	0.06	-0.88
^{4}PC	0.95	0.10	-0.00	-0.04	-0.00	-0.00	0.65	-0.65	0.77	-0.06	0.06	-0.77
^{2}PC	2.79	0.18	0.03	-0.01	0.01	0.00	0.79	-0.73	0.81	-0.12	0.03	-0.79
^{6}PC	4.03	0.25	0.04	0.66	0.01	0.01	1.06	-0.78	0.86	-0.49	0.08	-0.73

(c) For the three-fluorine substituent case

	Spin densities						Charges					
	Fe	O	I	Por+An	Ph	OTf	Fe	O	I	Por+An	Ph	OTf
^{2}RC	1.12	0.94	0.00	-1.06	0.00	0.00	0.56	-0.36	0.04	0.75	-0.09	-0.89
^{4}RC	1.08	0.94	0.00	0.97	0.00	0.00	0.56	-0.36	0.04	0.74	-0.09	-0.89
^{6}RC	3.01	0.65	0.00	1.33	-0.00	-0.00	0.76	-0.37	0.04	0.55	-0.09	-0.89
^{2}TS	0.95	0.66	-0.05	-0.53	-0.01	-0.00	0.63	-0.43	0.30	0.36	0.01	-0.87
^{4}TS	1.82	0.55	0.57	-0.07	0.06	0.08	0.74	-0.53	0.48	0.01	0.08	-0.78
^{6}TS	3.88	0.22	-0.35	1.26	-0.00	-0.01	0.91	-0.63	0.41	0.18	0.02	-0.87
^{4}PC	0.95	0.09	-0.00	-0.04	-0.00	-0.00	0.64	-0.65	0.77	-0.05	0.04	-0.76
^{2}PC	2.78	0.18	0.04	-0.01	0.01	0.00	0.79	-0.73	0.82	-0.11	0.02	-0.79
^{6}PC	4.03	0.25	0.04	0.66	0.01	0.01	1.06	-0.77	0.88	-0.49	0.05	-0.74

(d) For the four-fluorine substituent case

	Spin densities						Charges					
	Fe	O	I	Por+An	Ph	OTf	Fe	O	I	Por+An	Ph	OTf
^{2}RC	1.12	0.94	-0.00	-1.06	-0.00	0.00	0.56	-0.36	0.09	0.73	-0.17	-0.85
^{4}RC	1.09	0.94	-0.00	0.97	0.00	0.00	0.56	-0.36	0.09	0.73	-0.17	-0.85
^{6}RC	3.02	0.65	-0.00	1.33	-0.00	-0.00	0.76	-0.36	0.09	0.53	-0.17	-0.85
^{2}TS	0.94	0.66	-0.02	-0.56	-0.01	-0.01	0.63	-0.44	0.31	0.39	-0.02	-0.87
^{4}TS	1.84	0.55	0.55	-0.07	0.05	0.08	0.74	-0.53	0.50	0.03	0.03	-0.78
^{6}TS	3.88	0.21	-0.33	1.26	-0.01	-0.01	0.91	-0.64	0.44	0.18	-0.02	-0.87
^{4}PC	0.96	0.09	-0.00	-0.04	-0.00	-0.00	0.65	-0.65	0.79	-0.03	-0.00	-0.75
^{2}PC	2.78	0.18	0.03	-0.01	0.01	0.00	0.78	-0.72	0.83	-0.10	-0.00	-0.78
^{6}PC	4.08	0.25	0.03	0.61	0.01	0.01	0.97	-0.75	0.85	-0.37	0.03	-0.73

(e) For the five-fluorine substituent case

	Spin densities						Charges					
	Fe	O	I	Por+An	Ph	OTf	Fe	O	I	Por+An	Ph	OTf
^{2}RC	1.12	0.94	-0.00	-1.05	0.00	0.00	0.57	-0.36	0.11	0.74	-0.20	-0.85
^{4}RC	1.09	0.94	-0.00	0.97	-0.00	0.00	0.56	-0.36	0.12	0.73	-0.20	-0.85
^{6}RC	3.02	0.65	-0.00	1.33	-0.00	-0.00	0.76	-0.36	0.12	0.53	-0.20	-0.84
^{2}TS	0.93	0.65	-0.00	-0.57	-0.01	-0.00	0.63	-0.44	0.32	0.41	-0.05	-0.87
^{4}TS	1.85	0.54	0.54	-0.07	0.05	0.08	0.75	-0.53	0.50	0.05	-0.00	-0.77
^{6}TS	3.89	0.21	-0.33	1.25	-0.01	-0.01	0.91	-0.64	0.46	0.18	-0.05	-0.86
^{4}PC	0.96	0.09	-0.00	-0.04	-0.00	-0.00	0.65	-0.65	0.80	-0.02	-0.04	-0.74
^{2}PC	2.79	0.17	0.03	-0.01	0.01	0.00	0.78	-0.72	0.85	-0.09	-0.03	-0.78
^{6}PC	4.09	0.25	0.03	0.62	0.01	0.01	0.97	-0.75	0.89	-0.37	0.01	-0.74

Supplementary Cartesian Coordinates

$^{2}2_{(1a)}$

Fe	1.316156	-0.348524	0.201756
N	0.720204	1.547989	0.393785
C	-0.200882	2.024194	1.320316
C	-0.518946	3.403943	1.040691
C	0.230934	3.780113	-0.033976
C	0.993949	2.626625	-0.442745
H	-1.210641	4.006960	1.606546
H	0.264030	4.746143	-0.511565
C	1.866505	2.615675	-1.530723
N	2.395576	0.199482	-1.412765
C	2.506618	1.462906	-1.983906
C	3.342324	1.408235	-3.158220
C	3.720313	0.108174	-3.320194
C	3.147179	-0.639407	-2.226384
H	3.597485	2.252885	-3.777770
H	4.346741	-0.306156	-4.093654
C	3.381694	-1.996628	-2.001161
N	2.272332	-2.110316	0.213774
C	2.980688	-2.664989	-0.845336
C	3.313307	-4.040301	-0.556858
C	2.813541	-4.321887	0.678935
C	2.148525	-3.129749	1.148229
H	3.866153	-4.694637	-1.211460
H	2.877983	-5.250573	1.222649
C	1.450819	-3.053399	2.353138
N	0.575796	-0.762364	2.015751
C	0.714453	-1.936251	2.742496
C	-0.054767	-1.861873	3.963199
C	-0.678784	-0.651594	3.967595
C	-0.285172	0.032108	2.755976
H	-0.106426	-2.636799	4.710947
H	-1.334357	-0.247686	4.722121
C	-0.686914	1.325721	2.426694
O	-0.151409	-1.032126	-0.647176
C	-1.625301	2.030039	3.360115
C	-3.021118	1.897202	3.266334
C	-1.165355	2.858933	4.398998
C	-3.908333	2.539759	4.125584
C	-2.015482	3.520388	5.280594
C	-3.396899	3.357581	5.137522
H	-4.975498	2.403817	4.007946
H	-1.608643	4.146992	6.063568
H	-4.073198	3.864958	5.815187
C	1.455791	-4.250759	3.254010
C	0.479375	-5.258638	3.169516
C	2.438604	-4.441064	4.240232
C	0.466295	-6.378522	3.996028
C	2.464535	-5.544370	5.088743
C	1.468413	-6.517439	4.961389
H	-0.308755	-7.126254	3.889172
H	3.244437	-5.642331	5.832619
H	1.473062	-7.382933	5.613252
C	4.148482	-2.761920	-3.036139
C	3.510327	-3.393188	-4.117636
C	5.547192	-2.895979	-2.997461
C	4.193496	-4.108829	-5.096394
C	6.271893	-3.601221	-3.954261
C	5.585446	-4.210506	-5.009198
H	3.652124	-4.576739	-5.908250
H	7.349016	-3.673112	-3.878334
H	6.134248	-4.763400	-5.762253
C	2.135931	3.907215	-2.242758
C	1.397430	4.340143	-3.357188
C	3.164985	4.772149	-1.828691
C	1.647546	5.537772	-4.021442
C	3.450973	5.977895	-2.462267
C	2.683165	6.359370	-3.566800
H	1.047006	5.822956	-4.875337
H	4.255790	6.605449	-2.102243
H	2.891559	7.294711	-4.072439
Cl	-3.732040	0.831802	1.962527
Cl	0.634863	3.087508	4.634360
Cl	6.484064	-2.110641	-1.636702
Cl	1.688484	-3.287170	-4.266910
Cl	-0.847801	-5.115766	1.918401
Cl	3.757558	-3.188619	4.439221
Cl	4.197093	4.309695	-0.390756
Cl	0.031792	3.301403	-3.991890
C	-5.263438	1.127451	-1.637562
C	-5.008524	-0.247978	-1.729081
C	-3.705403	-0.710334	-1.939566
C	-2.672926	0.236145	-2.042087
C	-2.904709	1.617630	-1.945591
C	-4.218640	2.054807	-1.746580
H	-3.506381	-1.771725	-2.023061
H	-2.095924	2.332908	-2.027525
H	-4.420345	3.117351	-1.674498
I	-0.723012	-0.439600	-2.429368
H	-6.278030	1.476721	-1.482923
H	-5.819507	-0.962047	-1.645314

$^{4}2_{(1a)}$

Fe	1.316246	-0.353748	0.190644
N	0.718894	1.551142	0.398688
C	-0.166154	2.039626	1.354070
C	-0.486283	3.416963	1.072451
C	0.225805	3.777674	-0.033359
C	0.974272	2.619213	-0.453948
H	-1.155325	4.028782	1.655746
H	0.244489	4.737913	-0.523218
C	1.829516	2.605152	-1.555118
N	2.406716	0.196659	-1.410006
C	2.488522	1.457522	-1.992394
C	3.335530	1.409913	-3.156918
C	3.755465	0.119270	-3.297485
C	3.192932	-0.632504	-2.204670
H	3.571664	2.252930	-3.786057
H	4.401264	-0.285127	-4.060090
C	3.449587	-1.983880	-1.977233
N	2.268980	-2.126942	0.199629
C	3.020529	-2.663212	-0.838100
C	3.349463	-4.038504	-0.552373
C	2.807788	-4.336165	0.662640
C	2.125182	-3.152116	1.124756
H	3.927324	-4.683257	-1.194633
H	2.857851	-5.270607	1.197916
C	1.413622	-3.084023	2.321081
N	0.583202	-0.766794	2.015002
C	0.699076	-1.956474	2.722138
C	-0.058775	-1.879749	3.946427
C	-0.646507	-0.649574	3.978483
C	-0.246061	0.043782	2.779234
H	-0.130126	-2.665999	4.680559
H	-1.285445	-0.242281	4.745254
C	-0.631140	1.347922	2.471649
O	-0.301245	-1.086277	-0.692928
C	-1.539879	2.061139	3.426443
C	-2.939911	1.974272	3.339927
C	-1.046680	2.857044	4.475669
C	-3.800443	2.626819	4.218506
C	-1.869416	3.526984	5.376581
C	-3.256191	3.408281	5.242149
H	-4.872179	2.526816	4.106607
H	-1.437751	4.127078	6.166987
H	-3.911408	3.922726	5.935027
C	1.396703	-4.290551	3.209106
C	0.407704	-5.284394	3.106872
C	2.369863	-4.504376	4.200494
C	0.373757	-6.412805	3.921166
C	2.374865	-5.616944	5.037103
C	1.366904	-6.575247	4.892100
H	-0.410302	-7.148976	3.800702
H	3.147877	-5.733272	5.785488
H	1.355438	-7.447590	5.534666
C	4.260764	-2.732421	-2.989975
C	3.666880	-3.386345	-4.083341
C	5.661205	-2.829180	-2.915334
C	4.393634	-4.088183	-5.040558
C	6.428443	-3.519423	-3.849542
C	5.785171	-4.151906	-4.917963
H	3.885735	-4.574668	-5.863058
H	7.504797	-3.562633	-3.745976
H	6.367319	-4.693616	-5.653936
C	2.073373	3.890030	-2.287369
C	1.328451	4.285733	-3.411381
C	3.081834	4.785351	-1.886839
C	1.552631	5.476954	-4.096203
C	3.341499	5.986019	-2.541012
C	2.567732	6.330223	-3.653613
H	0.948187	5.733032	-4.956556
H	4.131058	6.638084	-2.190899
H	2.756003	7.261108	-4.175141
Cl	-3.692296	0.960109	2.018153
Cl	0.761489	3.031568	4.694529
Cl	6.541712	-2.014640	-1.534230
Cl	1.847512	-3.331307	-4.278455
Cl	-0.908481	-5.109636	1.848340
Cl	3.703775	-3.272144	4.422699

Cl	4.122930	4.371262	-0.440655
Cl	-0.008605	3.201819	-4.030541
C	-5.333596	1.229510	-1.653313
C	-5.182968	-0.163322	-1.701318
C	-3.923082	-0.728133	-1.928812
C	-2.827251	0.132670	-2.098712
C	-2.956378	1.529189	-2.051855
C	-4.227249	2.071313	-1.828744
H	-3.804884	-1.804138	-1.972880
H	-2.100335	2.178434	-2.187759
H	-4.347708	3.148021	-1.791737
I	-0.930740	-0.711088	-2.465024
H	-6.314414	1.658620	-1.481252
H	-6.041543	-0.811351	-1.567024

^{6}2$_{(1a)}$

Fe	1.150745	-0.378800	0.090578
N	0.763023	1.637301	0.443730
C	-0.050372	2.141512	1.448280
C	-0.303108	3.545271	1.206683
C	0.367967	3.886672	0.067628
C	1.033725	2.694642	-0.410803
H	-0.904802	4.185838	1.831568
H	0.409934	4.855136	-0.404818
C	1.836353	2.636271	-1.559110
N	2.411822	0.222558	-1.449130
C	2.472923	1.480733	-2.033440
C	3.309592	1.426151	-3.210399
C	3.753485	0.139715	-3.333675
C	3.207407	-0.610472	-2.225891
H	3.532325	2.261418	-3.855057
H	4.403868	-0.259333	-4.095594
C	3.485159	-1.958875	-1.961621
N	2.248759	-2.153567	0.179889
C	3.047443	-2.662890	-0.830360
C	3.391153	-4.036485	-0.531168
C	2.802134	-4.348657	0.660218
C	2.082475	-3.173351	1.102670
H	4.006089	-4.672979	-1.147246
H	2.849868	-5.285998	1.191267
C	1.331402	-3.096375	2.283913
N	0.551969	-0.751246	2.049226
C	0.623603	-1.964789	2.714414
C	-0.139878	-1.889251	3.940183
C	-0.667983	-0.631211	4.010650
C	-0.229986	0.082755	2.832005
H	-0.253058	-2.690143	4.653369
H	-1.288251	-0.222292	4.792207
C	-0.527920	1.425262	2.554571
O	-0.444050	-1.023649	-0.762736
C	-1.390705	2.159057	3.538144
C	-2.791475	2.191738	3.428534
C	-0.853672	2.857559	4.633646
C	-3.612511	2.862752	4.330507
C	-1.635645	3.542295	5.559617
C	-3.025112	3.541625	5.402507
H	-4.686733	2.855945	4.199386
H	-1.170706	4.064483	6.385668
H	-3.648897	4.069183	6.114300
C	1.288080	-4.314350	3.158099
C	0.296162	-5.301046	3.024744
C	2.239239	-4.545235	4.167076
C	0.238731	-6.438528	3.825241
C	2.220961	-5.667236	4.990715
C	1.210848	-6.617983	4.814309
H	-0.546988	-7.168494	3.680273
H	2.977913	-5.796432	5.753288
H	1.181460	-7.497436	5.446527
C	4.340180	-2.695169	-2.949278
C	3.789683	-3.385258	-4.042962
C	5.741296	-2.742705	-2.847655
C	4.557880	-4.075937	-4.975702
C	6.549395	-3.420039	-3.756609
C	5.948270	-4.090101	-4.826664
H	4.082512	-4.591511	-5.799953
H	7.624449	-3.424775	-3.632466
H	6.562252	-4.622406	-5.543405
C	2.065967	3.913796	-2.311770
C	1.263612	4.317698	-3.392225
C	3.112228	4.792369	-1.976902
C	1.468489	5.500758	-4.097049
C	3.354711	5.984654	-2.652849
C	2.523443	6.337303	-3.720426
H	0.819152	5.763380	-4.922011
H	4.174989	6.624052	-2.353675
H	2.697681	7.261796	-4.257987
Cl	-3.599472	1.319646	2.038410
Cl	0.959615	2.882996	4.876974
Cl	6.567097	-1.878983	-1.462302
Cl	1.973276	-3.393346	-4.272627
Cl	-0.993818	-5.103353	1.741997
Cl	3.575994	-3.324121	4.431028
Cl	4.227644	4.368109	-0.590138
Cl	-0.127609	3.254963	-3.924891
C	-5.526545	0.947343	-1.771918
C	-5.326070	-0.437992	-1.847008
C	-4.046450	-0.952540	-2.079780
C	-2.984087	-0.046792	-2.232157
C	-3.162311	1.344143	-2.163104
C	-4.451896	1.833601	-1.929373
H	-3.887155	-2.022300	-2.138821
H	-2.330013	2.026415	-2.285878
H	-4.612625	2.903945	-1.872220
I	-1.059363	-0.810082	-2.575754
H	-6.522273	1.337126	-1.592679
H	-6.160376	-1.119217	-1.726057

^{2}2$_{(1b)}$

Fe	1.428146	-0.049442	0.327671
N	0.868756	1.870115	0.507787
C	0.042231	2.381336	1.494317
C	-0.141514	3.801529	1.289735
C	0.602833	4.151615	0.201975
C	1.228328	2.945864	-0.289285
H	-0.748070	4.443669	1.908105
H	0.713573	5.130698	-0.236039
C	2.048446	2.891216	-1.420466
N	2.320641	0.426714	-1.425966
C	2.546638	1.698960	-1.949143
C	3.340691	1.600902	-3.148205
C	3.609237	0.276813	-3.347623
C	3.005181	-0.452987	-2.258310
H	3.648170	2.435295	-3.758260
H	4.182036	-0.164797	-4.147339
C	3.166058	-1.825105	-2.050084
N	2.090631	-1.945911	0.182483
C	2.741852	-2.501319	-0.901225
C	2.983233	-3.909232	-0.659653
C	2.485626	-4.193884	0.576295
C	1.916238	-2.969063	1.095576
H	3.473826	-4.581161	-1.345572
H	2.489685	-5.142396	1.089158
C	1.250365	-2.872409	2.319914
N	0.565301	-0.508105	2.089089
C	0.602406	-1.715034	2.758064
C	-0.174220	-1.627120	3.977817
C	-0.690297	-0.367978	4.029825
C	-0.217515	0.333146	2.851768
H	-0.308311	-2.428061	4.687262
H	-1.322974	0.056718	4.792742
C	-0.490856	1.676277	2.577749
O	-0.137137	-0.567754	-0.441973
C	-1.370755	2.421301	3.536692
C	-2.765719	2.485642	3.376592
C	-0.861911	3.099538	4.658265
C	-3.606160	3.167869	4.251858
C	-1.663280	3.794283	5.560083
C	-3.045426	3.826067	5.350625
H	-4.674593	3.184807	4.080403
H	-1.218709	4.299575	6.407611
H	-3.684117	4.362074	6.042624
C	1.187145	-4.091435	3.189011
C	0.150387	-5.035918	3.091022
C	2.164261	-4.368589	4.160727
C	0.075373	-6.174266	3.888969
C	2.130247	-5.492601	4.981170
C	1.075398	-6.399519	4.840075
H	-0.745383	-6.869765	3.771075
H	2.909533	-5.657003	5.713889
H	1.032843	-7.280152	5.469929
C	3.896255	-2.611197	-3.097565
C	3.233211	-3.206081	-4.184930
C	5.288501	-2.805471	-3.062814
C	3.886035	-3.939924	-5.171422
C	5.983716	-3.530355	-4.026861
C	5.272485	-4.099973	-5.087460
H	3.324999	-4.377474	-5.986887
H	7.056953	-3.647765	-3.951979
H	5.797551	-4.667567	-5.846544
C	2.399287	4.175016	-2.109448
C	1.622863	4.721826	-3.146224
C	3.540002	4.918881	-1.757915
C	1.938872	5.913240	-3.793137

C	3.895886	6.113884	-2.376854
C	3.085380	6.611127	-3.401923
H	1.304046	6.288390	-4.585223
H	4.786040	6.644900	-2.065621
H	3.346445	7.539946	-3.895018
Cl	-3.540457	1.635695	1.953613
Cl	0.941057	3.085162	4.972734
Cl	6.261675	-2.076789	-1.694730
Cl	1.417823	-3.026466	-4.331907
Cl	-1.179510	-4.780385	1.859714
Cl	3.562364	-3.207890	4.377941
Cl	4.631444	4.306890	-0.422485
Cl	0.110757	3.848505	-3.695573
C	-5.295410	-1.081720	-2.061450
C	-4.333065	-1.990075	-2.522662
C	-2.982786	-1.625198	-2.565357
C	-2.624431	-0.340352	-2.128768
C	-3.573255	0.584717	-1.666150
C	-4.918545	0.199779	-1.637324
H	-2.237313	-2.322935	-2.927672
H	-3.278801	1.573498	-1.336447
H	-5.665933	0.901190	-1.284308
I	-0.600579	0.218250	-2.188141
H	-6.340069	-1.371326	-2.035740
H	-4.628347	-2.979499	-2.853006
N	3.145881	0.410884	1.324559
C	4.118894	0.667072	1.893186
C	5.344126	0.988640	2.610512
H	5.568139	2.054927	2.516035
H	5.236287	0.743098	3.670734
H	6.181406	0.416340	2.200792

$^{4}2_{(1b)}$

Fe	1.400404	-0.315953	0.243616
N	0.719759	1.570492	0.399283
C	-0.156665	2.055814	1.358757
C	-0.487746	3.431015	1.070138
C	0.211964	3.787215	-0.045585
C	0.964154	2.628027	-0.463879
H	-1.156703	4.043179	1.653409
H	0.218340	4.743197	-0.544296
C	1.811104	2.605788	-1.573834
N	2.386058	0.195336	-1.436685
C	2.463474	1.454729	-2.017883
C	3.300811	1.402910	-3.190720
C	3.722543	0.112001	-3.328475
C	3.169944	-0.636271	-2.226418
H	3.529675	2.242772	-3.826906
H	4.362373	-0.294380	-4.095189
C	3.434678	-1.986565	-1.990191
N	2.270181	-2.133740	0.194260
C	3.011217	-2.667722	-0.848116
C	3.331999	-4.047856	-0.567259
C	2.793673	-4.344628	0.649762
C	2.123231	-3.154336	1.119201
H	3.899690	-4.696468	-1.214884
H	2.837179	-5.281805	1.181060
C	1.418470	-3.079475	2.321110
N	0.593738	-0.758392	2.027126
C	0.708935	-1.948740	2.728221
C	-0.048055	-1.871227	3.954721
C	-0.630408	-0.638176	3.990155
C	-0.228196	0.056713	2.790624
H	-0.124081	-2.659157	4.686752
H	-1.268200	-0.230982	4.758095
C	-0.611112	1.363105	2.482470
O	-0.267413	-1.058452	-0.632602
C	-1.520585	2.075304	3.437700
C	-2.920746	1.985798	3.351262
C	-1.030773	2.873556	4.486687
C	-3.783491	2.636873	4.228790
C	-1.855383	3.542400	5.386877
C	-3.241787	3.420418	5.252157
H	-4.854928	2.534180	4.116266
H	-1.425398	4.144206	6.176909
H	-3.898587	3.933842	5.944317
C	1.395529	-4.288237	3.206345
C	0.399680	-5.275463	3.103560
C	2.368573	-4.513080	4.195464
C	0.359142	-6.406427	3.914097
C	2.367538	-5.628293	5.028681
C	1.352798	-6.579169	4.882692
H	-0.430319	-7.136642	3.792516
H	3.141226	-5.752306	5.775143
H	1.336467	-7.453514	5.522445
C	4.244865	-2.735339	-3.003775
C	3.650921	-3.388778	-4.097579
C	5.645391	-2.833096	-2.930733
C	4.376771	-4.090688	-5.055534
C	6.412197	-3.523297	-3.865392
C	5.768330	-4.155239	-4.933734
H	3.868210	-4.576575	-5.877989
H	7.488613	-3.566713	-3.762334
H	6.349945	-4.696918	-5.670172
C	2.050696	3.888550	-2.311923
C	1.306494	4.276446	-3.439391
C	3.053566	4.791735	-1.914325
C	1.525649	5.465842	-4.129185
C	3.308298	5.991061	-2.573004
C	2.535123	6.326639	-3.688553
H	0.921310	5.714843	-4.991705
H	4.093810	6.648631	-2.224040
H	2.719450	7.256320	-4.213654
Cl	-3.671945	0.969212	2.030093
Cl	0.776905	3.053907	4.707267
Cl	6.528694	-2.018601	-1.550903
Cl	1.831225	-3.332964	-4.292685
Cl	-0.918616	-5.088663	1.848430
Cl	3.712735	-3.292158	4.420241
Cl	4.096485	4.391313	-0.465274
Cl	-0.025052	3.184588	-4.056825
C	-5.312532	1.199511	-1.704617
C	-5.149909	-0.191291	-1.764518
C	-3.879438	-0.744049	-1.962832
C	-2.785219	0.125177	-2.093148
C	-2.927239	1.519759	-2.034166
C	-4.207748	2.050681	-1.839510
H	-3.752054	-1.818721	-2.014986
H	-2.072792	2.176747	-2.139508
H	-4.336903	3.126136	-1.793608
I	-0.869490	-0.701846	-2.413199
H	-6.300838	1.619871	-1.554903
H	-6.006829	-0.847350	-1.661605
N	3.417562	0.453708	1.496723
C	4.356727	0.762367	2.102772
C	5.538107	1.149127	2.865749
H	5.694540	2.229724	2.802803
H	5.417297	0.874618	3.917547
H	6.425623	0.644642	2.473281

$^{6}2_{(1b)}$

Fe	1.306107	-0.324146	0.204157
N	0.716528	1.651343	0.420530
C	-0.095791	2.144414	1.424888
C	-0.374682	3.542594	1.166144
C	0.289825	3.883383	0.021231
C	0.977537	2.696410	-0.445625
H	-0.988276	4.180622	1.782296
H	0.311213	4.847399	-0.462075
C	1.789394	2.632047	-1.591280
N	2.373506	0.216916	-1.490807
C	2.431986	1.475694	-2.067441
C	3.269964	1.418934	-3.244896
C	3.716891	0.131257	-3.365606
C	3.173251	-0.618900	-2.254888
H	3.491284	2.251442	-3.893884
H	4.367287	-0.266298	-4.128535
C	3.458501	-1.968196	-1.979641
N	2.257428	-2.169506	0.181770
C	3.033502	-2.676373	-0.842550
C	3.364710	-4.057028	-0.550232
C	2.788996	-4.365113	0.650081
C	2.089733	-3.180307	1.107536
H	3.959114	-4.702405	-1.177430
H	2.830818	-5.306355	1.175074
C	1.349824	-3.091182	2.299445
N	0.554665	-0.748632	2.070559
C	0.641314	-1.958554	2.735788
C	-0.122743	-1.879107	3.962714
C	-0.661051	-0.623309	4.026204
C	-0.231652	0.089325	2.841728
H	-0.233556	-2.676202	4.680784
H	-1.286434	-0.218041	4.805818
C	-0.546925	1.427252	2.547127
O	-0.325055	-0.989445	-0.644414
C	-1.408492	2.160453	3.532867
C	-2.811259	2.170263	3.443728
C	-0.868728	2.881836	4.612343
C	-3.630581	2.840036	4.348365
C	-1.648229	3.566549	5.540505
C	-3.039548	3.542193	5.403177
H	-4.706275	2.814413	4.232383
H	-1.180079	4.106546	6.353207

H	-3.661713	4.069162	6.116853
C	1.304277	-4.309819	3.173189
C	0.304233	-5.289640	3.045976
C	2.260280	-4.551433	4.175112
C	0.243598	-6.428512	3.844359
C	2.239635	-5.674878	4.996929
C	1.221214	-6.617663	4.826126
H	-0.548724	-7.152110	3.703281
H	3.001166	-5.811315	5.753672
H	1.189638	-7.498229	5.456724
C	4.307682	-2.705621	-2.972236
C	3.752169	-3.390365	-4.067071
C	5.709028	-2.761202	-2.875577
C	4.514257	-4.082454	-5.003909
C	6.511771	-3.439943	-3.788345
C	5.904894	-4.104159	-4.858746
H	4.033957	-4.593458	-5.828169
H	7.587119	-3.450098	-3.666954
H	6.514402	-4.637559	-5.578515
C	2.024917	3.910319	-2.342150
C	1.238312	4.313044	-3.434864
C	3.063122	4.793446	-1.993027
C	1.450167	5.496442	-4.137308
C	3.312572	5.986311	-2.665528
C	2.496723	6.336415	-3.745664
H	0.812142	5.756774	-4.971782
H	4.126529	6.627973	-2.354096
H	2.676354	7.261229	-4.280924
Cl	-3.626246	1.266906	2.077463
Cl	0.947427	2.939126	4.832656
Cl	6.545388	-1.904571	-1.491479
Cl	1.934969	-3.390785	-4.293084
Cl	-0.994358	-5.081855	1.772841
Cl	3.609490	-3.342194	4.433300
Cl	4.161756	4.375751	-0.590277
Cl	-0.143782	3.248796	-3.987746
C	-5.408329	0.948578	-1.785053
C	-5.180462	-0.429170	-1.905111
C	-3.882652	-0.913909	-2.100514
C	-2.829866	0.012103	-2.170036
C	-3.035800	1.395531	-2.053516
C	-4.342793	1.856092	-1.858956
H	-3.702719	-1.977926	-2.194365
H	-2.210744	2.094795	-2.112285
H	-4.523739	2.920867	-1.766797
I	-0.875181	-0.705114	-2.465694
H	-6.417658	1.315540	-1.635841
H	-6.007338	-1.127790	-1.848490
N	3.335580	0.417154	1.428760
C	4.275976	0.724812	2.032809
C	5.458973	1.110497	2.793798
H	5.622964	2.189361	2.721188
H	5.334761	0.846515	3.847898
H	6.343545	0.596297	2.407372

$^{2}2_{(1c)}$

Fe	1.470162	0.027197	0.540294
N	0.757344	1.901639	0.686150
C	-0.097754	2.364708	1.670185
C	-0.383700	3.767008	1.452080
C	0.325713	4.155501	0.354996
C	1.038223	2.991701	-0.121842
H	-1.031388	4.370964	2.067255
H	0.363366	5.134162	-0.096321
C	1.878792	2.991061	-1.238709
N	2.366439	0.560370	-1.199249
C	2.497027	1.841020	-1.732732
C	3.354949	1.805113	-2.890958
C	3.762840	0.511948	-3.050505
C	3.176401	-0.258244	-1.978957
H	3.611337	2.657517	-3.499756
H	4.417825	0.118089	-3.811156
C	3.450678	-1.608308	-1.746772
N	2.249276	-1.832136	0.414302
C	3.009613	-2.324142	-0.628727
C	3.299263	-3.726832	-0.407911
C	2.695272	-4.080101	0.760623
C	2.030809	-2.898140	1.266806
H	3.883086	-4.350970	-1.065366
H	2.692218	-5.046801	1.238499
C	1.256503	-2.873040	2.429364
N	0.567307	-0.502851	2.260764
C	0.583715	-1.735774	2.882489
C	-0.236289	-1.699108	4.075996
C	-0.754774	-0.443393	4.162352
C	-0.256344	0.300305	3.021569
H	-0.389597	-2.527257	4.749456
H	-1.412897	-0.049814	4.920472
C	-0.585237	1.632762	2.757043
O	-0.039724	-0.617319	-0.271894
C	-1.507935	2.329258	3.713040
C	-2.905123	2.300459	3.560897
C	-1.039086	3.054383	4.822745
C	-3.784251	2.936123	4.433325
C	-1.880035	3.705916	5.721024
C	-3.262343	3.643198	5.520757
H	-4.852343	2.880752	4.267916
H	-1.465055	4.250353	6.559296
H	-3.931251	4.144132	6.210506
C	1.073202	-4.154737	3.186335
C	0.011904	-5.034208	2.902808
C	1.933108	-4.567635	4.218418
C	-0.194863	-6.231071	3.582357
C	1.765341	-5.755814	4.925520
C	0.691656	-6.590283	4.602152
H	-1.029141	-6.869286	3.321753
H	2.458735	-6.023396	5.712223
H	0.546223	-7.518218	5.142492
C	4.296661	-2.331860	-2.751933
C	3.739231	-3.005004	-3.853069
C	5.698535	-2.386950	-2.659713
C	4.499205	-3.688440	-4.798055
C	6.498775	-3.056917	-3.581458
C	5.890057	-3.712109	-4.656157
H	4.016798	-4.191005	-5.626296
H	7.574516	-3.066661	-3.463191
H	6.498009	-4.238868	-5.382166
C	2.145580	4.293424	-1.931610
C	1.371277	4.760803	-3.007528
C	3.203972	5.135189	-1.543003
C	1.613650	5.966977	-3.659300
C	3.483874	6.348558	-2.165261
C	2.679792	6.763480	-3.231199
H	0.984104	6.277971	-4.482807
H	4.312190	6.956567	-1.825355
H	2.883224	7.705185	-3.727116
Cl	-3.631500	1.388024	2.150523
Cl	0.761658	3.165427	5.125140
Cl	6.540498	-1.535033	-1.277888
Cl	1.922326	-3.000601	-4.077565
Cl	-1.173898	-4.610963	1.573447
Cl	3.353423	-3.513083	4.678891
Cl	4.281716	4.629505	-0.155866
Cl	-0.038670	3.757457	-3.604932
C	-5.181381	-1.203926	-1.911825
C	-4.216969	-2.112297	-2.368372
C	-2.867520	-1.744076	-2.413764
C	-2.511587	-0.455299	-1.987039
C	-3.463223	0.469615	-1.529926
C	-4.807428	0.081187	-1.496159
H	-2.120500	-2.442940	-2.770737
H	-3.170922	1.461440	-1.207376
H	-5.556272	0.782732	-1.146369
I	-0.488082	0.109553	-2.042952
H	-6.225165	-1.496369	-1.882797
H	-4.509834	-3.104702	-2.691868
N	8.821420	0.895365	0.381310
C	8.603158	0.567774	1.474622
C	8.331670	0.150391	2.847224
H	7.389659	-0.404066	2.894084
H	9.138470	-0.487892	3.219093
H	8.245793	1.021745	3.502345
C	4.910874	1.962944	2.832673
S	3.947024	0.376645	2.682617
O	3.180319	0.308377	3.930051
O	3.152964	0.726724	1.445873
O	4.975465	-0.649537	2.457976
F	5.732407	1.923704	3.950707
F	5.719953	2.174642	1.726684
F	4.071896	3.055880	2.964085

$^{4}2_{(1c)}$

Fe	1.436462	-0.281581	0.451851
N	0.677790	1.578580	0.589930
C	-0.231277	2.030079	1.533002
C	-0.595180	3.398583	1.248494
C	0.117788	3.783533	0.151082
C	0.912829	2.649193	-0.258526
H	-1.294482	3.986319	1.821222
H	0.107795	4.743275	-0.340387
C	1.791622	2.662345	-1.343828
N	2.436434	0.269954	-1.211815
C	2.495519	1.537173	-1.775457

C	3.385197	1.528082	-2.911044
C	3.862322	0.255806	-3.038548
C	3.287960	-0.522933	-1.968216
H	3.610094	2.382099	-3.529602
H	4.551337	-0.119205	-3.778169
C	3.588733	-1.866200	-1.733640
N	2.317213	-2.094585	0.384573
C	3.124259	-2.583702	-0.630334
C	3.440942	-3.971360	-0.381121
C	2.820265	-4.321601	0.781025
C	2.114317	-3.153073	1.254150
H	4.056753	-4.589943	-1.014039
H	2.833353	-5.280157	1.274556
C	1.338746	-3.126599	2.414139
N	0.540850	-0.789765	2.171529
C	0.624571	-2.003426	2.835331
C	-0.170049	-1.959565	4.039797
C	-0.741324	-0.722634	4.099360
C	-0.302691	0.005284	2.932045
H	-0.273642	-2.769878	4.743552
H	-1.397556	-0.334505	4.861688
C	-0.694509	1.312565	2.638138
O	-0.200649	-1.056865	-0.505445
C	-1.641742	1.994303	3.579299
C	-3.036438	1.850272	3.477447
C	-1.195677	2.818758	4.627900
C	-3.934313	2.469800	4.342457
C	-2.056878	3.457654	5.515780
C	-3.435636	3.278504	5.368104
H	-4.999508	2.324627	4.218010
H	-1.659865	4.080766	6.306582
H	-4.120011	3.768012	6.050856
C	1.235487	-4.382402	3.226183
C	0.195449	-5.309912	3.035508
C	2.167401	-4.721040	4.223008
C	0.073196	-6.485336	3.771081
C	2.084800	-5.884981	4.982725
C	1.027843	-6.770319	4.752205
H	-0.748022	-7.164178	3.581462
H	2.830217	-6.095290	5.738592
H	0.948740	-7.680686	5.334521
C	4.473595	-2.572434	-2.715184
C	3.955852	-3.255674	-3.829138
C	5.873378	-2.598425	-2.587532
C	4.752433	-3.923190	-4.754934
C	6.709149	-3.252058	-3.489090
C	6.139619	-3.918859	-4.578181
H	4.301292	-4.434757	-5.595178
H	7.781655	-3.240433	-3.344799
H	6.775622	-4.433021	-5.288995
C	2.023476	3.962013	-2.054868
C	1.308620	4.351762	-3.200037
C	2.991484	4.880749	-1.607955
C	1.520644	5.558633	-3.861208
C	3.237395	6.097696	-2.237175
C	2.492959	6.435546	-3.371470
H	0.939542	5.808398	-4.739359
H	3.995093	6.767030	-1.850928
H	2.671203	7.379102	-3.873493
Cl	-3.734234	0.805000	2.148336
Cl	0.599238	3.079129	4.859705
Cl	6.659525	-1.728411	-1.184497
Cl	2.144737	-3.285921	-4.097416
Cl	-1.072056	-4.985938	1.754779
Cl	3.566845	-3.595351	4.560075
Cl	3.995773	4.471970	-0.136832
Cl	0.028158	3.237423	-3.882688
C	-5.232706	1.164504	-1.690909
C	-5.051374	-0.219886	-1.811916
C	-3.766982	-0.749870	-1.981625
C	-2.677990	0.134391	-2.023531
C	-2.839305	1.522738	-1.902318
C	-4.132923	2.031397	-1.735938
H	-3.624712	-1.819579	-2.078720
H	-1.989221	2.192636	-1.939109
H	-4.276174	3.102036	-1.642635
I	-0.738794	-0.658787	-2.294510
H	-6.231246	1.567666	-1.563196
H	-5.904138	-0.888494	-1.777791
N	8.563489	1.192993	0.399171
C	8.473497	1.091649	1.553265
C	8.362044	0.956925	3.002671
H	9.280559	0.533746	3.419593
H	8.184985	1.931787	3.465645
H	7.520845	0.303489	3.251895
C	4.725060	2.132630	3.074914
S	4.056482	0.409998	2.841895
O	3.230711	0.207216	4.041409
O	3.309204	0.577385	1.560710
O	5.271861	-0.417807	2.729655
F	5.490452	2.219511	4.230965
F	5.539112	2.515737	2.014337
F	3.705819	3.067620	3.177216

^{6}2$_{(1c)}$

Fe	1.030280	-0.482108	0.237318
N	0.626582	1.521298	0.635548
C	-0.226764	1.999823	1.618123
C	-0.457026	3.413176	1.412321
C	0.268726	3.785569	0.317429
C	0.951389	2.604781	-0.165354
H	-1.083012	4.038027	2.029205
H	0.340236	4.768619	-0.120037
C	1.830944	2.582859	-1.257028
N	2.393262	0.163893	-1.192581
C	2.501830	1.443009	-1.721957
C	3.436974	1.431553	-2.823492
C	3.894378	0.150620	-2.954408
C	3.255033	-0.640287	-1.927963
H	3.713243	2.290081	-3.414626
H	4.610351	-0.220110	-3.670422
C	3.507375	-1.999773	-1.697308
N	2.090864	-2.279493	0.318809
C	2.966841	-2.751052	-0.643809
C	3.272537	-4.141349	-0.382070
C	2.584255	-4.500301	0.740969
C	1.843472	-3.336216	1.178729
H	3.931649	-4.756205	-0.974002
H	2.580261	-5.461188	1.230468
C	1.016285	-3.296111	2.309794
N	0.288597	-0.929580	2.127202
C	0.303063	-2.169842	2.744795
C	-0.514029	-2.125188	3.936953
C	-1.009478	-0.856260	4.039970
C	-0.503104	-0.106719	2.911819
H	-0.679005	-2.951589	4.609791
H	-1.651481	-0.462913	4.811896
C	-0.755800	1.253393	2.679747
O	-0.516025	-1.075934	-0.743797
C	-1.610997	1.976464	3.677197
C	-3.010145	2.039556	3.567671
C	-1.059247	2.635532	4.790456
C	-3.818677	2.701236	4.487794
C	-1.828977	3.308980	5.734703
C	-3.218366	3.338453	5.578141
H	-4.892739	2.719630	4.356399
H	-1.354560	3.799913	6.574459
H	-3.832193	3.857943	6.304424
C	0.913325	-4.543264	3.136019
C	-0.064986	-5.524326	2.902588
C	1.795819	-4.808166	4.198219
C	-0.172121	-6.690117	3.656069
C	1.725917	-5.959383	4.977564
C	0.733313	-6.904526	4.699912
H	-0.944768	-7.414490	3.433532
H	2.430442	-6.114953	5.784200
H	0.665090	-7.806362	5.296676
C	4.454479	-2.695049	-2.629057
C	4.015592	-3.335825	-3.800114
C	5.838886	-2.750703	-2.390997
C	4.873028	-3.988376	-4.681234
C	6.733375	-3.391605	-3.243855
C	6.241758	-4.013457	-4.395815
H	4.482310	-4.466606	-5.570002
H	7.790899	-3.405043	-3.014305
H	6.924240	-4.516671	-5.070387
C	2.120364	3.886526	-1.940797
C	1.417511	4.325358	-3.075271
C	3.125973	4.755330	-1.479054
C	1.678508	5.532891	-3.716942
C	3.421016	5.971367	-2.089040
C	2.689208	6.358727	-3.215855
H	1.105549	5.822578	-4.588139
H	4.206077	6.602544	-1.693333
H	2.906014	7.302143	-3.702720
Cl	-3.832425	1.223716	2.151247
Cl	0.754654	2.623800	5.026396
Cl	6.521521	-1.948013	-0.895944
Cl	2.230876	-3.328123	-4.208064
Cl	-1.269971	-5.280098	1.546673
Cl	3.102891	-3.592626	4.596307
Cl	4.107289	4.282801	-0.011383

Cl	0.085757	3.277939	-3.766966
C	-5.426056	1.134870	-1.989275
C	-5.278378	-0.249561	-2.151393
C	-4.007294	-0.806290	-2.328256
C	-2.899760	0.056855	-2.338827
C	-3.024866	1.446461	-2.181820
C	-4.306573	1.978365	-2.004241
H	-3.888574	-1.875864	-2.451709
H	-2.158499	2.096298	-2.196431
H	-4.426015	3.048544	-1.880510
I	-0.985590	-0.771524	-2.585790
H	-6.415219	1.557503	-1.853285
H	-6.147087	-0.897627	-2.140328
N	7.641056	2.144893	-0.454897
C	8.078531	2.193222	0.620569
C	8.628884	2.245451	1.971707
H	9.718056	2.147664	1.946612
H	8.373485	3.194625	2.451234
H	8.206950	1.434061	2.572018
C	5.200349	2.220079	3.704498
S	5.029022	0.379297	3.483507
O	4.724888	-0.083894	4.851953
O	3.915289	0.286806	2.516032
O	6.356292	-0.007331	2.958065
F	6.214843	2.541021	4.597945
F	5.508284	2.854576	2.500814
F	4.030158	2.796831	4.182492

^{2}RC$_{(1d)}$

Fe	1.673300	0.196888	-0.262527
N	1.214259	2.158465	-0.036194
C	0.296001	2.697856	0.840107
C	0.189443	4.125503	0.637051
C	1.054091	4.445585	-0.366883
C	1.685726	3.212953	-0.782480
H	-0.454941	4.787423	1.192249
H	1.248813	5.418106	-0.788399
C	2.642065	3.128497	-1.808835
N	3.000727	0.682476	-1.715684
C	3.246215	1.937512	-2.232831
C	4.221532	1.858035	-3.297331
C	4.556958	0.543233	-3.426367
C	3.791901	-0.181595	-2.436366
H	4.594049	2.695468	-3.864287
H	5.256387	0.102538	-4.117841
C	3.871796	-1.571480	-2.246868
N	2.301961	-1.728652	-0.342034
C	3.173103	-2.278067	-1.258762
C	3.293730	-3.702700	-1.042841
C	2.494155	-4.008961	0.017783
C	1.876760	-2.773259	0.445362
H	3.911615	-4.370217	-1.620875
H	2.333602	-4.974424	0.468959
C	0.966591	-2.678366	1.511341
N	0.522369	-0.250917	1.345983
C	0.336790	-1.493421	1.914737
C	-0.622399	-1.411290	2.993655
C	-1.021619	-0.109944	3.066919
C	-0.300852	0.606039	2.038030
H	-0.944346	-2.237995	3.605584
H	-1.729886	0.328057	3.751032
C	-0.426939	1.986223	1.806296
O	0.464686	-0.061377	-1.307249
C	-1.389225	2.752323	2.662546
C	-2.728226	2.944385	2.285032
C	-1.006425	3.321979	3.887847
C	-3.638582	3.653242	3.062930
C	-1.884469	4.038360	4.695442
C	-3.208387	4.201948	4.275281
H	-4.661047	3.774848	2.729933
H	-1.542972	4.459947	5.631791
H	-3.904655	4.756828	4.892617
C	0.645753	-3.932764	2.266749
C	-0.414537	-4.776094	1.896874
C	1.391313	-4.334232	3.387284
C	-0.726400	-5.943905	2.586665
C	1.113052	-5.493614	4.104506
C	0.045504	-6.300086	3.697130
H	-1.553852	-6.562350	2.264236
H	1.715929	-5.761772	4.962246
H	-0.184517	-7.206118	4.244890
C	4.776453	-2.350405	-3.153401
C	4.328751	-2.863569	-4.382131
C	6.115997	-2.613838	-2.824842
C	5.148123	-3.595649	-5.236163
C	6.967887	-3.340828	-3.650772
C	6.474780	-3.833668	-4.863263
H	4.758747	-3.971831	-6.173257
H	7.993629	-3.518209	-3.354964
H	7.124834	-4.401997	-5.517690
C	3.036275	4.399685	-2.498557
C	2.366489	4.860486	-3.644523
C	4.091710	5.200799	-2.034062
C	2.716039	6.040570	-4.294797
C	4.471801	6.386200	-2.655802
C	3.775023	6.804297	-3.794242
H	2.171283	6.356881	-5.174847
H	5.292943	6.969931	-2.260712
H	4.057543	7.724901	-4.290772
Cl	-3.316402	2.240001	0.705475
Cl	0.717727	3.124635	4.460431
Cl	6.787414	-1.978096	-1.247997
Cl	2.604753	-2.557846	-4.893475
Cl	-1.437987	-4.334983	0.450318
Cl	2.791453	-3.298759	3.941518
Cl	5.018328	4.677773	-0.547030
Cl	0.982702	3.883500	-4.318504
C	-5.194625	-2.338059	-0.187753
C	-5.535154	-3.627850	-0.613974
C	-5.109835	-4.095778	-1.865136
C	-4.341952	-3.253915	-2.679694
C	-3.991982	-1.960781	-2.271379
C	-4.425889	-1.510376	-1.015592
H	-5.374578	-5.094448	-2.191608
H	-3.401277	-1.310877	-2.907655
H	-4.160275	-0.509249	-0.690958
I	-3.695821	-3.957839	-4.588256
H	-5.526392	-1.980674	0.781349
H	-6.130929	-4.275177	0.021217
N	3.262938	0.535888	1.131644
C	4.116973	0.723386	1.887845
C	5.192110	0.959448	2.840798
H	5.668116	1.923720	2.641387
H	4.797763	0.966634	3.860828
H	5.947078	0.172102	2.761444
C	-0.204112	-0.014422	-5.681480
S	-1.861365	0.794998	-5.426200
O	-2.682383	0.181676	-6.489291
O	-2.201620	0.389927	-4.044002
O	-1.550236	2.227907	-5.607107
F	0.298276	0.228425	-6.952604
F	0.742815	0.443292	-4.771377
F	-0.279108	-1.397901	-5.527849

^{4}RC$_{(1d)}$

Fe	1.675792	0.197323	-0.260191
N	1.216275	2.158421	-0.034202
C	0.296085	2.697724	0.840095
C	0.188012	4.125002	0.635600
C	1.053524	4.445378	-0.367404
C	1.687495	3.213357	-0.781217
H	-0.458188	4.786498	1.189194
H	1.247368	5.417783	-0.789601
C	2.644170	3.129056	-1.806558
N	3.002639	0.682875	-1.713733
C	3.247978	1.937806	-2.231154
C	4.221226	1.858109	-3.297490
C	4.556116	0.543309	-3.427352
C	3.792366	-0.181679	-2.436508
H	4.592824	2.695535	-3.865066
H	5.254065	0.102556	-4.120291
C	3.871714	-1.571192	-2.247473
N	2.303247	-1.727862	-0.341189
C	3.172611	-2.277865	-1.259451
C	3.291312	-3.702865	-1.045108
C	2.492761	-4.009170	0.016174
C	1.877486	-2.773213	0.445964
H	3.907332	-4.370665	-1.624804
H	2.331300	-4.974940	0.466380
C	0.968781	-2.678102	1.512542
N	0.524278	-0.250559	1.346686
C	0.338848	-1.492961	1.915892
C	-0.621149	-1.411070	2.994055
C	-1.021466	-0.110115	3.066652
C	-0.300522	0.606381	2.038297
H	-0.943033	-2.237906	3.605843
H	-1.730703	0.327468	3.750037
C	-0.427056	1.985940	1.806392
O	0.467907	-0.059773	-1.306452
C	-1.390146	2.752022	2.661769
C	-2.729026	2.943341	2.283441
C	-1.008236	3.322650	3.886883
C	-3.640119	3.652253	3.060425

C	-1.887020	4.039123	4.693600
C	-3.210801	4.201867	4.272674
H	-4.662450	3.773227	2.726797
H	-1.546187	4.461434	5.629865
H	-3.907635	4.756806	4.889320
C	0.648168	-3.932289	2.268409
C	-0.413128	-4.775060	1.900089
C	1.394917	-4.334021	3.388048
C	-0.724715	-5.942627	2.590423
C	1.116997	-5.493181	4.105764
C	0.048489	-6.299132	3.699881
H	-1.552941	-6.560648	2.269169
H	1.720839	-5.761547	4.962759
H	-0.181293	-7.204984	4.248038
C	4.775796	-2.350382	-3.154370
C	4.327879	-2.862812	-4.383344
C	6.115142	-2.614821	-2.825834
C	5.146859	-3.595075	-5.237603
C	6.966662	-3.341976	-3.652000
C	6.473349	-3.834040	-4.864717
H	4.757311	-3.970668	-6.174862
H	7.992283	-3.520065	-3.356201
H	7.123117	-4.402476	-5.519338
C	3.038115	4.400078	-2.496735
C	2.367620	4.860746	-3.642354
C	4.094032	5.201060	-2.033185
C	2.716957	6.040598	-4.293163
C	4.473887	6.386286	-2.655416
C	3.776407	6.804256	-3.793476
H	2.171709	6.356782	-5.172953
H	5.295389	6.969969	-2.261003
H	4.058761	7.724694	-4.290410
Cl	-3.315967	2.238015	0.703850
Cl	0.715710	3.126474	4.460514
Cl	6.786887	-1.980139	-1.248695
Cl	2.604054	-2.556062	-4.894689
Cl	-1.438412	-4.333542	0.454933
Cl	2.796183	-3.299118	3.940511
Cl	5.021553	4.678183	-0.546659
Cl	0.983333	3.883709	-4.315343
C	-5.198359	-2.338580	-0.190658
C	-5.539727	-3.627868	-0.617719
C	-5.112966	-4.095994	-1.868315
C	-4.342783	-3.254852	-2.681450
C	-3.991886	-1.962232	-2.272277
C	-4.427315	-1.511636	-1.017082
H	-5.378417	-5.094260	-2.195466
H	-3.399317	-1.312804	-2.907356
H	-4.161053	-0.510910	-0.691791
I	-3.694585	-3.959154	-4.589177
H	-5.531258	-1.981018	0.777992
H	-6.137298	-4.274635	0.016354
N	3.265097	0.535806	1.133132
C	4.119303	0.723152	1.889180
C	5.194174	0.959585	2.842344
H	5.670668	1.923489	2.642294
H	4.799445	0.967710	3.862227
H	5.948872	0.171870	2.763893
C	-0.204991	-0.014383	-5.680130
S	-1.861884	0.795014	-5.422507
O	-2.684098	0.182900	-6.485370
O	-2.200923	0.388534	-4.040406
O	-1.550672	2.228028	-5.602447
F	0.296826	0.230574	-6.951072
F	0.742508	0.441443	-4.769681
F	-0.280358	-1.398113	-5.528916

^{6}RC$_{(1d)}$

Fe	1.624424	0.190352	-0.321788
N	1.191191	2.211531	-0.047585
C	0.287058	2.732086	0.846536
C	0.176137	4.163507	0.638498
C	1.020301	4.484514	-0.386458
C	1.655611	3.252428	-0.814361
H	-0.457310	4.830304	1.200999
H	1.198192	5.459817	-0.809865
C	2.609880	3.146025	-1.851869
N	3.037761	0.707017	-1.766548
C	3.248608	1.961968	-2.284793
C	4.234872	1.883903	-3.345979
C	4.601285	0.572466	-3.454705
C	3.843530	-0.163237	-2.460163
H	4.598218	2.717572	-3.924939
H	5.316837	0.144386	-4.138073
C	3.928939	-1.556233	-2.238423
N	2.326117	-1.772273	-0.361352
C	3.222757	-2.294433	-1.261548
C	3.346471	-3.723094	-1.042174
C	2.518189	-4.040704	-0.003250
C	1.877143	-2.809863	0.419492
H	3.982827	-4.389198	-1.602157
H	2.357582	-5.012405	0.435145
C	0.941630	-2.698950	1.472853
N	0.484101	-0.266730	1.363950
C	0.296624	-1.516847	1.902060
C	-0.666013	-1.433893	2.984308
C	-1.048291	-0.125720	3.079159
C	-0.321042	0.603661	2.057578
H	-1.001961	-2.261449	3.588095
H	-1.750929	0.304569	3.774423
C	-0.419765	1.993859	1.822322
O	0.424114	-0.071197	-1.370035
C	-1.361519	2.763679	2.700786
C	-2.702831	2.979262	2.344982
C	-0.953374	3.313306	3.927032
C	-3.592086	3.690836	3.144650
C	-1.809641	4.031409	4.756199
C	-3.137081	4.218208	4.357425
H	-4.617424	3.830692	2.828012
H	-1.448835	4.436572	5.692581
H	-3.816719	4.774691	4.991624
C	0.607199	-3.959918	2.214474
C	-0.447351	-4.799589	1.821236
C	1.334005	-4.370406	3.344037
C	-0.770861	-5.972718	2.496688
C	1.043760	-5.535168	4.047661
C	-0.017202	-6.338058	3.616660
H	-1.593233	-6.588138	2.155955
H	1.632556	-5.810200	4.912977
H	-0.256307	-7.248277	4.153489
C	4.861200	-2.328779	-3.124888
C	4.439572	-2.865472	-4.352798
C	6.201131	-2.561717	-2.776275
C	5.284358	-3.590189	-5.188142
C	7.078177	-3.280546	-3.582907
C	6.610810	-3.796586	-4.795944
H	4.914695	-3.985073	-6.125513
H	8.103293	-3.434147	-3.271933
H	7.280576	-4.358687	-5.435715
C	2.979699	4.415527	-2.561613
C	2.298799	4.845515	-3.712921
C	4.020963	5.243512	-2.112769
C	2.623583	6.022085	-4.382125
C	4.376446	6.426547	-2.753503
C	3.668589	6.813873	-3.895991
H	2.070928	6.314123	-5.265645
H	5.187362	7.031892	-2.369941
H	3.931864	7.732187	-4.407173
Cl	-3.323603	2.303066	0.765268
Cl	0.776529	3.086725	4.471329
Cl	6.838184	-1.896601	-1.197141
Cl	2.714728	-2.603929	-4.886931
Cl	-1.447789	-4.346355	0.362077
Cl	2.725589	-3.340161	3.929182
Cl	4.963386	4.759890	-0.622094
Cl	0.935115	3.829487	-4.370716
C	-5.253308	-2.187848	-0.160931
C	-5.542589	-3.521783	-0.473962
C	-5.081311	-4.084275	-1.672331
C	-4.329243	-3.291970	-2.549048
C	-4.029769	-1.955981	-2.253817
C	-4.499631	-1.410945	-1.049458
H	-5.306968	-5.116691	-1.911312
H	-3.448873	-1.344463	-2.935860
H	-4.273046	-0.376265	-0.812535
I	-3.630118	-4.141032	-4.378471
H	-5.612846	-1.757342	0.767691
H	-6.126292	-4.130447	0.208884
N	3.223340	0.537565	1.094538
C	4.074174	0.725875	1.854215
C	5.145306	0.963150	2.811083
H	5.623436	1.926194	2.610758
H	4.746389	0.973664	3.829304
H	5.899320	0.174343	2.737013
C	-0.166996	-0.136327	-5.600608
S	-1.842796	0.663144	-5.461619
O	-2.610437	-0.020073	-6.521940
O	-2.238174	0.331808	-4.074367
O	-1.540107	2.087800	-5.709715
F	0.382905	0.035705	-6.863675
F	0.736881	0.390222	-4.684199
F	-0.230842	-1.508979	-5.365666

$^{2}TS_{(1d)}$

Fe	1.375703	0.060268	0.044431
N	0.995233	2.017974	0.385633
C	0.338960	2.564337	1.470862
C	0.190611	3.992968	1.287794
C	0.741413	4.298183	0.079431
C	1.249388	3.061222	-0.475556
H	-0.280962	4.663191	1.988334
H	0.808398	5.265110	-0.392628
C	1.945852	2.970092	-1.687906
N	2.409850	0.533260	-1.604335
C	2.514696	1.791662	-2.178879
C	3.394471	1.737351	-3.324959
C	3.866696	0.461350	-3.408983
C	3.255806	-0.289202	-2.336153
H	3.634572	2.573206	-3.962043
H	4.559577	0.059109	-4.130434
C	3.475969	-1.648731	-2.100340
N	1.933980	-1.860248	-0.177841
C	2.807543	-2.380290	-1.112268
C	2.915721	-3.812312	-0.946800
C	2.092745	-4.155708	0.084326
C	1.500205	-2.931657	0.579301
H	3.530689	-4.462320	-1.548231
H	1.914125	-5.139360	0.487692
C	0.675896	-2.865030	1.708918
N	0.468546	-0.404655	1.804423
C	0.219333	-1.673108	2.281703
C	-0.543944	-1.597441	3.510911
C	-0.740720	-0.275467	3.774070
C	-0.118852	0.466126	2.695843
H	-0.870070	-2.444201	4.093184
H	-1.262653	0.162785	4.609439
C	-0.159660	1.859690	2.571447
O	-0.090707	-0.128152	-0.672672
C	-0.823031	2.641757	3.664408
C	-2.199870	2.923570	3.659610
C	-0.104914	3.139886	4.764565
C	-2.832404	3.646236	4.667253
C	-0.695654	3.867167	5.793804
C	-2.070072	4.119136	5.740005
H	-3.896631	3.836000	4.616197
H	-0.096848	4.228686	6.619566
H	-2.546481	4.683204	6.533019
C	0.306798	-4.151328	2.384449
C	-0.860207	-4.859616	2.052280
C	1.100717	-4.726961	3.391265
C	-1.225257	-6.056031	2.662951
C	0.774823	-5.920726	4.028293
C	-0.397544	-6.586722	3.657267
H	-2.135601	-6.562152	2.369210
H	1.421440	-6.321977	4.797747
H	-0.665948	-7.517177	4.143233
C	4.488382	-2.362230	-2.944988
C	4.175982	-2.959682	-4.178080
C	5.829986	-2.475438	-2.538887
C	5.116769	-3.626100	-4.959288
C	6.801701	-3.131662	-3.288010
C	6.436826	-3.710863	-4.507307
H	4.823731	-4.070089	-5.901749
H	7.820820	-3.188858	-2.928472
H	7.179941	-4.226184	-5.104150
C	2.161448	4.232844	-2.467032
C	1.275075	4.652153	-3.473193
C	3.261991	5.076899	-2.237403
C	1.455137	5.819926	-4.209239
C	3.481596	6.252589	-2.949184
C	2.568656	6.622158	-3.941841
H	0.741625	6.097488	-4.974154
H	4.346220	6.866836	-2.734031
H	2.724653	7.534279	-4.505527
Cl	-3.229796	2.322774	2.272707
Cl	1.694456	2.828545	4.870224
Cl	6.350688	-1.727130	-0.952550
Cl	2.466292	-2.871995	-4.813599
Cl	-1.969386	-4.192415	0.760567
Cl	2.639725	-3.884025	3.907914
Cl	4.479395	4.630099	-0.947193
Cl	-0.195053	3.632099	-3.847736
C	-5.146413	-1.000558	-2.180896
C	-4.344450	-2.146971	-2.091587
C	-2.974589	-2.074023	-2.367348
C	-2.422408	-0.835718	-2.735599
C	-3.213908	0.320846	-2.831276
C	-4.581362	0.228201	-2.549297
H	-2.354097	-2.959337	-2.297451
H	-2.777017	1.269889	-3.117580
H	-5.201008	1.115394	-2.619562
I	-0.373483	-0.714042	-3.161203
H	-6.207311	-1.064871	-1.965591
H	-4.780853	-3.098424	-1.808171
N	3.150997	0.338359	1.162960
C	4.118870	0.498101	1.774383
C	5.338672	0.700066	2.543355
H	5.846090	1.611088	2.213956
H	5.103737	0.794151	3.607292
H	6.015956	-0.147674	2.406880
C	0.147436	-0.662686	-7.646497
S	-1.317340	-1.749102	-7.279373
O	-0.840307	-2.547400	-6.127131
O	-2.375339	-0.763908	-6.972781
O	-1.485690	-2.496432	-8.541502
F	1.276112	-1.407899	-7.964313
F	-0.099693	0.187814	-8.716697
F	0.483623	0.140044	-6.558317

$^{4}TS_{(1d)}$

Fe	1.525234	-0.126970	-0.027591
N	0.988365	1.808723	0.183742
C	0.102879	2.324847	1.111427
C	-0.123143	3.729788	0.850409
C	0.624424	4.057937	-0.239755
C	1.316305	2.857464	-0.656864
H	-0.767955	4.371685	1.429057
H	0.706304	5.019153	-0.721315
C	2.188462	2.801499	-1.744972
N	2.743075	0.393898	-1.557944
C	2.844555	1.639002	-2.152241
C	3.744221	1.573910	-3.282814
C	4.175664	0.284683	-3.376094
C	3.548419	-0.451143	-2.300128
H	4.006157	2.406808	-3.915519
H	4.857079	-0.134300	-4.099106
C	3.752570	-1.811613	-2.064642
N	2.303344	-1.993277	-0.063073
C	3.159469	-2.514910	-1.015368
C	3.370155	-3.925412	-0.769104
C	2.633171	-4.253458	0.328323
C	1.962714	-3.047386	0.763655
H	4.000570	-4.570169	-1.360296
H	2.546529	-5.217248	0.803969
C	1.102109	-2.985609	1.860051
N	0.549046	-0.575389	1.671042
C	0.449413	-1.821215	2.266897
C	-0.445281	-1.754439	3.400206
C	-0.889901	-0.469031	3.483893
C	-0.272852	0.264900	2.402223
H	-0.694847	-2.583820	4.042446
H	-1.571207	-0.050382	4.207181
C	-0.492117	1.621391	2.159081
O	0.251375	-0.510863	-1.026716
C	-1.415541	2.364159	3.076335
C	-2.795645	2.471575	2.830809
C	-0.960310	3.001875	4.243633
C	-3.670447	3.155300	3.670837
C	-1.797543	3.696166	5.112503
C	-3.162738	3.770171	4.819394
H	-4.725202	3.206833	3.433987
H	-1.393471	4.168890	5.998233
H	-3.829392	4.306187	5.484498
C	0.856702	-4.242706	2.637827
C	-0.185080	-5.131265	2.318879
C	1.651261	-4.616134	3.735756
C	-0.432926	-6.304670	3.025716
C	1.441153	-5.779066	4.471750
C	0.389434	-6.626471	4.109859
H	-1.249709	-6.953317	2.736988
H	2.083723	-6.018518	5.309033
H	0.210897	-7.535771	4.671505
C	4.657097	-2.560535	-2.995572
C	4.182087	-3.189629	-4.159535
C	6.039002	-2.681908	-2.767726
C	5.001989	-3.888346	-5.041185
C	6.897412	-3.370390	-3.620546
C	6.369898	-3.976275	-4.764989
H	4.582755	-4.353750	-5.923724
H	7.954473	-3.432372	-3.396942
H	7.023334	-4.515906	-5.440177
C	2.438947	4.062936	-2.514947
C	1.686467	4.418699	-3.648325
C	3.445094	4.974238	-2.148930
C	1.903659	5.589265	-4.370772

C	3.697202	6.155276	-2.841156
C	2.916488	6.461106	-3.960125
H	1.294883	5.815355	-5.236604
H	4.485608	6.821222	-2.515304
H	3.098298	7.376070	-4.511457
Cl	-3.503124	1.684041	1.338735
Cl	0.819385	2.931753	4.665918
Cl	6.772584	-1.904092	-1.282305
Cl	2.397864	-3.103344	-4.560716
Cl	-1.286056	-4.749791	0.907521
Cl	3.038300	-3.536028	4.245110
Cl	4.495276	4.612234	-0.693532
Cl	0.358042	3.306017	-4.230522
C	-5.342930	-0.492720	-1.613188
C	-4.662476	-1.709989	-1.466005
C	-3.345550	-1.841139	-1.917838
C	-2.726281	-0.729082	-2.513517
C	-3.392379	0.498003	-2.670700
C	-4.710703	0.604672	-2.215665
H	-2.818652	-2.781070	-1.807105
H	-2.904488	1.337541	-3.149451
H	-5.240646	1.543005	-2.334600
I	-0.757164	-0.899691	-3.185458
H	-6.364648	-0.400436	-1.262007
H	-5.153643	-2.558213	-1.002700
N	3.307498	0.402114	1.315985
C	4.205134	0.677407	1.993308
C	5.335007	1.025046	2.846333
H	5.893765	1.859771	2.413779
H	4.983726	1.317026	3.840096
H	6.008859	0.169989	2.950924
C	-0.098791	0.121256	-7.227376
S	-1.868323	0.051690	-6.659068
O	-1.858484	-1.168728	-5.793467
O	-2.039597	1.322646	-5.933203
O	-2.622713	-0.104392	-7.912984
F	0.245520	-1.005220	-7.958700
F	0.136334	1.229205	-8.025689
F	0.775917	0.194322	-6.146521

^{6}TS$_{(1d)}$

Fe	1.328970	-0.085095	-0.133861
N	0.938490	1.949131	0.250017
C	0.120657	2.435610	1.235794
C	-0.036791	3.869921	1.069661
C	0.701756	4.227175	-0.023659
C	1.316625	3.014423	-0.534368
H	-0.624673	4.514737	1.703196
H	0.821547	5.214873	-0.439467
C	2.182365	2.944452	-1.648756
N	2.679757	0.515766	-1.650360
C	2.824118	1.785170	-2.152198
C	3.769622	1.764726	-3.253634
C	4.196047	0.471690	-3.387155
C	3.510818	-0.305345	-2.370342
H	4.074282	2.618850	-3.837101
H	4.909443	0.086742	-4.098256
C	3.699911	-1.690691	-2.136225
N	2.216490	-1.993751	-0.173590
C	3.096539	-2.465437	-1.120517
C	3.322165	-3.883428	-0.900270
C	2.573134	-4.242905	0.184833
C	1.884690	-3.046968	0.638449
H	3.965422	-4.515679	-1.491215
H	2.499089	-5.219422	0.636189
C	1.018436	-2.976714	1.758068
N	0.441196	-0.569074	1.691243
C	0.365786	-1.825235	2.248145
C	-0.478028	-1.775085	3.431060
C	-0.891353	-0.482083	3.573727
C	-0.306914	0.276155	2.479519
H	-0.713747	-2.612886	4.067740
H	-1.524277	-0.077651	4.347419
C	-0.467355	1.662065	2.268645
O	-0.137219	-0.470360	-1.048128
C	-1.337417	2.396805	3.246385
C	-2.718290	2.553020	3.041278
C	-0.824088	2.970967	4.420909
C	-3.545401	3.229618	3.932984
C	-1.614752	3.655539	5.339198
C	-2.984744	3.782666	5.088654
H	-4.604272	3.323200	3.730005
H	-1.171288	4.080300	6.230321
H	-3.614723	4.312425	5.793199
C	0.781876	-4.255831	2.506516
C	-0.273341	-5.122934	2.178294
C	1.597517	-4.661662	3.575476
C	-0.515199	-6.314231	2.855853
C	1.391845	-5.844080	4.280320
C	0.326370	-6.672497	3.913794
H	-1.342149	-6.948704	2.564716
H	2.048388	-6.112864	5.097561
H	0.151931	-7.596451	4.452128
C	4.668311	-2.400549	-3.037686
C	4.276083	-2.959851	-4.264934
C	6.024808	-2.547897	-2.702768
C	5.159498	-3.626561	-5.109399
C	6.940919	-3.205721	-3.517958
C	6.499284	-3.748643	-4.728737
H	4.808545	-4.041513	-6.045309
H	7.976424	-3.291542	-3.215408
H	7.198977	-4.264457	-5.375469
C	2.475919	4.236045	-2.355966
C	1.702127	4.684452	-3.439042
C	3.540604	5.070523	-1.977533
C	1.956040	5.876674	-4.110624
C	3.830136	6.270136	-2.621109
C	3.028949	6.671403	-3.694862
H	1.330009	6.178480	-4.940186
H	4.662848	6.877990	-2.292103
H	3.240568	7.602346	-4.207173
Cl	-3.480218	1.843174	1.539226
Cl	0.963218	2.823019	4.777812
Cl	6.638345	-1.842508	-1.130873
Cl	2.537792	-2.808976	-4.800785
Cl	-1.390827	-4.682494	0.799974
Cl	2.998549	-3.600562	4.079931
Cl	4.608826	4.574671	-0.578590
Cl	0.292691	3.668537	-4.004987
C	-5.550868	-0.617775	-1.662423
C	-4.832451	-1.795263	-1.907760
C	-3.504580	-1.735144	-2.348379
C	-2.911355	-0.477814	-2.535539
C	-3.617006	0.710904	-2.297091
C	-4.944612	0.630371	-1.857823
I	-0.913418	-0.371816	-3.184602
N	3.294430	0.397935	1.316071
C	4.230147	0.629266	1.960067
C	5.409052	0.920508	2.768424
H	5.820848	1.897953	2.501508
H	5.149427	0.929881	3.830807
H	6.179044	0.161244	2.604415
C	-0.078133	-1.140953	-7.135067
S	-1.767160	-0.482258	-7.563410
O	-2.460588	-0.521756	-6.256233
O	-1.458674	0.867455	-8.075952
O	-2.244364	-1.457666	-8.563175
F	-0.144249	-2.411936	-6.568649
F	0.743581	-1.229305	-8.248815
F	0.574510	-0.323923	-6.210432
H	-5.499996	1.543307	-1.672432
H	-3.149341	1.676362	-2.448695
H	-2.950573	-2.646453	-2.539847
H	-5.300420	-2.762333	-1.759289
H	-6.579350	-0.672323	-1.322733

^{2}PC$_{(1d)}$

Fe	1.452612	-0.150109	-0.006390
N	0.891440	1.769757	0.114392
C	-0.029158	2.290732	1.006386
C	-0.195941	3.707342	0.762535
C	0.650854	4.042894	-0.252623
C	1.319285	2.829144	-0.665186
H	-0.861532	4.356912	1.308444
H	0.801302	5.015362	-0.693650
C	2.235303	2.756196	-1.720112
N	2.493186	0.290779	-1.691609
C	2.760681	1.555969	-2.203399
C	3.653779	1.449993	-3.333111
C	3.939529	0.125501	-3.497845
C	3.247901	-0.593321	-2.451431
H	4.010621	2.280214	-3.921838
H	4.577689	-0.323621	-4.242138
C	3.402574	-1.960357	-2.203616
N	2.149518	-2.038631	-0.062393
C	2.891497	-2.614147	-1.076834
C	3.125581	-4.012030	-0.780175
C	2.534382	-4.270742	0.420306
C	1.913988	-3.039910	0.861769
H	3.674503	-4.696028	-1.407586
H	2.507473	-5.206519	0.955528
C	1.154730	-2.923058	2.029866
N	0.458618	-0.576105	1.698354

C	0.455723	-1.767739	2.391031
C	-0.427012	-1.670771	3.537819
C	-0.970445	-0.422288	3.514616
C	-0.403817	0.264180	2.368383
H	-0.608089	-2.459138	4.251100
H	-1.676554	0.005329	4.208626
C	-0.665627	1.597905	2.041691
O	-0.064101	-0.648108	-0.852157
C	-1.654414	2.346390	2.884101
C	-3.020977	2.402482	2.558242
C	-1.287002	3.037228	4.052067
C	-3.962850	3.086443	3.321988
C	-2.193146	3.734269	4.846732
C	-3.540796	3.755835	4.474659
H	-5.003182	3.096351	3.023785
H	-1.854825	4.249469	5.736338
H	-4.260023	4.293177	5.081394
C	1.050064	-4.120694	2.924675
C	0.036262	-5.084857	2.786364
C	1.965798	-4.357399	3.964846
C	-0.074018	-6.203011	3.608693
C	1.895769	-5.460174	4.811399
C	0.865589	-6.387524	4.627699
H	-0.875271	-6.914543	3.457100
H	2.628631	-5.592578	5.596664
H	0.795359	-7.252147	5.276994
C	4.236215	-2.757028	-3.162564
C	3.688946	-3.385141	-4.295025
C	5.622209	-2.927323	-2.994054
C	4.443488	-4.126705	-5.200107
C	6.416692	-3.659028	-3.872339
C	5.817914	-4.261657	-4.982908
H	3.968460	-4.589236	-6.055503
H	7.479759	-3.756174	-3.694251
H	6.420977	-4.834836	-5.677102
C	2.679188	4.038231	-2.357555
C	2.013438	4.619796	-3.450589
C	3.797617	4.748902	-1.886472
C	2.417154	5.815215	-4.040859
C	4.237015	5.945285	-2.445581
C	3.536984	6.479247	-3.531876
H	1.867349	6.219013	-4.881220
H	5.105501	6.449562	-2.042272
H	3.863935	7.410141	-3.980004
Cl	-3.617688	1.543406	1.056841
Cl	0.466396	3.039979	4.579082
Cl	6.453698	-2.154789	-1.557494
Cl	1.894249	-3.239378	-4.618489
Cl	-1.214649	-4.885603	1.464736
Cl	3.330169	-3.169036	4.242339
Cl	4.745008	4.091111	-0.463951
Cl	0.549048	3.784948	-4.149613
C	-5.070577	-1.334317	-2.153119
C	-4.109122	-2.347177	-2.041086
C	-2.753136	-2.058984	-2.242108
C	-2.390875	-0.740777	-2.545759
C	-3.333482	0.287466	-2.663222
C	-4.685408	-0.024243	-2.465940
H	-2.009290	-2.842554	-2.160878
H	-3.033592	1.297067	-2.915108
H	-5.430301	0.758579	-2.555957
I	-0.340011	-0.290818	-2.774454
H	-6.118739	-1.566480	-1.999785
H	-4.408075	-3.362001	-1.803222
N	3.105234	0.340894	1.118364
C	4.035839	0.607933	1.749825
C	5.209035	0.943258	2.544678
H	5.488550	1.988270	2.383937
H	5.001234	0.794543	3.607963
H	6.051917	0.307184	2.259624
C	-0.344795	1.173585	-7.362007
S	-1.668665	0.750970	-6.125848
O	-0.976700	-0.304598	-5.311415
O	-1.905162	2.015587	-5.409171
O	-2.766010	0.241221	-6.960599
F	-0.049387	0.086604	-8.170266
F	-0.745652	2.214557	-8.185136
F	0.831447	1.560903	-6.737682

^{4}PC$_{(1d)}$

Fe	1.375093	-0.232381	-0.087452
N	0.810749	1.691146	0.123392
C	-0.101947	2.186428	1.041397
C	-0.345381	3.587581	0.786359
C	0.441861	3.945622	-0.267704
C	1.159683	2.762364	-0.682806
H	-1.019604	4.212342	1.349961
H	0.528280	4.916641	-0.728347
C	2.067142	2.732926	-1.743573
N	2.522040	0.294118	-1.659791
C	2.688526	1.566160	-2.191825
C	3.595610	1.514712	-3.312259
C	3.972432	0.212293	-3.466746
C	3.322584	-0.544941	-2.424671
H	3.898009	2.363720	-3.904123
H	4.642445	-0.197462	-4.205439
C	3.530432	-1.908381	-2.205524
N	2.223180	-2.066642	-0.105730
C	3.018665	-2.599942	-1.106040
C	3.292121	-3.991973	-0.829615
C	2.669664	-4.296049	0.344382
C	1.995414	-3.097718	0.790092
H	3.888442	-4.641770	-1.449813
H	2.659979	-5.241939	0.861873
C	1.219366	-3.025663	1.947791
N	0.485920	-0.673498	1.664378
C	0.517058	-1.883795	2.337665
C	-0.316933	-1.813321	3.514553
C	-0.863375	-0.563928	3.544428
C	-0.357491	0.148126	2.394408
H	-0.464013	-2.616210	4.219060
H	-1.538346	-0.155320	4.279288
C	-0.667099	1.478029	2.102920
O	-0.234411	-0.829325	-1.051682
C	-1.621497	2.197297	3.007634
C	-3.009811	2.194017	2.786601
C	-1.192286	2.920385	4.134466
C	-3.916244	2.855270	3.610895
C	-2.061995	3.595912	4.986110
C	-3.433751	3.560431	4.717521
H	-4.975921	2.820547	3.393755
H	-1.677663	4.137750	5.840488
H	-4.125118	4.080772	5.369726
C	1.121154	-4.246541	2.810977
C	0.111921	-5.210663	2.642948
C	2.035830	-4.506036	3.846630
C	0.004879	-6.351155	3.434266
C	1.968043	-5.631818	4.662482
C	0.942641	-6.558515	4.450615
H	-0.792520	-7.062080	3.261130
H	2.699012	-5.782118	5.446239
H	0.874647	-7.440601	5.076193
C	4.385729	-2.660517	-3.179386
C	3.844416	-3.307317	-4.304132
C	5.779617	-2.772078	-3.033300
C	4.613936	-4.012268	-5.225244
C	6.588787	-3.466022	-3.928709
C	5.996601	-4.088766	-5.031720
H	4.144724	-4.491656	-6.074504
H	7.657781	-3.519874	-3.768849
H	6.611307	-4.633149	-5.738733
C	2.401007	4.026730	-2.423751
C	1.726470	4.479145	-3.571336
C	3.414732	4.876085	-1.945451
C	2.023938	5.683861	-4.203790
C	3.745095	6.087582	-2.545897
C	3.039806	6.490929	-3.683920
H	1.472681	5.985140	-5.085135
H	4.535499	6.702279	-2.135211
H	3.282573	7.431172	-4.164722
Cl	-3.683692	1.282499	1.351862
Cl	0.593944	2.992823	4.526582
Cl	6.597231	-1.975133	-1.603162
Cl	2.038813	-3.238630	-4.592127
Cl	-1.135362	-4.980165	1.323557
Cl	3.391924	-3.318295	4.159998
Cl	4.369550	4.387299	-0.461629
Cl	0.401318	3.453907	-4.293688
C	-5.424148	0.078832	-2.046458
C	-4.774100	-1.014914	-1.459133
C	-3.420028	-1.257902	-1.726221
C	-2.745004	-0.379630	-2.580526
C	-3.368127	0.721353	-3.175781
C	-4.725120	0.940497	-2.901471
H	-2.914791	-2.103115	-1.274214
H	-2.827776	1.379501	-3.845246
H	-5.228241	1.787625	-3.354769
I	-0.678590	-0.740353	-2.922622
H	-6.473656	0.257440	-1.839502
H	-5.315365	-1.685383	-0.800705
N	3.462704	0.457226	1.375565
C	4.391794	0.723581	2.017627

C	5.561467	1.058448	2.823611
H	5.827294	2.110918	2.689735
H	5.356621	0.883205	3.883592
H	6.416087	0.443190	2.527962
C	0.390743	0.109535	-6.936527
S	-1.413244	0.169107	-6.488904
O	-1.486745	-0.884207	-5.422405
O	-1.602462	1.546266	-6.001397
O	-2.096374	-0.198242	-7.736790
F	0.737560	-1.119281	-7.475296
F	0.715994	1.084411	-7.864673
F	1.188398	0.312658	-5.815563

^{6}PC$_{(1d)}$

Fe	1.129592	-0.234971	-0.271496
N	0.814828	1.799286	0.120069
C	-0.040406	2.313517	1.079508
C	-0.220302	3.733368	0.856652
C	0.535035	4.069310	-0.229502
C	1.182423	2.858477	-0.691021
H	-0.833746	4.385607	1.457799
H	0.647431	5.044666	-0.675650
C	2.057860	2.788638	-1.784917
N	2.552278	0.356022	-1.682332
C	2.693880	1.621511	-2.232939
C	3.621511	1.564172	-3.341339
C	4.037701	0.267978	-3.455070
C	3.379185	-0.486528	-2.411335
H	3.919874	2.404640	-3.947695
H	4.736759	-0.136561	-4.169709
C	3.584585	-1.851664	-2.162567
N	2.168735	-2.052572	-0.137418
C	3.028081	-2.566974	-1.091669
C	3.289406	-3.963104	-0.807055
C	2.586810	-4.282256	0.318870
C	1.881342	-3.087351	0.735512
H	3.930553	-4.607801	-1.387023
H	2.551484	-5.234658	0.823671
C	1.038361	-3.007221	1.853608
N	0.404986	-0.615991	1.651428
C	0.360615	-1.852063	2.272815
C	-0.495392	-1.776692	3.437869
C	-0.965298	-0.496453	3.510831
C	-0.400057	0.230401	2.393799
H	-0.704301	-2.592478	4.111653
H	-1.626283	-0.080769	4.254774
C	-0.624686	1.590203	2.129397
O	-0.392268	-0.726586	-1.231488
C	-1.540667	2.333145	3.056164
C	-2.921206	2.443635	2.815296
C	-1.079514	2.966667	4.223200
C	-3.791967	3.126934	3.659674
C	-1.912782	3.660409	5.096404
C	-3.278765	3.738013	4.807893
H	-4.847420	3.181192	3.426568
H	-1.504932	4.130404	5.981884
H	-3.941986	4.274004	5.476439
C	0.843916	-4.254561	2.663667
C	-0.181337	-5.175414	2.385480
C	1.670982	-4.584424	3.751237
C	-0.383986	-6.339620	3.121206
C	1.506158	-5.736741	4.515106
C	0.469154	-6.617857	4.193548
H	-1.189969	-7.014394	2.863742
H	2.172337	-5.942102	5.342940
H	0.326035	-7.519428	4.777376
C	4.483098	-2.598591	-3.102965
C	3.992969	-3.225652	-4.261783
C	5.867118	-2.721951	-2.890698
C	4.801255	-3.925676	-5.152871
C	6.714038	-3.412080	-3.753759
C	6.172014	-4.016842	-4.891963
H	4.371066	-4.389976	-6.030729
H	7.773536	-3.476055	-3.542563
H	6.816502	-4.557987	-5.574512
C	2.358184	4.066484	-2.512131
C	1.616612	4.490277	-3.628820
C	3.400323	4.923962	-2.118077
C	1.878031	5.675708	-4.311226
C	3.697072	6.117228	-2.770666
C	2.925872	6.491956	-3.875276
H	1.276065	5.955384	-5.166124
H	4.511931	6.740085	-2.425203
H	3.142058	7.417544	-4.395619
Cl	-3.634293	1.660631	1.322822
Cl	0.701529	2.892540	4.637071
Cl	6.618684	-1.944331	-1.414673
Cl	2.204388	-3.133747	-4.640343
Cl	-1.322215	-4.850523	0.991698
Cl	3.040783	-3.459653	4.207218
Cl	4.437507	4.471057	-0.679141
Cl	0.246940	3.448912	-4.241509
C	-5.607253	-0.590224	-2.132209
C	-4.902510	-1.786875	-1.947105
C	-3.538622	-1.857998	-2.257638
C	-2.910202	-0.706049	-2.746387
C	-3.591758	0.500854	-2.941836
C	-4.956641	0.546646	-2.629502
H	-2.992534	-2.783357	-2.118982
H	-3.087304	1.373091	-3.337728
H	-5.504404	1.470935	-2.775313
I	-0.835407	-0.787219	-3.131516
H	-6.663640	-0.544552	-1.891677
H	-5.408015	-2.667087	-1.566018
N	4.437070	0.568102	2.006824
C	5.385958	0.812569	2.630733
C	6.579493	1.119360	3.414235
H	6.858734	2.169734	3.290407
H	6.398529	0.932102	4.476666
H	7.419358	0.497334	3.091197
C	0.106707	0.273795	-7.043785
S	-1.660977	0.142908	-6.481327
O	-1.565050	-1.011394	-5.508166
O	-1.928508	1.439928	-5.844183
O	-2.403213	-0.192348	-7.700367
F	0.510745	-0.872793	-7.705246
F	0.282718	1.345589	-7.900008
F	0.955843	0.453155	-5.957788

^{2}RC$_{(1b)}$

Fe	1.397911	0.171895	0.343635
N	1.058800	2.145898	0.659073
C	0.349461	2.709662	1.698947
C	0.262840	4.142612	1.526891
C	0.926338	4.441173	0.374165
C	1.417110	3.190526	-0.160494
H	-0.234683	4.821798	2.199748
H	1.073042	5.410339	-0.073743
C	2.151421	3.081580	-1.353531
N	2.463260	0.628273	-1.320708
C	2.629582	1.876391	-1.883598
C	3.380968	1.773866	-3.114825
C	3.665119	0.452696	-3.293400
C	3.090721	-0.253149	-2.169586
H	3.651369	2.601280	-3.750252
H	4.212372	-0.003612	-4.101920
C	3.182918	-1.643006	-1.985435
N	1.936973	-1.772508	0.147258
C	2.645423	-2.336302	-0.893302
C	2.761079	-3.765031	-0.703503
C	2.111207	-4.061605	0.457469
C	1.598062	-2.814272	0.978654
H	3.271896	-4.442229	-1.368379
H	1.990630	-5.026974	0.921160
C	0.855571	-2.706691	2.166379
N	0.525064	-0.255589	2.122952
C	0.363973	-1.503128	2.688878
C	-0.393406	-1.401300	3.916517
C	-0.690714	-0.082021	4.087061
C	-0.116715	0.623773	2.963051
H	-0.654986	-2.227273	4.557471
H	-1.241685	0.373756	4.893365
C	-0.210655	2.013369	2.777641
O	0.019393	-0.029354	-0.481364
C	-0.960128	2.804265	3.806631
C	-2.339597	3.044734	3.697856
C	-0.326951	3.347316	4.936380
C	-3.056103	3.774649	4.641249
C	-1.005866	4.083553	5.902615
C	-2.379745	4.295506	5.749027
H	-4.119022	3.933392	4.514483
H	-0.474298	4.482860	6.756444
H	-2.923089	4.866268	6.492525
C	0.561981	-3.967248	2.922391
C	-0.579473	-4.740736	2.654101
C	1.406140	-4.443773	3.938041
C	-0.876715	-5.911692	3.344249
C	1.146031	-5.609706	4.651619
C	-0.005076	-6.344248	4.348868
H	-1.769174	-6.474298	3.103182
H	1.826463	-5.938417	5.426282
H	-0.222222	-7.253969	4.895790
C	3.908482	-2.436862	-3.029060

C	3.243613	-2.989682	-4.135730
C	5.291493	-2.670486	-2.960529
C	3.896398	-3.728246	-5.117863
C	5.982526	-3.403136	-3.920786
C	5.275256	-3.933250	-5.004685
H	3.341194	-4.134422	-5.953212
H	7.049398	-3.557029	-3.825074
H	5.798475	-4.505857	-5.761074
C	2.447836	4.343305	-2.106326
C	1.590036	4.835056	-3.103295
C	3.600895	5.104253	-1.853815
C	1.848126	6.004222	-3.812435
C	3.896829	6.277961	-2.540006
C	3.010985	6.726345	-3.524926
H	1.156672	6.344692	-4.572110
H	4.798797	6.830441	-2.311209
H	3.226490	7.638642	-4.068191
Cl	-3.248068	2.375376	2.260963
Cl	1.467286	3.084643	5.162494
Cl	6.239345	-1.990888	-1.553849
Cl	1.442915	-2.734248	-4.308558
Cl	-1.731736	-4.196792	1.345204
Cl	2.918196	-3.503894	4.349859
Cl	4.775253	4.540079	-0.572457
Cl	0.063064	3.911702	-3.494749
C	-4.067003	-3.094404	-1.307474
C	-3.331925	-3.422551	-2.453676
C	-2.923099	-2.420390	-3.344466
C	-3.258554	-1.088466	-3.069999
C	-3.989891	-0.743622	-1.926132
C	-4.392350	-1.757455	-1.045292
H	-2.358169	-2.678999	-4.232039
H	-4.246734	0.288885	-1.721159
H	-4.962608	-1.496814	-0.159884
I	-2.647888	0.441607	-4.422970
H	-4.386773	-3.875853	-0.626512
H	-3.077104	-4.456152	-2.663028
N	3.221023	0.440993	1.433064
C	4.206350	0.602273	2.015761
C	5.448416	0.807502	2.746819
H	5.943951	1.718747	2.400406
H	5.245397	0.903373	3.817135
H	6.122633	-0.039463	2.591945

^{4}RC$_{(1b)}$

Fe	1.544653	0.066876	-0.052296
N	1.038920	2.016112	0.183867
C	0.183512	2.542300	1.125146
C	0.006271	3.960548	0.906100
C	0.764230	4.288823	-0.178197
C	1.404623	3.071431	-0.623872
H	-0.611009	4.610863	1.504050
H	0.883502	5.258232	-0.633752
C	2.276974	2.998247	-1.718808
N	2.760894	0.575448	-1.592150
C	2.908130	1.822739	-2.155864
C	3.816605	1.762408	-3.279163
C	4.215938	0.464155	-3.392864
C	3.551936	-0.270674	-2.339392
H	4.107299	2.600404	-3.891348
H	4.894440	0.040920	-4.115361
C	3.703040	-1.648438	-2.127921
N	2.222550	-1.841271	-0.155585
C	3.070388	-2.369420	-1.102918
C	3.234152	-3.790812	-0.894158
C	2.475114	-4.119308	0.189465
C	1.848238	-2.898774	0.645569
H	3.848457	-4.441945	-1.494282
H	2.351560	-5.089781	0.641604
C	0.991618	-2.821948	1.752759
N	0.514500	-0.397713	1.630607
C	0.382259	-1.641224	2.206142
C	-0.488215	-1.571670	3.358612
C	-0.887409	-0.273373	3.472239
C	-0.260775	0.452201	2.389898
H	-0.752623	-2.403418	3.990903
H	-1.539971	0.156270	4.214597
C	-0.432648	1.824852	2.162476
O	0.284224	-0.232870	-1.023620
C	-1.335256	2.578517	3.091657
C	-2.713365	2.701115	2.849945
C	-0.854670	3.203096	4.253976
C	-3.570056	3.396326	3.697891
C	-1.676873	3.907223	5.128348
C	-3.042835	4.001655	4.843212
H	-4.625753	3.464042	3.469842
H	-1.260755	4.371705	6.012789
H	-3.696477	4.546514	5.513778
C	0.705819	-4.086607	2.504834
C	-0.397697	-4.899262	2.197070
C	1.522067	-4.527822	3.558971
C	-0.682270	-6.076975	2.881308
C	1.272655	-5.698394	4.268896
C	0.161910	-6.474674	3.923038
H	-1.544293	-6.671285	2.607727
H	1.930125	-5.997646	5.074672
H	-0.046099	-7.389008	4.465767
C	4.603492	-2.402546	-3.059304
C	4.125751	-2.987120	-4.243633
C	5.974316	-2.565092	-2.801002
C	4.943959	-3.689211	-5.123265
C	6.827097	-3.259244	-3.653830
C	6.303034	-3.822979	-4.821555
H	4.529910	-4.122225	-6.024506
H	7.877345	-3.357939	-3.412329
H	6.953655	-4.366434	-5.496184
C	2.559670	4.262748	-2.472462
C	1.776790	4.667880	-3.565811
C	3.624210	5.111728	-2.128080
C	2.023426	5.836434	-4.280017
C	3.905392	6.288395	-2.815583
C	3.096358	6.648209	-3.898206
H	1.392245	6.107324	-5.116270
H	4.737506	6.910734	-2.513295
H	3.301886	7.561163	-4.444184
Cl	-3.426741	1.917808	1.361496
Cl	0.925507	3.093074	4.651160
Cl	6.685291	-1.839016	-1.282236
Cl	2.354290	-2.827824	-4.659792
Cl	-1.518197	-4.400480	0.843500
Cl	2.976402	-3.529500	4.036528
Cl	4.697306	4.665409	-0.717932
Cl	0.369797	3.625272	-4.087270
C	-4.957207	-0.985715	-1.137283
C	-4.845551	-2.372366	-0.976228
C	-3.965072	-3.111551	-1.778818
C	-3.198775	-2.442906	-2.742283
C	-3.298130	-1.056604	-2.914844
C	-4.184347	-0.331770	-2.105179
H	-3.884956	-4.184540	-1.652163
H	-2.703785	-0.546006	-3.663094
H	-4.268121	0.741784	-2.238297
I	-1.857265	-3.556875	-3.967730
H	-5.643050	-0.419897	-0.515961
H	-5.441762	-2.886147	-0.229424
N	3.210929	0.470633	1.228927
C	4.113991	0.702065	1.912559
C	5.251418	0.995183	2.772761
H	5.770424	1.890710	2.419714
H	4.914775	1.166056	3.799203
H	5.954394	0.157332	2.768437

^{6}RC$_{(1b)}$

Fe	1.431023	0.116910	-0.038460
N	0.996159	2.134570	0.262507
C	0.172859	2.650937	1.233316
C	0.028921	4.080168	1.030393
C	0.772766	4.404230	-0.068723
C	1.378037	3.176084	-0.548216
H	-0.557044	4.743645	1.645734
H	0.901914	5.379259	-0.510167
C	2.233479	3.072344	-1.668135
N	2.704099	0.640690	-1.604425
C	2.845204	1.893132	-2.151015
C	3.727109	1.818731	-3.300524
C	4.103352	0.511945	-3.431103
C	3.455526	-0.224640	-2.362246
H	4.020183	2.651415	-3.919407
H	4.758222	0.088347	-4.175368
C	3.584470	-1.613546	-2.135608
N	2.150368	-1.838380	-0.127980
C	2.976450	-2.354256	-1.096849
C	3.133292	-3.780738	-0.884449
C	2.391138	-4.104482	0.215912
C	1.773964	-2.878880	0.686659
H	3.731281	-4.441574	-1.490990
H	2.275291	-5.076689	0.667143
C	0.922901	-2.774451	1.809851
N	0.444509	-0.344467	1.739953
C	0.312819	-1.594770	2.293703
C	-0.549050	-1.516078	3.457984
C	-0.927770	-0.209828	3.586713
C	-0.300822	0.522246	2.502401

H	-0.823315	-2.344827	4.090610
H	-1.566368	0.217290	4.343021
C	-0.433431	1.910339	2.273215
O	0.152924	-0.161303	-0.987007
C	-1.298943	2.673894	3.232025
C	-2.673656	2.856001	3.010127
C	-0.782824	3.248256	4.405113
C	-3.494464	3.558724	3.886949
C	-1.568162	3.958384	5.308101
C	-2.932670	4.111549	5.042279
H	-4.549197	3.672370	3.673180
H	-1.124849	4.382845	6.199423
H	-3.558067	4.661587	5.735190
C	0.637644	-4.040723	2.562784
C	-0.458088	-4.860467	2.246507
C	1.447438	-4.475744	3.624271
C	-0.742658	-6.038028	2.931165
C	1.198116	-5.646047	4.334758
C	0.094178	-6.428692	3.981452
H	-1.599061	-6.637551	2.651311
H	1.850735	-5.940491	5.146239
H	-0.113845	-7.342761	4.524640
C	4.453716	-2.376304	-3.091765
C	3.939603	-2.954240	-4.264028
C	5.828890	-2.553846	-2.869230
C	4.727387	-3.663755	-5.165335
C	6.652088	-3.255882	-3.744409
C	6.092257	-3.812442	-4.898895
H	4.285571	-4.091129	-6.056019
H	7.707075	-3.366053	-3.530068
H	6.719447	-4.361944	-5.590610
C	2.525312	4.339834	-2.416481
C	1.728335	4.770402	-3.489665
C	3.612768	5.164983	-2.086449
C	1.982879	5.940689	-4.198277
C	3.902598	6.342643	-2.768749
C	3.078847	6.728153	-3.831240
H	1.340123	6.231531	-5.018877
H	4.752571	6.946027	-2.477898
H	3.290791	7.642159	-4.373000
Cl	-3.433713	2.144079	1.508747
Cl	0.996917	3.063945	4.777060
Cl	6.586727	-1.836828	-1.368775
Cl	2.159821	-2.775791	-4.636386
Cl	-1.567885	-4.370922	0.880698
Cl	2.895440	-3.471185	4.108586
Cl	4.705566	4.684906	-0.702499
Cl	0.290592	3.760268	-3.991311
C	-4.065710	-1.106922	-1.377782
C	-4.327585	-2.454266	-1.098820
C	-3.931856	-3.455251	-1.997706
C	-3.271965	-3.087243	-3.177246
C	-3.002739	-1.744682	-3.470548
C	-3.404698	-0.755628	-2.561482
H	-4.138763	-4.495902	-1.778557
H	-2.493935	-1.467275	-4.385905
H	-3.201862	0.286274	-2.786353
I	-2.669958	-4.598885	-4.555662
H	-4.376552	-0.336960	-0.679671
H	-4.841471	-2.734045	-0.185189
N	3.143759	0.495508	1.227054
C	4.061032	0.716440	1.895124
C	5.215867	0.997136	2.735652
H	5.758461	1.865937	2.352541
H	4.895046	1.206848	3.759996
H	5.892274	0.137809	2.747912

^{2}TS$_{(1b)}$

Fe	1.359594	0.039896	0.260606
N	0.903460	1.982505	0.520710
C	0.109154	2.509372	1.520816
C	-0.000514	3.943071	1.358360
C	0.755347	4.281245	0.275353
C	1.308502	3.053809	-0.250598
H	-0.568019	4.598906	1.998673
H	0.916812	5.263433	-0.138748
C	2.106098	2.976301	-1.397843
N	2.286613	0.503849	-1.453999
C	2.535917	1.772977	-1.963070
C	3.306245	1.674147	-3.180947
C	3.540455	0.349454	-3.401344
C	2.939379	-0.377924	-2.306441
H	3.622512	2.510208	-3.783665
H	4.088136	-0.097311	-4.215331
C	3.086721	-1.753235	-2.109494
N	1.996549	-1.873961	0.106555
C	2.651066	-2.436356	-0.966004
C	2.876060	-3.846246	-0.727704
C	2.359794	-4.126948	0.501736
C	1.799873	-2.895009	1.016004
H	3.367737	-4.521443	-1.409259
H	2.346991	-5.076051	1.012875
C	1.121919	-2.793648	2.235676
N	0.514267	-0.405845	2.059710
C	0.493004	-1.629304	2.691552
C	-0.310497	-1.551188	3.895167
C	-0.787462	-0.277744	3.970779
C	-0.261227	0.437753	2.825476
H	-0.486924	-2.366328	4.578369
H	-1.424144	0.146836	4.730173
C	-0.470510	1.798524	2.579571
O	-0.124659	-0.359286	-0.379272
C	-1.339609	2.555653	3.538302
C	-2.724211	2.689019	3.339599
C	-0.828689	3.174215	4.691994
C	-3.555407	3.384239	4.213068
C	-1.622440	3.879372	5.592153
C	-2.995195	3.982241	5.346215
H	-4.616634	3.457151	4.014012
H	-1.179149	4.338340	6.466234
H	-3.627524	4.527363	6.036836
C	1.026468	-4.021130	3.090625
C	-0.024416	-4.945826	2.966636
C	1.985714	-4.319509	4.073035
C	-0.128537	-6.089493	3.753325
C	1.921559	-5.450688	4.881364
C	0.854387	-6.339113	4.716239
H	-0.958569	-6.770526	3.617713
H	2.687405	-5.634363	5.623563
H	0.788906	-7.224544	5.337228
C	3.822259	-2.538463	-3.154207
C	3.163007	-3.146893	-4.235443
C	5.215858	-2.718579	-3.113909
C	3.824217	-3.881919	-5.215255
C	5.917724	-3.444378	-4.071969
C	5.212050	-4.028194	-5.128695
H	3.268082	-4.330910	-6.027832
H	6.991767	-3.552246	-3.995038
H	5.742796	-4.596817	-5.882953
C	2.525086	4.256378	-2.056232
C	1.769996	4.877333	-3.065480
C	3.713093	4.916193	-1.695461
C	2.152454	6.065690	-3.681564
C	4.134068	6.104640	-2.284600
C	3.344196	6.679772	-3.284911
H	1.533063	6.502467	-4.454009
H	5.058106	6.571600	-1.969651
H	3.656802	7.604949	-3.754199
Cl	-3.491958	1.915443	1.871108
Cl	0.961897	3.062461	5.048153
Cl	6.175717	-1.973116	-1.746912
Cl	1.348217	-2.981421	-4.379924
Cl	-1.329471	-4.652778	1.719204
Cl	3.395727	-3.180448	4.318120
Cl	4.774469	4.196843	-0.391065
Cl	0.204067	4.109036	-3.613032
C	-5.041027	-1.922851	-1.653596
C	-3.968563	-2.649167	-2.188836
C	-2.756328	-2.011245	-2.476108
C	-2.638165	-0.637022	-2.214922
C	-3.702563	0.105137	-1.678894
C	-4.907473	-0.550691	-1.401080
H	-1.927737	-2.572521	-2.890693
H	-3.598592	1.165228	-1.481788
H	-5.737052	0.012427	-0.988058
I	-0.819811	0.330347	-2.631179
H	-5.977603	-2.423904	-1.435159
H	-4.071068	-3.710704	-2.385226
N	3.140930	0.423638	1.294712
C	4.119555	0.630919	1.873693
C	5.352152	0.892145	2.602993
H	5.801654	1.828932	2.261949
H	5.147822	0.969981	3.674516
H	6.066518	0.080280	2.439938

^{4}TS$_{(1b)}$

Fe	1.443111	-0.284001	0.013639
N	0.844091	1.662167	0.227911
C	-0.132816	2.115935	1.095188
C	-0.468750	3.485385	0.775102
C	0.308689	3.852362	-0.284228
C	1.112279	2.704050	-0.639932
H	-1.198218	4.083497	1.297387

H	0.328127	4.803434	-0.791850
C	2.001770	2.661592	-1.716656
N	2.472161	0.219454	-1.644731
C	2.639272	1.498072	-2.157154
C	3.559581	1.454490	-3.271228
C	3.950152	0.158188	-3.424050
C	3.296195	-0.611818	-2.389740
H	3.863568	2.308584	-3.854629
H	4.637168	-0.243786	-4.151090
C	3.525783	-1.972874	-2.168956
N	2.348837	-2.120737	-0.000538
C	3.057419	-2.670618	-1.052688
C	3.295431	-4.073993	-0.799682
C	2.722839	-4.366896	0.403119
C	2.109968	-3.151098	0.890733
H	3.831230	-4.740422	-1.456448
H	2.700887	-5.318033	0.910439
C	1.366028	-3.058849	2.069481
N	0.516539	-0.747741	1.738980
C	0.643598	-1.925226	2.453978
C	-0.140041	-1.836609	3.667340
C	-0.737128	-0.612556	3.674208
C	-0.314442	0.078334	2.474916
H	-0.216770	-2.614412	4.409869
H	-1.388618	-0.198539	4.426738
C	-0.671319	1.393278	2.163430
O	-0.104679	-0.854544	-0.784570
C	-1.659285	2.083363	3.054714
C	-3.047018	1.968623	2.862057
C	-1.262479	2.887726	4.137304
C	-3.984130	2.601979	3.673494
C	-2.164431	3.538166	4.974586
C	-3.534402	3.391644	4.736070
H	-5.042138	2.482053	3.480130
H	-1.805886	4.144786	5.795936
H	-4.250280	3.891437	5.377749
C	1.305590	-4.265445	2.956453
C	0.284863	-5.226189	2.851018
C	2.270635	-4.512374	3.947974
C	0.213999	-6.354653	3.662927
C	2.238206	-5.625619	4.782878
C	1.200102	-6.550655	4.634903
H	-0.592666	-7.065434	3.539369
H	3.005816	-5.767700	5.532357
H	1.159802	-7.423293	5.275869
C	4.362494	-2.716832	-3.164976
C	3.807154	-3.312279	-4.310429
C	5.752406	-2.868827	-3.017575
C	4.560320	-4.009244	-5.250621
C	6.544986	-3.556278	-3.932363
C	5.939758	-4.128868	-5.055331
H	4.081508	-4.450188	-6.115154
H	7.611836	-3.642508	-3.772580
H	6.542039	-4.667631	-5.777104
C	2.280606	3.941204	-2.446952
C	1.568380	4.334738	-3.593014
C	3.279462	4.834262	-2.020048
C	1.816759	5.522313	-4.275547
C	3.563040	6.030764	-2.672158
C	2.822948	6.372970	-3.808006
H	1.237021	5.778069	-5.152835
H	4.344721	6.681352	-2.302180
H	3.029798	7.300865	-4.327819
Cl	-3.676907	0.949401	1.480852
Cl	0.519770	3.097958	4.491516
Cl	6.584909	-2.128784	-1.567039
Cl	2.003533	-3.190040	-4.598456
Cl	-1.020548	-5.008887	1.588059
Cl	3.641492	-3.323177	4.175742
Cl	4.275713	4.422180	-0.542470
Cl	0.240119	3.256395	-4.238941
C	-5.317957	0.744192	-2.403535
C	-5.028299	-0.625859	-2.345379
C	-3.714187	-1.077483	-2.511896
C	-2.703664	-0.129718	-2.734843
C	-2.972628	1.246132	-2.793929
C	-4.294512	1.675041	-2.626797
H	-3.489047	-2.136106	-2.468371
H	-2.180611	1.965181	-2.963969
H	-4.519230	2.734823	-2.671257
I	-0.725851	-0.796645	-3.001045
H	-6.339245	1.085469	-2.275718
H	-5.820345	-1.345866	-2.172712
N	3.366625	0.400482	1.328190
C	4.290450	0.704629	1.958700
C	5.453706	1.086365	2.751271
H	5.649990	2.157209	2.646907
H	5.282440	0.864323	3.808388
H	6.337672	0.535318	2.417877

^{6}TS$_{(1b)}$

Fe	1.275756	-0.237900	0.161857
N	0.819706	1.791053	0.465199
C	0.052812	2.296440	1.481850
C	-0.152533	3.718684	1.271536
C	0.508006	4.050875	0.122001
C	1.120940	2.834660	-0.382289
H	-0.716861	4.373293	1.916359
H	0.576102	5.024439	-0.336688
C	1.911692	2.742290	-1.547654
N	2.474253	0.328633	-1.488976
C	2.540567	1.576942	-2.054857
C	3.383141	1.527696	-3.235199
C	3.824197	0.237655	-3.355542
C	3.256708	-0.506952	-2.246837
H	3.613383	2.361666	-3.878881
H	4.477309	-0.163442	-4.114047
C	3.503261	-1.875182	-1.969391
N	2.215527	-2.119539	0.134648
C	3.027650	-2.611323	-0.862678
C	3.326881	-4.006202	-0.590333
C	2.689220	-4.331450	0.574152
C	1.992265	-3.138501	1.022374
H	3.942315	-4.646723	-1.201753
H	2.693218	-5.283735	1.080070
C	1.206405	-3.042731	2.199098
N	0.510384	-0.669510	2.044909
C	0.530639	-1.898162	2.668979
C	-0.239735	-1.821048	3.899623
C	-0.703951	-0.542074	4.003973
C	-0.222819	0.184409	2.840220
H	-0.396196	-2.633648	4.591018
H	-1.306344	-0.125767	4.795524
C	-0.446609	1.551793	2.580583
O	-0.244467	-0.723363	-0.645164
C	-1.279603	2.301632	3.578707
C	-2.672430	2.424195	3.442701
C	-0.718100	2.924739	4.705471
C	-3.466314	3.112357	4.355503
C	-1.474191	3.622735	5.642615
C	-2.857959	3.713526	5.461943
H	-4.536176	3.177972	4.206342
H	-0.993817	4.085772	6.494664
H	-3.461466	4.252798	6.182269
C	1.093903	-4.284011	3.035068
C	0.061851	-5.218136	2.846984
C	2.013309	-4.585543	4.053274
C	-0.062296	-6.376053	3.609135
C	1.927122	-5.731069	4.838980
C	0.879838	-6.629431	4.611177
H	-0.876093	-7.065190	3.424841
H	2.661120	-5.917990	5.611918
H	0.798235	-7.526058	5.213898
C	4.373783	-2.612055	-2.945355
C	3.839621	-3.279653	-4.059542
C	5.769788	-2.677841	-2.804649
C	4.623280	-3.968983	-4.979977
C	6.591408	-3.355442	-3.700795
C	6.009009	-4.003726	-4.794542
H	4.162833	-4.468028	-5.822634
H	7.662630	-3.376913	-3.548701
H	6.634313	-4.535608	-5.501616
C	2.137118	4.014719	-2.312338
C	1.281133	4.430511	-3.345128
C	3.221547	4.864965	-2.038204
C	1.474090	5.606070	-4.064855
C	3.452510	6.048654	-2.732697
C	2.569430	6.417322	-3.752453
H	0.785070	5.882420	-4.852295
H	4.303011	6.669649	-2.483367
H	2.734886	7.335732	-4.302954
Cl	-3.497830	1.653595	2.005115
Cl	1.088684	2.828368	4.969933
Cl	6.563046	-1.840625	-1.386036
Cl	2.030688	-3.256675	-4.329657
Cl	-1.184965	-4.916627	1.544061
Cl	3.393540	-3.431046	4.378020
Cl	4.395539	4.413667	-0.711059
Cl	-0.158723	3.392192	-3.781205
C	-5.579646	0.226239	-1.554425
C	-5.167051	-1.112457	-1.584279
C	-3.850567	-1.439100	-1.931102

C	-2.960494	-0.401677	-2.246567
C	-3.356244	0.943923	-2.224334
C	-4.677058	1.249576	-1.873803
H	-3.531335	-2.474114	-1.952086
H	-2.658850	1.735613	-2.470121
H	-4.995509	2.285990	-1.852941
I	-0.970846	-0.876800	-2.745916
H	-6.601129	0.471224	-1.285061
H	-5.864674	-1.905432	-1.338282
N	3.287960	0.373520	1.434205
C	4.242096	0.646900	2.032691
C	5.443084	0.989758	2.786057
H	5.667122	2.055003	2.680205
H	5.302346	0.766674	3.847460
H	6.298506	0.415280	2.419404

^{2}PC$_{(1b)}$

Fe	1.428146	-0.049442	0.327671
N	0.868756	1.870115	0.507787
C	0.042231	2.381336	1.494317
C	-0.141514	3.801529	1.289735
C	0.602833	4.151615	0.201975
C	1.228328	2.945864	-0.289285
H	-0.748070	4.443669	1.908105
H	0.713573	5.130698	-0.236039
C	2.048446	2.891216	-1.420466
N	2.320641	0.426714	-1.425966
C	2.546638	1.698960	-1.949143
C	3.340691	1.600902	-3.148205
C	3.609237	0.276813	-3.347623
C	3.005181	-0.452987	-2.258310
H	3.648170	2.435295	-3.758260
H	4.182036	-0.164797	-4.147339
C	3.166058	-1.825105	-2.050084
N	2.090631	-1.945911	0.182483
C	2.741852	-2.501319	-0.901225
C	2.983233	-3.909232	-0.659653
C	2.485626	-4.193884	0.576295
C	1.916238	-2.969063	1.095576
H	3.473826	-4.581161	-1.345572
H	2.489685	-5.142396	1.089158
C	1.250365	-2.872409	2.319914
N	0.565301	-0.508105	2.089089
C	0.602406	-1.715034	2.758064
C	-0.174220	-1.627120	3.977817
C	-0.690297	-0.367978	4.029825
C	-0.217515	0.333146	2.851768
H	-0.308311	-2.428061	4.687262
H	-1.322974	0.056718	4.792742
C	-0.490856	1.676277	2.577749
O	-0.137137	-0.567754	-0.441973
C	-1.370755	2.421301	3.536692
C	-2.765719	2.485642	3.376592
C	-0.861911	3.099538	4.658265
C	-3.606160	3.167869	4.251858
C	-1.663280	3.794283	5.560083
C	-3.045426	3.826067	5.350625
H	-4.674593	3.184807	4.080403
H	-1.218709	4.299575	6.407611
H	-3.684117	4.362074	6.042624
C	1.187145	-4.091435	3.189011
C	0.150387	-5.035918	3.091022
C	2.164261	-4.368589	4.160727
C	0.075373	-6.174266	3.888969
C	2.130247	-5.492601	4.981170
C	1.075398	-6.399519	4.840075
H	-0.745383	-6.869765	3.771075
H	2.909533	-5.657003	5.713889
H	1.032843	-7.280152	5.469929
C	3.896255	-2.611197	-3.097565
C	3.233211	-3.206081	-4.184930
C	5.288501	-2.805471	-3.062814
C	3.886035	-3.939924	-5.171422
C	5.983716	-3.530355	-4.026861
C	5.272485	-4.099973	-5.087460
H	3.324999	-4.377474	-5.986887
H	7.056953	-3.647765	-3.951979
H	5.797551	-4.667567	-5.846544
C	2.399287	4.175016	-2.109448
C	1.622863	4.721826	-3.146224
C	3.540002	4.918881	-1.757915
C	1.938872	5.913240	-3.793137
C	3.895886	6.113884	-2.376854
C	3.085380	6.611127	-3.401923
H	1.304046	6.288390	-4.585223
H	4.786040	6.644900	-2.065621
H	3.346445	7.539946	-3.895018
Cl	-3.540457	1.635695	1.953613
Cl	0.941057	3.085162	4.972734
Cl	6.261675	-2.076789	-1.694730
Cl	1.417823	-3.026466	-4.331907
Cl	-1.179510	-4.780385	1.859714
Cl	3.562364	-3.207890	4.377941
Cl	4.631444	4.306890	-0.422485
Cl	0.110757	3.848505	-3.695573
C	-5.295410	-1.081720	-2.061450
C	-4.333065	-1.990075	-2.522662
C	-2.982786	-1.625198	-2.565357
C	-2.624431	-0.340352	-2.128768
C	-3.573255	0.584717	-1.666150
C	-4.918545	0.199779	-1.637324
H	-2.237313	-2.322935	-2.927672
H	-3.278801	1.573498	-1.336447
H	-5.665933	0.901190	-1.284308
I	-0.600579	0.218250	-2.188141
H	-6.340069	-1.371326	-2.035740
H	-4.628347	-2.979499	-2.853006
N	3.145881	0.410884	1.324559
C	4.118894	0.667072	1.893186
C	5.344126	0.988640	2.610512
H	5.568139	2.054927	2.516035
H	5.236287	0.743098	3.670734
H	6.181406	0.416340	2.200792

^{4}PC$_{(1b)}$

Fe	1.421084	-0.342070	-0.015489
N	0.716058	1.538253	0.103564
C	-0.214203	2.014522	1.015534
C	-0.547288	3.384761	0.706219
C	0.204843	3.747560	-0.372757
C	0.991496	2.596803	-0.749026
H	-1.253158	3.989740	1.252311
H	0.225186	4.702587	-0.872872
C	1.894421	2.582097	-1.814252
N	2.483363	0.176895	-1.646394
C	2.580516	1.437398	-2.222331
C	3.479107	1.393516	-3.349247
C	3.917622	0.106059	-3.465706
C	3.313579	-0.647848	-2.394956
H	3.734677	2.235865	-3.971831
H	4.600335	-0.294411	-4.197779
C	3.573311	-1.997214	-2.147919
N	2.304603	-2.153152	-0.022970
C	3.097594	-2.682292	-1.028961
C	3.411930	-4.060931	-0.733840
C	2.818882	-4.361048	0.456684
C	2.120917	-3.174531	0.894514
H	4.012947	-4.706100	-1.354265
H	2.842738	-5.298172	0.989346
C	1.363845	-3.102663	2.064393
N	0.531710	-0.790416	1.726740
C	0.628736	-1.976535	2.437568
C	-0.180611	-1.901446	3.630313
C	-0.777963	-0.675029	3.633930
C	-0.331617	0.018922	2.449514
H	-0.278637	-2.686599	4.362715
H	-1.452778	-0.271346	4.371492
C	-0.715642	1.319203	2.117710
O	-0.198605	-1.097627	-0.973380
C	-1.682505	2.021831	3.022559
C	-3.075070	1.906875	2.868219
C	-1.259167	2.835931	4.088134
C	-3.991182	2.549197	3.696698
C	-2.138705	3.496749	4.941105
C	-3.514427	3.349850	4.738928
H	-5.053802	2.426781	3.532285
H	-1.758725	4.111359	5.746757
H	-4.213434	3.856973	5.393368
C	1.314508	-4.308519	2.952302
C	0.325979	-5.299565	2.820405
C	2.254984	-4.526241	3.974075
C	0.262205	-6.427495	3.633745
C	2.230114	-5.638304	4.811029
C	1.223837	-6.593148	4.635350
H	-0.520296	-7.160923	3.488811
H	2.979012	-5.756771	5.583222
H	1.189252	-7.465089	5.277649
C	4.434715	-2.740770	-3.122459
C	3.896173	-3.396011	-4.243513
C	5.830608	-2.832299	-2.983072
C	4.669814	-4.093946	-5.166275
C	6.644014	-3.518549	-3.880567
C	6.054276	-4.152571	-4.978498

H	4.203030	-4.581519	-6.012189
H	7.714506	-3.557394	-3.726584
H	6.672461	-4.691329	-5.686757
C	2.155805	3.865891	-2.543374
C	1.463003	4.242672	-3.706941
C	3.127814	4.781343	-2.100051
C	1.701829	5.433077	-4.388330
C	3.400514	5.982215	-2.748728
C	2.678626	6.306510	-3.901336
H	1.137513	5.673137	-5.280005
H	4.160445	6.649621	-2.363650
H	2.877516	7.237203	-4.419281
Cl	-3.742960	0.867403	1.520352
Cl	0.531774	3.049439	4.396964
Cl	6.643630	-2.014969	-1.562398
Cl	2.087560	-3.348615	-4.524049
Cl	-0.949733	-5.122994	1.520456
Cl	3.586316	-3.299427	4.239056
Cl	4.103340	4.396048	-0.600869
Cl	0.176743	3.133618	-4.386412
C	-5.177029	1.158428	-2.305448
C	-5.015572	-0.230938	-2.393904
C	-3.736890	-0.784588	-2.525918
C	-2.633754	0.082276	-2.563512
C	-2.774697	1.475419	-2.474029
C	-4.062991	2.007327	-2.345130
H	-3.609606	-1.858149	-2.597719
H	-1.912891	2.130417	-2.506589
H	-4.191174	3.081684	-2.276612
I	-0.703996	-0.744360	-2.783855
H	-6.171478	1.579468	-2.207246
H	-5.879516	-0.885160	-2.363825
N	3.364679	0.449174	1.329367
C	4.277644	0.767671	1.969358
C	5.426343	1.167187	2.774441
H	5.616996	2.238021	2.660079
H	5.240949	0.956592	3.831534
H	6.318936	0.618405	2.460834

^{6}PC$_{(1b)}$

Fe	1.306107	-0.324146	0.204157
N	0.716528	1.651343	0.420530
C	-0.095791	2.144414	1.424888
C	-0.374682	3.542594	1.166144
C	0.289825	3.883383	0.021231
C	0.977537	2.696410	-0.445625
H	-0.988276	4.180622	1.782296
H	0.311213	4.847399	-0.462075
C	1.789394	2.632047	-1.591280
N	2.373506	0.216916	-1.490807
C	2.431986	1.475694	-2.067441
C	3.269964	1.418934	-3.244896
C	3.716891	0.131257	-3.365606
C	3.173251	-0.618900	-2.254888
H	3.491284	2.251442	-3.893884
H	4.367287	-0.266298	-4.128535
C	3.458501	-1.968196	-1.979641
N	2.257428	-2.169506	0.181770
C	3.033502	-2.676373	-0.842550
C	3.364710	-4.057028	-0.550232
C	2.788996	-4.365113	0.650081
C	2.089733	-3.180307	1.107536
H	3.959114	-4.702405	-1.177430
H	2.830818	-5.306355	1.175074
C	1.349824	-3.091182	2.299445
N	0.554665	-0.748632	2.070559
C	0.641314	-1.958554	2.735788
C	-0.122743	-1.879107	3.962714
C	-0.661051	-0.623309	4.026204
C	-0.231652	0.089325	2.841728
H	-0.233556	-2.676202	4.680784
H	-1.286434	-0.218041	4.805818
C	-0.546925	1.427252	2.547127
O	-0.325055	-0.989445	-0.644414
C	-1.408492	2.160453	3.532867
C	-2.811259	2.170263	3.443728
C	-0.868728	2.881836	4.612343
C	-3.630581	2.840036	4.348365
C	-1.648229	3.566549	5.540505
C	-3.039548	3.542193	5.403177
H	-4.706275	2.814413	4.232383
H	-1.180079	4.106546	6.353207
H	-3.661713	4.069162	6.116853
C	1.304277	-4.309819	3.173189
C	0.304233	-5.289640	3.045976
C	2.260280	-4.551433	4.175112
C	0.243598	-6.428512	3.844359
C	2.239635	-5.674878	4.996929
C	1.221214	-6.617663	4.826126
H	-0.548724	-7.152110	3.703281
H	3.001166	-5.811315	5.753672
H	1.189638	-7.498229	5.456724
C	4.307682	-2.705621	-2.972236
C	3.752169	-3.390365	-4.067071
C	5.709028	-2.761202	-2.875577
C	4.514257	-4.082454	-5.003909
C	6.511771	-3.439943	-3.788345
C	5.904894	-4.104159	-4.858746
H	4.033957	-4.593458	-5.828169
H	7.587119	-3.450098	-3.666954
H	6.514402	-4.637559	-5.578515
C	2.024917	3.910319	-2.342150
C	1.238312	4.313044	-3.434864
C	3.063122	4.793446	-1.993027
C	1.450167	5.496442	-4.137308
C	3.312572	5.986311	-2.665528
C	2.496723	6.336415	-3.745664
H	0.812142	5.756774	-4.971782
H	4.126529	6.627973	-2.354096
H	2.676354	7.261229	-4.280924
Cl	-3.626246	1.266906	2.077463
Cl	0.947427	2.939126	4.832656
Cl	6.545388	-1.904571	-1.491479
Cl	1.934969	-3.390785	-4.293084
Cl	-0.994358	-5.081855	1.772841
Cl	3.609490	-3.342194	4.433300
Cl	4.161756	4.375751	-0.590277
Cl	-0.143782	3.248796	-3.987746
C	-5.408329	0.948578	-1.785053
C	-5.180462	-0.429170	-1.905111
C	-3.882652	-0.913909	-2.100514
C	-2.829866	0.012103	-2.170036
C	-3.035800	1.395531	-2.053516
C	-4.342793	1.856092	-1.858956
H	-3.702719	-1.977926	-2.194365
H	-2.210744	2.094795	-2.112285
H	-4.523739	2.920867	-1.766797
I	-0.875181	-0.705114	-2.465694
H	-6.417658	1.315540	-1.635841
H	-6.007338	-1.127790	-1.848490
N	3.335580	0.417154	1.428760
C	4.275976	0.724812	2.032809
C	5.458973	1.110497	2.793798
H	5.622964	2.189361	2.721188
H	5.334761	0.846515	3.847898
H	6.343545	0.596297	2.407372

^{2}RC$_{(a)}$

Fe	1.675277	0.197371	-0.266315
N	1.216539	2.159068	-0.040457
C	0.294358	2.698089	0.829532
C	0.189789	4.126091	0.627993
C	1.060853	4.447155	-0.370117
C	1.693967	3.214782	-0.783976
H	-0.457520	4.787592	1.180267
H	1.258916	5.420225	-0.788846
C	2.653242	3.129677	-1.805350
N	3.007199	0.682848	-1.715176
C	3.256851	1.936567	-2.229371
C	4.233235	1.857097	-3.292878
C	4.565097	0.541649	-3.424797
C	3.796644	-0.183503	-2.437752
H	4.608704	2.694849	-3.857384
H	5.264247	0.100734	-4.116436
C	3.870877	-1.572540	-2.251413
N	2.302311	-1.728585	-0.345439
C	3.170207	-2.279050	-1.262347
C	3.288500	-3.704114	-1.047978
C	2.490421	-4.009741	0.014017
C	1.875383	-2.773492	0.443195
H	3.903981	-4.372349	-1.627715
H	2.328847	-4.975302	0.464661
C	0.966179	-2.677103	1.507848
N	0.519203	-0.250356	1.338450
C	0.334121	-1.490596	1.908671
C	-0.628917	-1.409048	2.984207
C	-1.032450	-0.108770	3.053111
C	-0.309461	0.607386	2.025983
H	-0.950715	-2.235390	3.596680
H	-1.744639	0.328487	3.733637
C	-0.435816	1.985581	1.791978
O	0.470170	-0.059908	-1.315274
C	-1.405499	2.751935	2.639637

C	-2.740999	2.943860	2.249755
C	-1.034044	3.322419	3.868013
C	-3.658704	3.652561	3.019013
C	-1.919671	4.038909	4.667235
C	-3.239787	4.201803	4.235070
H	-4.678106	3.773684	2.676621
H	-1.586805	4.461166	5.606379
H	-3.941864	4.756625	4.845842
C	0.644577	-3.929878	2.265634
C	-0.418643	-4.771312	1.899877
C	1.391848	-4.331136	3.385087
C	-0.731383	-5.937364	2.592228
C	1.112876	-5.488845	4.104731
C	0.042587	-6.293629	3.701225
H	-1.561073	-6.554409	2.272884
H	1.717175	-5.756916	4.961497
H	-0.188069	-7.198315	4.250938
C	4.770103	-2.353992	-3.161083
C	4.319154	-2.856936	-4.392870
C	6.107092	-2.630407	-2.832771
C	5.133070	-3.591452	-5.250016
C	6.953576	-3.360104	-3.661858
C	6.457382	-3.842494	-4.877291
H	4.741298	-3.959618	-6.189294
H	7.977605	-3.547429	-3.366252
H	7.103224	-4.412827	-5.534141
C	3.051358	4.399832	-2.494626
C	2.384455	4.861338	-3.641992
C	4.108125	5.198545	-2.029179
C	2.737791	6.040116	-4.292563
C	4.491939	6.382658	-2.651107
C	3.797864	6.801644	-3.790880
H	2.195089	6.357184	-5.173608
H	5.313939	6.964623	-2.255203
H	4.083313	7.721248	-4.287582
Cl	-3.314421	2.240183	0.664383
Cl	0.685056	3.126555	4.456091
Cl	6.782644	-2.008027	-1.252377
Cl	2.597753	-2.535046	-4.903692
Cl	-1.445042	-4.330009	0.455467
Cl	2.794712	-3.297118	3.935128
Cl	5.031289	4.674085	-0.540505
Cl	0.999235	3.886821	-4.316818
C	-5.115451	-2.380332	-0.190260
C	-5.478012	-3.659760	-0.595599
C	-5.075610	-4.098179	-1.863492
C	-4.325921	-3.242990	-2.682709
C	-3.970537	-1.954801	-2.258802
C	-4.373140	-1.518183	-0.989664
H	-5.347843	-5.091903	-2.196571
H	-3.394970	-1.291334	-2.894536
H	-4.114769	-0.528571	-0.632796
I	-3.719336	-3.912729	-4.609495
N	3.260791	0.534235	1.133017
C	4.112389	0.720435	1.892284
C	5.183963	0.954782	2.849660
H	5.664874	1.916524	2.649766
H	4.784802	0.966436	3.867779
H	5.936078	0.164134	2.776088
C	-0.227517	0.015884	-5.650451
S	-1.892056	0.805407	-5.381030
O	-2.706459	0.208206	-6.458148
O	-2.231267	0.367265	-4.008415
O	-1.593113	2.244497	-5.529356
F	0.276414	0.294000	-6.913670
F	0.712543	0.459149	-4.726436
F	-0.291922	-1.371453	-5.530913
F	-5.514715	-1.942621	1.074446
H	-6.057845	-4.298943	0.058428

^{4}RC$_{(a)}$

Fe	1.678646	0.197948	-0.266389
N	1.219460	2.159409	-0.041627
C	0.294184	2.698462	0.825190
C	0.188642	4.126142	0.621961
C	1.062247	4.447287	-0.373840
C	1.697994	3.215329	-0.784908
H	-0.461149	4.787403	1.171601
H	1.260342	5.420193	-0.792942
C	2.659312	3.130215	-1.803990
N	3.011391	0.683011	-1.714425
C	3.262432	1.936785	-2.228009
C	4.238031	1.856751	-3.292211
C	4.567504	0.540932	-3.425898
C	3.798893	-0.184079	-2.438866
H	4.614316	2.694459	-3.856238
H	5.265311	0.099629	-4.118648
C	3.871167	-1.573146	-2.253645
N	2.304505	-1.727753	-0.345852
C	3.170302	-2.279238	-1.264406
C	3.286532	-3.704623	-1.051006
C	2.489852	-4.009622	0.012141
C	1.877237	-2.772784	0.443085
H	3.899878	-4.373516	-1.632244
H	2.327461	-4.975221	0.462418
C	0.969130	-2.675711	1.508275
N	0.520934	-0.249249	1.336372
C	0.336402	-1.489113	1.907925
C	-0.627768	-1.407296	2.982430
C	-1.033049	-0.107522	3.049302
C	-0.309758	0.608534	2.022340
H	-0.949320	-2.233344	3.595425
H	-1.746609	0.329613	3.728474
C	-0.437051	1.986116	1.787049
O	0.475050	-0.058895	-1.317516
C	-1.408997	2.752393	2.632206
C	-2.744781	2.939837	2.241122
C	-1.039615	3.327461	3.859056
C	-3.664655	3.648586	3.007734
C	-1.927422	4.044217	4.655633
C	-3.247711	4.202598	4.222298
H	-4.684179	3.766097	2.664453
H	-1.596095	4.470100	5.593680
H	-3.951457	4.757570	4.831010
C	0.647794	-3.927983	2.267012
C	-0.416225	-4.769162	1.902968
C	1.396157	-4.328964	3.385840
C	-0.728631	-5.934737	2.596274
C	1.117488	-5.486138	4.106471
C	0.046431	-6.290713	3.704600
H	-1.558916	-6.551634	2.278189
H	1.722602	-5.753954	4.962740
H	-0.183980	-7.195009	4.255059
C	4.768329	-2.355315	-3.164748
C	4.315824	-2.855578	-4.397087
C	6.104892	-2.635009	-2.837468
C	5.127843	-3.590487	-5.255686
C	6.949492	-3.365276	-3.667981
C	6.451796	-3.844832	-4.883907
H	4.734898	-3.956484	-6.195323
H	7.973267	-3.555127	-3.373109
H	7.096181	-4.415525	-5.541876
C	3.059182	4.400262	-2.492469
C	2.394501	4.862223	-3.640981
C	4.115694	5.198280	-2.025320
C	2.749649	6.040743	-4.290999
C	4.501345	6.382112	-2.646663
C	3.809444	6.801537	-3.787585
H	2.208577	6.358199	-5.172905
H	5.323072	6.963551	-2.249421
H	4.096346	7.720935	-4.283833
Cl	-3.315558	2.229778	0.657683
Cl	0.679536	3.137304	4.448864
Cl	6.782602	-2.016117	-1.256625
Cl	2.594674	-2.529932	-4.906633
Cl	-1.444163	-4.328264	0.459511
Cl	2.799936	-3.295140	3.933940
Cl	5.036056	4.673147	-0.535169
Cl	1.009255	3.888891	-4.317550
C	-5.118432	-2.397966	-0.185672
C	-5.476790	-3.676800	-0.596762
C	-5.073897	-4.107725	-1.867057
C	-4.327936	-3.246021	-2.682883
C	-3.976813	-1.958631	-2.253170
C	-4.379875	-1.529461	-0.981604
H	-5.342801	-5.100821	-2.204753
H	-3.403781	-1.290041	-2.885860
H	-4.124601	-0.540610	-0.620498
I	-3.720654	-3.904550	-4.613257
N	3.262720	0.534777	1.133544
C	4.113736	0.721317	1.893382
C	5.184507	0.957102	2.851319
H	5.665110	1.918884	2.650864
H	4.784603	0.969550	3.869137
H	5.937057	0.166747	2.779084
C	-0.234895	0.026905	-5.631969
S	-1.899971	0.815222	-5.362251
O	-2.713216	0.220181	-6.441453
O	-2.240252	0.373688	-3.990960
O	-1.601461	2.254774	-5.506904
F	0.269723	0.307211	-6.894438
F	0.704367	0.469148	-4.706695

F	-0.298720	-1.360661	-5.514598
F	-5.518189	-1.967666	1.081338
H	-6.053749	-4.321098	0.054807

$^{6}RC_{(a)}$

Fe	1.622114	0.186549	-0.318885
N	1.196151	2.208391	-0.038368
C	0.290919	2.729069	0.854473
C	0.188498	4.162138	0.653491
C	1.038942	4.484016	-0.365980
C	1.669080	3.250712	-0.798026
H	-0.443708	4.829335	1.216914
H	1.224052	5.460577	-0.783358
C	2.625189	3.144302	-1.833775
N	3.039078	0.702472	-1.760258
C	3.257508	1.958726	-2.272107
C	4.243482	1.880085	-3.333527
C	4.601947	0.567003	-3.448906
C	3.839778	-0.169127	-2.458065
H	4.611849	2.714451	-3.908294
H	5.315118	0.138102	-4.134256
C	3.917355	-1.563592	-2.242708
N	2.315939	-1.778751	-0.364327
C	3.209051	-2.301940	-1.267402
C	3.327322	-3.731715	-1.052240
C	2.500071	-4.048773	-0.012326
C	1.864153	-2.816685	0.414472
H	3.959819	-4.398884	-1.615305
H	2.336642	-5.020969	0.423933
C	0.928845	-2.705364	1.467950
N	0.476555	-0.271963	1.362829
C	0.284756	-1.522861	1.897549
C	-0.682504	-1.440599	2.975745
C	-1.063567	-0.132134	3.071226
C	-0.330228	0.598311	2.054766
H	-1.022507	-2.268832	3.576315
H	-1.768970	0.297720	3.763948
C	-0.423974	1.989481	1.823401
O	0.422819	-0.066909	-1.370235
C	-1.369243	2.758784	2.698471
C	-2.706009	2.984175	2.331800
C	-0.969549	3.297940	3.932140
C	-3.598908	3.694938	3.128082
C	-1.829628	4.015048	4.758224
C	-3.152350	4.211560	4.348608
H	-4.620524	3.842398	2.802990
H	-1.475280	4.412113	5.700520
H	-3.834882	4.767312	4.980329
C	0.592972	-3.966276	2.209069
C	-0.459778	-4.807157	1.813666
C	1.316785	-4.375180	3.341152
C	-0.784676	-5.979687	2.489480
C	1.025143	-5.539308	4.045239
C	-0.034147	-6.343259	3.612127
H	-1.605726	-6.595927	2.147060
H	1.611618	-5.813045	4.912540
H	-0.274372	-7.252933	4.149375
C	4.843138	-2.337859	-3.134444
C	4.418070	-2.858704	-4.368032
C	6.179703	-2.588890	-2.785404
C	5.256378	-3.585520	-5.208078
C	7.050241	-3.310391	-3.596688
C	6.579579	-3.810448	-4.815125
H	4.884168	-3.967949	-6.149602
H	8.072974	-3.478120	-3.285174
H	7.244262	-4.374479	-5.458487
C	3.003683	4.415285	-2.536228
C	2.321712	4.859599	-3.681462
C	4.054636	5.230364	-2.086421
C	2.654916	6.037350	-4.344391
C	4.418686	6.414162	-2.720916
C	3.709733	6.815745	-3.857796
H	2.101178	6.340532	-5.223467
H	5.236927	7.009217	-2.336812
H	3.979694	7.734779	-4.364164
Cl	-3.315893	2.323071	0.741306
Cl	0.754239	3.059127	4.490432
Cl	6.821418	-1.944242	-1.199666
Cl	2.697457	-2.573202	-4.903756
Cl	-1.456095	-4.356106	0.350980
Cl	2.706454	-3.343847	3.928838
Cl	4.997894	4.728523	-0.602304
Cl	0.944759	3.861506	-4.338980
C	-5.146649	-2.254836	-0.166061
C	-5.505376	-3.551874	-0.515695
C	-5.096479	-4.045356	-1.760818
C	-4.344550	-3.225967	-2.614187
C	-3.993240	-1.919585	-2.246569
C	-4.402170	-1.427818	-0.999579
H	-5.365117	-5.053397	-2.050995
H	-3.415617	-1.283957	-2.908491
H	-4.146720	-0.422965	-0.685889
I	-3.729712	-3.981131	-4.506449
N	3.219956	0.522838	1.100681
C	4.070583	0.706126	1.861816
C	5.141497	0.937026	2.820481
H	5.617464	1.902890	2.628743
H	4.742864	0.937469	3.838866
H	5.897199	0.150569	2.739047
C	-0.173722	-0.077184	-5.624953
S	-1.851192	0.709712	-5.440716
O	-2.626349	0.064738	-6.519225
O	-2.232595	0.323333	-4.063640
O	-1.556556	2.144010	-5.636116
F	0.365644	0.148919	-6.883958
F	0.735164	0.414481	-4.694279
F	-0.231288	-1.458381	-5.446036
F	-5.552101	-1.762341	1.076226
H	-6.087029	-4.162096	0.163905

$^{2}TS_{(a)}$

Fe	1.424052	-0.129648	-0.005887
N	0.899556	1.815333	0.199482
C	0.102619	2.361819	1.186291
C	-0.095078	3.773487	0.935530
C	0.583549	4.073070	-0.207391
C	1.202514	2.846607	-0.661945
H	-0.677164	4.438411	1.552955
H	0.660174	5.028383	-0.700929
C	2.008247	2.750282	-1.803710
N	2.472447	0.315420	-1.658213
C	2.603350	1.566222	-2.246362
C	3.509607	1.492274	-3.370105
C	3.961412	0.208736	-3.438143
C	3.333749	-0.520121	-2.359830
H	3.772170	2.319600	-4.009429
H	4.660660	-0.209462	-4.144080
C	3.593801	-1.859873	-2.064793
N	2.118901	-2.022823	-0.086220
C	2.999096	-2.555249	-1.005359
C	3.225383	-3.955397	-0.725470
C	2.471036	-4.267617	0.365868
C	1.788435	-3.057113	0.769064
H	3.870778	-4.606385	-1.292830
H	2.386646	-5.222122	0.859750
C	0.944050	-2.974766	1.882347
N	0.461625	-0.555777	1.743543
C	0.326399	-1.798950	2.321830
C	-0.535691	-1.714418	3.483613
C	-0.916018	-0.412001	3.600013
C	-0.294971	0.307353	2.506250
H	-0.804871	-2.542236	4.119724
H	-1.555955	0.026808	4.348494
C	-0.456940	1.676535	2.270479
O	-0.019085	-0.495655	-0.730188
C	-1.301118	2.456504	3.232782
C	-2.686165	2.615633	3.056023
C	-0.758784	3.074531	4.372118
C	-3.488261	3.333874	3.938224
C	-1.522683	3.802012	5.280183
C	-2.897241	3.929440	5.056935
H	-4.551059	3.426551	3.756472
H	-1.055498	4.259195	6.142681
H	-3.507030	4.492077	5.753769
C	0.700900	-4.227011	2.670291
C	-0.344487	-5.113850	2.362538
C	1.501705	-4.589681	3.766860
C	-0.591097	-6.279813	3.081574
C	1.292101	-5.745519	4.513556
C	0.236246	-6.593294	4.164367
H	-1.411019	-6.928940	2.803162
H	1.938610	-5.979494	5.349313
H	0.058384	-7.496989	4.735063
C	4.589980	-2.589115	-2.915608
C	4.225714	-3.287607	-4.078983
C	5.958645	-2.616768	-2.595402
C	5.140757	-3.968054	-4.877435
C	6.907844	-3.283509	-3.364382
C	6.490632	-3.962769	-4.513283
H	4.806972	-4.491169	-5.764038
H	7.950119	-3.273058	-3.073353
H	7.216205	-4.487130	-5.123637
C	2.298383	4.011984	-2.560840

C	1.540010	4.417831	-3.672112
C	3.350013	4.870487	-2.194958
C	1.794913	5.592615	-4.375281
C	3.639372	6.052314	-2.870268
C	2.851221	6.412500	-3.967876
H	1.180382	5.861192	-5.224743
H	4.461960	6.677371	-2.548062
H	3.061573	7.329500	-4.505396
Cl	-3.494693	1.850052	1.605320
Cl	1.035479	2.929828	4.697180
Cl	6.545358	-1.739326	-1.101456
Cl	2.470272	-3.321941	-4.588225
Cl	-1.450011	-4.738688	0.954826
Cl	2.893899	-3.507716	4.253371
Cl	4.410872	4.431264	-0.769787
Cl	0.160120	3.371668	-4.246666
C	-5.011073	-1.060894	-1.952713
C	-4.149227	-2.017317	-1.422905
C	-2.799850	-1.972360	-1.785858
C	-2.359813	-0.966584	-2.661413
C	-3.242320	-0.010739	-3.189797
C	-4.592533	-0.063313	-2.828376
H	-2.110093	-2.703759	-1.384602
H	-2.895803	0.741068	-3.889189
H	-5.303365	0.653858	-3.219101
I	-0.329453	-0.879575	-3.186089
N	3.123815	0.328176	1.142618
C	4.065014	0.577727	1.765406
C	5.253201	0.891951	2.546091
H	5.511023	1.948667	2.432044
H	5.075875	0.686064	3.605357
H	6.098163	0.285949	2.206987
C	-0.136240	0.699814	-7.426057
S	-1.924867	0.495478	-6.952307
O	-1.952552	-0.881119	-6.412529
O	-2.123844	1.572010	-5.956022
O	-2.620569	0.689599	-8.239672
F	0.239385	-0.218464	-8.399152
F	0.122043	1.967201	-7.931818
F	0.716667	0.511571	-6.341522
F	-6.354928	-1.107900	-1.592538
H	-4.522198	-2.776375	-0.747144

^{4}TS$_{(a)}$

Fe	1.510208	-0.132443	-0.031020
N	0.958813	1.798764	0.182156
C	0.066756	2.306632	1.108100
C	-0.166181	3.711142	0.851139
C	0.583996	4.047422	-0.234727
C	1.283689	2.852241	-0.653830
H	-0.816802	4.347355	1.429550
H	0.662511	5.010819	-0.712457
C	2.157866	2.804567	-1.740627
N	2.724975	0.399227	-1.560053
C	2.819458	1.646465	-2.151448
C	3.719129	1.589046	-3.282243
C	4.158324	0.302574	-3.378332
C	3.536341	-0.439176	-2.303557
H	3.975882	2.424776	-3.913327
H	4.842114	-0.110732	-4.102361
C	3.752065	-1.797921	-2.068454
N	2.303121	-1.992486	-0.067806
C	3.165038	-2.506273	-1.019222
C	3.389599	-3.914383	-0.771752
C	2.655278	-4.248951	0.325485
C	1.972387	-3.049418	0.759376
H	4.026829	-4.553224	-1.362048
H	2.577914	-5.213197	0.801796
C	1.109403	-2.995857	1.854288
N	0.534226	-0.590729	1.664247
C	0.444011	-1.838000	2.258989
C	-0.456185	-1.780501	3.388279
C	-0.913903	-0.499559	3.470559
C	-0.298876	0.241176	2.392563
H	-0.700497	-2.612612	4.028988
H	-1.602568	-0.088071	4.190972
C	-0.528247	1.596185	2.150936
O	0.238127	-0.525378	-1.031440
C	-1.463343	2.329260	3.064064
C	-2.842105	2.428303	2.807915
C	-1.021781	2.965647	4.237298
C	-3.728442	3.102715	3.643267
C	-1.870786	3.650858	5.101965
C	-3.234073	3.716595	4.798187
H	-4.781587	3.147902	3.398137
H	-1.477137	4.123058	5.992653
H	-3.909687	4.245457	5.459960
C	0.875462	-4.254926	2.632398
C	-0.154784	-5.155780	2.310576
C	1.670243	-4.617922	3.733673
C	-0.391681	-6.331187	3.017831
C	1.470807	-5.782374	4.470220
C	0.430281	-6.642251	4.105401
H	-1.199863	-6.989520	2.726847
H	2.112998	-6.013481	5.310134
H	0.260131	-7.552925	4.667425
C	4.664662	-2.538492	-2.998217
C	4.196493	-3.176492	-4.160048
C	6.048122	-2.642598	-2.771065
C	5.024070	-3.867495	-5.040581
C	6.914141	-3.322826	-3.622803
C	6.393164	-3.937985	-4.765291
H	4.609816	-4.340347	-5.921507
H	7.972028	-3.371484	-3.399814
H	7.052590	-4.471351	-5.439625
C	2.404459	4.070444	-2.504619
C	1.650022	4.430311	-3.635391
C	3.408685	4.982233	-2.134555
C	1.863952	5.605198	-4.351820
C	3.657459	6.167444	-2.820805
C	2.875109	6.477235	-3.937541
H	1.253879	5.834397	-5.215923
H	4.444494	6.833587	-2.492056
H	3.054303	7.395486	-4.484249
Cl	-3.531802	1.641381	1.307073
Cl	0.754933	2.906374	4.673223
Cl	6.773247	-1.852687	-1.287946
Cl	2.410883	-3.113725	-4.559600
Cl	-1.254967	-4.788545	0.894849
Cl	3.043027	-3.521464	4.246579
Cl	4.460465	4.615425	-0.681529
Cl	0.323909	3.317659	-4.222140
C	-5.315850	-0.591086	-1.719005
C	-4.643038	-1.795724	-1.526203
C	-3.318657	-1.895586	-1.957121
C	-2.712125	-0.780510	-2.562987
C	-3.406008	0.428227	-2.751102
C	-4.731990	0.520721	-2.322685
H	-2.776075	-2.822403	-1.820179
H	-2.933589	1.269551	-3.240868
H	-5.300587	1.431967	-2.456262
I	-0.734713	-0.917923	-3.202133
N	3.285611	0.407516	1.313967
C	4.181455	0.686461	1.992133
C	5.309393	1.038546	2.845832
H	5.953567	1.764863	2.342243
H	4.953390	1.477165	3.782331
H	5.900997	0.148729	3.078974
C	-0.116035	0.254176	-7.220945
S	-1.876835	0.098130	-6.642845
O	-1.815892	-1.153273	-5.825013
O	-2.087432	1.332974	-5.865884
O	-2.636553	-0.035614	-7.895952
F	0.258838	-0.825310	-8.006111
F	0.074132	1.404899	-7.969061
F	0.765297	0.307157	-6.144613
F	-6.633349	-0.495490	-1.292490
H	-5.142637	-2.631874	-1.054374

^{6}TS$_{(a)}$

Fe	1.327915	-0.084458	-0.130205
N	0.937715	1.950098	0.251066
C	0.121303	2.437928	1.237352
C	-0.035963	3.872064	1.069769
C	0.701347	4.227892	-0.024867
C	1.315302	3.014452	-0.534963
H	-0.622924	4.517757	1.703263
H	0.820856	5.215093	-0.441930
C	2.179984	2.943091	-1.650063
N	2.675438	0.513919	-1.650532
C	2.820627	1.783014	-2.153159
C	3.765528	1.761126	-3.254995
C	4.190889	0.467628	-3.387972
C	3.505645	-0.308276	-2.370400
H	4.070600	2.614648	-3.839126
H	4.903663	0.081753	-4.099191
C	3.693798	-1.693658	-2.135507
N	2.212999	-1.993920	-0.170387
C	3.091137	-2.467113	-1.118430
C	3.315554	-3.885186	-0.897613
C	2.567834	-4.243180	0.188894
C	1.881309	-3.046281	0.642798
H	3.957190	-4.518522	-1.489157

H	2.493448	-5.219339	0.640964
C	1.016745	-2.974452	1.763668
N	0.440249	-0.566661	1.694900
C	0.365386	-1.822176	2.253484
C	-0.476037	-1.770164	3.438011
C	-0.888267	-0.476760	3.580109
C	-0.305638	0.279961	2.483901
H	-0.710961	-2.607112	4.076102
H	-1.519341	-0.071102	4.354667
C	-0.465369	1.665760	2.272048
O	-0.140236	-0.470188	-1.044911
C	-1.332624	2.402195	3.250995
C	-2.714088	2.557985	3.049837
C	-0.815838	2.978589	4.422924
C	-3.538673	3.236234	3.942596
C	-1.603831	3.664880	5.342225
C	-2.974564	3.791519	5.095514
H	-4.598144	3.329348	3.742581
H	-1.157758	4.091314	6.231243
H	-3.602462	4.322602	5.800915
C	0.780861	-4.252617	2.513945
C	-0.275662	-5.119321	2.188911
C	1.598496	-4.657846	3.581616
C	-0.516935	-6.309695	2.868289
C	1.393464	-5.839333	4.288198
C	0.326618	-6.667385	3.924845
H	-1.344941	-6.943908	2.579601
H	2.051528	-6.107679	5.104362
H	0.152649	-7.590615	4.464573
C	4.659992	-2.405147	-3.038038
C	4.265169	-2.964238	-4.264558
C	6.016737	-2.554417	-2.704992
C	5.146341	-3.632573	-5.110064
C	6.930673	-3.213898	-3.521288
C	6.486481	-3.756564	-4.731245
H	4.793435	-4.047295	-6.045340
H	7.966484	-3.301178	-3.220209
H	7.184471	-4.273655	-5.378795
C	2.473666	4.233956	-2.358554
C	1.699061	4.682078	-3.441164
C	3.539287	5.068012	-1.981809
C	1.953072	5.873628	-4.113893
C	3.828952	6.266945	-2.626584
C	3.026939	6.667945	-3.699819
H	1.326389	6.175246	-4.943031
H	4.662392	6.874502	-2.298878
H	3.238651	7.598365	-4.213038
Cl	-3.480597	1.844975	1.551548
Cl	0.972444	2.831154	4.774923
Cl	6.633575	-1.849342	-1.134281
Cl	2.526322	-2.810695	-4.798000
Cl	-1.395660	-4.679651	0.812372
Cl	3.001272	-3.597133	4.081967
Cl	4.608560	4.572505	-0.583566
Cl	0.288314	3.666760	-4.004939
C	-5.509192	-0.660957	-1.714760
C	-4.812687	-1.841121	-1.956354
C	-3.483471	-1.757014	-2.382740
C	-2.895254	-0.493331	-2.551129
C	-3.614967	0.686761	-2.304793
C	-4.944633	0.600517	-1.879107
I	-0.898440	-0.365584	-3.181701
N	3.292380	0.398356	1.315563
C	4.227499	0.629943	1.960296
C	5.405640	0.921405	2.769637
H	5.845107	1.877255	2.470602
H	5.136061	0.977517	3.828094
H	6.157305	0.137135	2.642371
C	-0.081554	-1.111894	-7.125607
S	-1.767523	-0.432602	-7.533316
O	-2.447618	-0.471676	-6.218843
O	-1.449732	0.916477	-8.041576
O	-2.266127	-1.397309	-8.532890
F	-0.155628	-2.385784	-6.566873
F	0.728879	-1.201070	-8.247322
F	0.587729	-0.307632	-6.201400
F	-6.832229	-0.745925	-1.291368
H	-5.527733	1.491193	-1.682499
H	-3.156793	1.658479	-2.440250
H	-2.924108	-2.663407	-2.578414
H	-5.295410	-2.799959	-1.816645

$^{2}PC_{(a)}$

Fe	1.361615	0.074485	-0.009608
N	0.932140	2.025641	0.269052
C	0.223728	2.586995	1.313935
C	0.048050	4.005670	1.083650
C	0.637774	4.290972	-0.110946
C	1.197563	3.052712	-0.614819
H	-0.466552	4.683363	1.746131
H	0.697643	5.246534	-0.607084
C	1.944172	2.958083	-1.794458
N	2.407702	0.521073	-1.685595
C	2.545585	1.781275	-2.250717
C	3.484550	1.725386	-3.348330
C	3.951685	0.444815	-3.415781
C	3.283710	-0.306507	-2.380105
H	3.762859	2.561695	-3.969598
H	4.676417	0.041620	-4.105115
C	3.469745	-1.670481	-2.144592
N	1.901913	-1.847454	-0.232303
C	2.770408	-2.385500	-1.166670
C	2.853756	-3.818011	-0.992786
C	2.032575	-4.142492	0.046508
C	1.457179	-2.908292	0.537034
H	3.455029	-4.482117	-1.593131
H	1.842457	-5.121722	0.456170
C	0.642788	-2.825020	1.670974
N	0.388865	-0.363334	1.703596
C	0.174852	-1.625506	2.216082
C	-0.586402	-1.534888	3.447540
C	-0.817332	-0.212246	3.675878
C	-0.215711	0.516937	2.577242
H	-0.890274	-2.373825	4.053207
H	-1.349092	0.234333	4.500948
C	-0.289642	1.903476	2.419503
O	-0.225846	-0.128381	-0.861178
C	-0.996266	2.697989	3.475419
C	-2.379708	2.945905	3.436057
C	-0.319031	3.247449	4.577861
C	-3.053671	3.680416	4.408011
C	-0.950091	3.988148	5.573425
C	-2.328683	4.203408	5.483197
H	-4.120951	3.840937	4.327834
H	-0.378763	4.388091	6.400984
H	-2.836871	4.777390	6.248986
C	0.299775	-4.098780	2.384186
C	-0.855256	-4.841116	2.083429
C	1.108160	-4.632803	3.403358
C	-1.195921	-6.024725	2.732677
C	0.808263	-5.811815	4.079955
C	-0.354085	-6.509910	3.738037
H	-2.098568	-6.555922	2.459948
H	1.466886	-6.177528	4.856961
H	-0.603126	-7.429394	4.254453
C	4.471002	-2.409426	-2.979953
C	4.155720	-2.976421	-4.227322
C	5.801112	-2.586465	-2.558682
C	5.077890	-3.671160	-5.005928
C	6.756286	-3.272198	-3.303484
C	6.386391	-3.818284	-4.536388
H	4.780290	-4.088612	-5.959090
H	7.766691	-3.377238	-2.930262
H	7.116360	-4.355927	-5.129897
C	2.177295	4.214973	-2.578545
C	1.348861	4.599401	-3.647403
C	3.238768	5.093036	-2.295106
C	1.545413	5.762689	-4.387234
C	3.474038	6.265588	-3.007525
C	2.617294	6.598879	-4.061092
H	0.875907	6.010589	-5.200676
H	4.307823	6.904484	-2.746987
H	2.785111	7.507840	-4.626631
Cl	-3.369120	2.282407	2.046486
Cl	1.486264	2.989108	4.738070
Cl	6.334892	-1.885029	-0.953898
Cl	2.460219	-2.801854	-4.884377
Cl	-1.984959	-4.241979	0.775114
Cl	2.638616	-3.752556	3.887776
Cl	4.391084	4.697130	-0.928459
Cl	-0.064216	3.535897	-4.112011
C	-4.872924	-2.088761	-2.279636
C	-3.883244	-3.060723	-2.394392
C	-2.554974	-2.646511	-2.539148
C	-2.272926	-1.274120	-2.569790
C	-3.280356	-0.305627	-2.460267
C	-4.606271	-0.723159	-2.306534
H	-1.767853	-3.384822	-2.625159
H	-3.051470	0.751965	-2.496228
H	-5.411921	-0.005811	-2.217253
I	-0.277182	-0.636198	-2.766212
N	3.081867	0.361705	1.090708

C	4.051993	0.533534	1.695224
C	5.275109	0.752396	2.454593
H	5.536309	1.814481	2.450093
H	5.140761	0.428727	3.490552
H	6.100353	0.186332	2.013551
C	0.421134	0.136137	-6.999681
S	-1.172664	-0.531512	-6.314706
O	-0.667718	-1.429676	-5.218455
O	-1.873143	0.670633	-5.836540
O	-1.765044	-1.255527	-7.447109
F	1.195627	-0.869858	-7.554686
F	0.188728	1.081653	-7.985331
F	1.175079	0.744389	-6.003611
F	-6.191912	-2.502432	-2.132794
H	-4.141967	-4.111447	-2.368712

^{4}PC$_{(a)}$

Fe	1.381751	-0.204359	-0.074449
N	0.830980	1.723390	0.145116
C	-0.065424	2.223948	1.075775
C	-0.304107	3.626676	0.824451
C	0.465688	3.978766	-0.244258
C	1.170144	2.791088	-0.669771
H	-0.964867	4.255795	1.399018
H	0.548998	4.948566	-0.707988
C	2.056950	2.755075	-1.747497
N	2.516441	0.316788	-1.658499
C	2.674140	1.587043	-2.198292
C	3.573011	1.533353	-3.324992
C	3.958295	0.232541	-3.472313
C	3.317889	-0.522397	-2.423056
H	3.866374	2.380198	-3.924449
H	4.627113	-0.177703	-4.211790
C	3.529336	-1.884874	-2.201554
N	2.212447	-2.046663	-0.107697
C	3.012286	-2.578182	-1.105702
C	3.278257	-3.972633	-0.834704
C	2.645079	-4.280868	0.332427
C	1.974279	-3.081790	0.780953
H	3.876051	-4.621607	-1.454320
H	2.627169	-5.229741	0.844175
C	1.195662	-3.011598	1.936988
N	0.493457	-0.647067	1.676487
C	0.508774	-1.864313	2.337962
C	-0.319831	-1.792768	3.518457
C	-0.845289	-0.534879	3.563864
C	-0.333836	0.180372	2.418461
H	-0.476876	-2.600239	4.215518
H	-1.510328	-0.122991	4.305899
C	-0.627543	1.516388	2.139336
O	-0.247030	-0.770003	-1.031589
C	-1.569159	2.240092	3.053720
C	-2.958818	2.249594	2.841276
C	-1.126652	2.955013	4.180450
C	-3.854563	2.915824	3.673024
C	-1.985370	3.634776	5.039900
C	-3.358927	3.612556	4.779300
H	-4.915776	2.891564	3.462103
H	-1.591258	4.169692	5.894188
H	-4.041691	4.136649	5.437522
C	1.080358	-4.239326	2.788246
C	0.060763	-5.189946	2.606570
C	1.987134	-4.519220	3.825566
C	-0.063358	-6.336524	3.386486
C	1.902339	-5.651858	4.630290
C	0.867213	-6.564494	4.404992
H	-0.868380	-7.036178	3.203065
H	2.627827	-5.818170	5.415903
H	0.786009	-7.451557	5.021914
C	4.390410	-2.635527	-3.171570
C	3.855550	-3.288241	-4.295972
C	5.784390	-2.739801	-3.020999
C	4.631364	-3.991870	-5.212832
C	6.599628	-3.432300	-3.911989
C	6.013796	-4.061005	-5.015016
H	4.167055	-4.475825	-6.062196
H	7.668353	-3.480670	-3.748634
H	6.633266	-4.604333	-5.718672
C	2.373374	4.044043	-2.445113
C	1.666605	4.488742	-3.576284
C	3.400888	4.895822	-2.002069
C	1.946861	5.688294	-4.226028
C	3.715396	6.102201	-2.621095
C	2.978249	6.497757	-3.741529
H	1.370971	5.983816	-5.093449
H	4.517846	6.719074	-2.237956
H	3.208270	7.433979	-4.236259
Cl	-3.648669	1.347874	1.407528
Cl	0.662480	3.009729	4.561328
Cl	6.593586	-1.935561	-1.590203
Cl	2.050684	-3.229386	-4.589404
Cl	-1.178234	-4.932328	1.284239
Cl	3.355703	-3.350730	4.156205
Cl	4.396019	4.417178	-0.541757
Cl	0.320264	3.459403	-4.253607
C	-5.401108	-0.108800	-2.082974
C	-4.712971	-1.086440	-1.370218
C	-3.349967	-1.267211	-1.631050
C	-2.735083	-0.455046	-2.590788
C	-3.431892	0.530621	-3.298060
C	-4.796896	0.701525	-3.039129
H	-2.790806	-2.018342	-1.087274
H	-2.940712	1.144607	-4.042850
H	-5.374764	1.451272	-3.564484
I	-0.654970	-0.733554	-2.910262
N	3.466924	0.454622	1.368373
C	4.398669	0.712818	2.009732
C	5.572178	1.036927	2.814350
H	5.846681	2.087231	2.680999
H	5.367168	0.862449	3.874422
H	6.421033	0.414587	2.516925
C	0.430072	0.106681	-6.929878
S	-1.378101	0.092223	-6.494454
O	-1.413815	-0.947927	-5.412201
O	-1.631285	1.465937	-6.024982
O	-2.036948	-0.322153	-7.740178
F	0.829222	-1.105792	-7.468633
F	0.720233	1.096152	-7.853904
F	1.210813	0.339489	-5.803160
F	-6.757885	0.065418	-1.826628
H	-5.227134	-1.694798	-0.637237

^{6}PC$_{(a)}$

Fe	1.125515	-0.291268	-0.269483
N	0.787810	1.737814	0.115310
C	-0.085981	2.242290	1.063522
C	-0.286064	3.657957	0.832562
C	0.479096	4.002429	-0.244147
C	1.150089	2.800281	-0.694135
H	-0.917678	4.302369	1.423257
H	0.582145	4.978067	-0.691929
C	2.038858	2.739830	-1.777817
N	2.537909	0.307698	-1.685027
C	2.680908	1.576639	-2.227203
C	3.611214	1.526171	-3.333599
C	4.024565	0.229976	-3.457179
C	3.365436	-0.530588	-2.418436
H	3.911814	2.370598	-3.933294
H	4.723502	-0.170408	-4.174247
C	3.576023	-1.895482	-2.172909
N	2.182315	-2.098663	-0.132922
C	3.034467	-2.611176	-1.094728
C	3.317447	-4.001163	-0.801579
C	2.640292	-4.316914	0.340774
C	1.925678	-3.127319	0.756767
H	3.956580	-4.643607	-1.386241
H	2.626821	-5.264108	0.856300
C	1.102964	-3.046019	1.889610
N	0.409576	-0.674191	1.656101
C	0.402651	-1.900697	2.297898
C	-0.443281	-1.827831	3.470248
C	-0.947272	-0.559719	3.525789
C	-0.409257	0.163594	2.393266
H	-0.624027	-2.637617	4.159215
H	-1.612621	-0.149199	4.268688
C	-0.662618	1.515609	2.115261
O	-0.397730	-0.801395	-1.227733
C	-1.596851	2.247210	3.032803
C	-2.980627	2.312430	2.794237
C	-1.151996	2.913231	4.187991
C	-3.869348	2.983925	3.629291
C	-2.003525	3.596734	5.051638
C	-3.371823	3.629322	4.765535
H	-4.926472	3.002837	3.398211
H	-1.607882	4.093071	5.928229
H	-4.049064	4.156674	5.426848
C	0.969592	-4.276621	2.736582
C	-0.037426	-5.233631	2.523401
C	1.847184	-4.551789	3.799884
C	-0.176819	-6.382359	3.297608
C	1.746504	-5.686398	4.600041
C	0.724815	-6.605781	4.342787
H	-0.971316	-7.087129	3.089527

H	2.449635	-5.849073	5.406493
H	0.631562	-7.494523	4.955601
C	4.471803	-2.638896	-3.118556
C	3.974983	-3.279221	-4.267146
C	5.859445	-2.746117	-2.921450
C	4.780441	-3.976140	-5.163214
C	6.703732	-3.432437	-3.790073
C	6.155114	-4.050317	-4.918034
H	4.345124	-4.451063	-6.032812
H	7.766229	-3.483713	-3.590829
H	6.797513	-4.588692	-5.604725
C	2.345719	4.023446	-2.491976
C	1.634573	4.443859	-3.629396
C	3.365641	4.890681	-2.062338
C	1.902715	5.635911	-4.297566
C	3.667851	6.090867	-2.699473
C	2.926312	6.462527	-3.825238
H	1.324115	5.912718	-5.169364
H	4.464508	6.721181	-2.326217
H	3.147046	7.393502	-4.333919
Cl	-3.673595	1.482386	1.318049
Cl	0.630996	2.897155	4.599648
Cl	6.619460	-1.952541	-1.458281
Cl	2.180942	-3.210897	-4.624596
Cl	-1.238840	-4.981276	1.165786
Cl	3.197989	-3.374546	4.171783
Cl	4.366190	4.440616	-0.596782
Cl	0.297955	3.389418	-4.290073
C	-5.545531	-0.168280	-2.133795
C	-4.953286	-1.375861	-1.774489
C	-3.604381	-1.575332	-2.084699
C	-2.904634	-0.549636	-2.734260
C	-3.508454	0.662770	-3.090964
C	-4.860219	0.852788	-2.786010
H	-3.123770	-2.509044	-1.820711
H	-2.955646	1.435747	-3.608733
H	-5.367240	1.773027	-3.046103
I	-0.851501	-0.837104	-3.122403
N	4.366663	0.874714	1.912578
C	5.314759	1.112672	2.540229
C	6.507174	1.412071	3.328307
H	6.776838	2.467444	3.228068
H	6.330085	1.198881	4.386498
H	7.351829	0.805088	2.989542
C	0.167821	0.060202	-7.037878
S	-1.615080	0.073898	-6.509260
O	-1.619760	-1.042238	-5.488139
O	-1.802905	1.412439	-5.931365
O	-2.356823	-0.259701	-7.728760
F	0.507401	-1.141660	-7.633677
F	0.431184	1.074435	-7.940134
F	1.005070	0.237452	-5.942206
F	-6.887493	0.025192	-1.829706
H	-5.530590	-2.141479	-1.272495

^{2}RC$_{(b)}$

Fe	1.658293	0.192795	-0.268450
N	1.201077	2.154381	-0.038215
C	0.285375	2.693335	0.838441
C	0.183304	4.122163	0.641444
C	1.047862	4.443491	-0.362205
C	1.675966	3.210755	-0.782626
H	-0.458601	4.783819	1.199791
H	1.245009	5.417036	-0.780237
C	2.630062	3.126306	-1.808671
N	2.989396	0.680257	-1.717697
C	3.234784	1.933947	-2.233687
C	4.211017	1.856262	-3.297499
C	4.548471	0.541944	-3.426597
C	3.782738	-0.184439	-2.438352
H	4.583274	2.694419	-3.863524
H	5.249502	0.102501	-4.117264
C	3.862407	-1.572679	-2.249525
N	2.285877	-1.733133	-0.350307
C	3.159768	-2.280924	-1.262942
C	3.280795	-3.705785	-1.048669
C	2.477321	-4.014237	0.008414
C	1.857227	-2.779743	0.435378
H	3.901235	-4.372034	-1.625395
H	2.315731	-4.980505	0.457514
C	0.943602	-2.686157	1.496258
N	0.502091	-0.257778	1.335619
C	0.312002	-1.500063	1.899403
C	-0.652491	-1.420725	2.973822
C	-1.050429	-0.119133	3.049812
C	-0.323413	0.599788	2.027411
H	-0.978637	-2.249158	3.581137
H	-1.761679	0.317183	3.731904
C	-0.443539	1.979712	1.801170
O	0.452306	-0.061669	-1.317106
C	-1.404818	2.746631	2.657795
C	-2.737478	2.960706	2.269945
C	-1.027218	3.295130	3.894397
C	-3.647172	3.669061	3.049011
C	-1.904681	4.010493	4.703514
C	-3.222536	4.195238	4.273265
H	-4.664829	3.807460	2.707963
H	-1.567257	4.415330	5.648692
H	-3.918354	4.749338	4.891796
C	0.619002	-3.940804	2.249649
C	-0.438969	-4.784466	1.874085
C	1.358200	-4.341726	3.374602
C	-0.754489	-5.952214	2.562292
C	1.076242	-5.501087	4.090400
C	0.011267	-6.307966	3.677147
H	-1.579996	-6.570894	2.235365
H	1.674316	-5.768901	4.951601
H	-0.221605	-7.213938	4.223794
C	4.769750	-2.351694	-3.153290
C	4.326165	-2.863808	-4.383950
C	6.107741	-2.616780	-2.819748
C	5.148072	-3.596129	-5.235337
C	6.962061	-3.344042	-3.642921
C	6.473093	-3.835604	-4.857605
H	4.761858	-3.971450	-6.174084
H	7.986514	-3.522582	-3.343364
H	7.125084	-4.404098	-5.509957
C	3.023216	4.396757	-2.500273
C	2.350507	4.856314	-3.645023
C	4.080325	5.197917	-2.039750
C	2.698529	6.035497	-4.297683
C	4.458918	6.382557	-2.663887
C	3.759036	6.799557	-3.800830
H	2.151538	6.350884	-5.176675
H	5.281352	6.966501	-2.271809
H	4.040400	7.719527	-4.299186
Cl	-3.318395	2.287850	0.673769
Cl	0.689589	3.072086	4.479433
Cl	6.773665	-1.982864	-1.239867
Cl	2.604160	-2.556984	-4.901274
Cl	-1.454266	-4.343857	0.421547
Cl	2.754621	-3.305556	3.936711
Cl	5.011296	4.675931	-0.555104
Cl	0.965202	3.878201	-4.314607
C	-5.019349	-2.280715	-0.157712
C	-5.363078	-3.569957	-0.554296
C	-4.993709	-4.058657	-1.801185
C	-4.264222	-3.218321	-2.654130
C	-3.912985	-1.917306	-2.268628
C	-4.298134	-1.449970	-1.003962
H	-5.275282	-5.065189	-2.080164
H	-3.352521	-1.266032	-2.929457
H	-4.041003	-0.449517	-0.678060
I	-3.689257	-3.939339	-4.565683
N	3.244645	0.526859	1.130534
C	4.097220	0.711676	1.889042
C	5.170538	0.944999	2.844711
H	5.650186	1.907589	2.645856
H	4.773480	0.954133	3.863676
H	5.923190	0.155167	2.767920
C	-0.211263	-0.024489	-5.699387
S	-1.872218	0.773924	-5.434261
O	-2.693194	0.164379	-6.499262
O	-2.206985	0.355965	-4.054046
O	-1.569405	2.209777	-5.603470
F	0.287539	0.233435	-6.968829
F	0.734356	0.429400	-4.786235
F	-0.279300	-1.409623	-5.559005
F	-5.407500	-1.835779	1.098366
F	-6.085613	-4.375220	0.315052

^{4}RC$_{(b)}$

Fe	1.659587	0.192764	-0.267085
N	1.202087	2.153959	-0.037025
C	0.285580	2.693045	0.839003
C	0.183408	4.121795	0.641771
C	1.048552	4.443246	-0.361246
C	1.677213	3.210707	-0.781371
H	-0.459156	4.783301	1.199543
H	1.245658	5.416796	-0.779293
C	2.631119	3.126336	-1.807381
N	2.990370	0.680220	-1.716552
C	3.235069	1.933961	-2.233280

C	4.209295	1.855971	-3.298879
C	4.546203	0.541635	-3.428647
C	3.782444	-0.184657	-2.438851
H	4.580483	2.694026	-3.865766
H	5.245652	0.102027	-4.120813
C	3.862458	-1.572728	-2.249777
N	2.286426	-1.732826	-0.349912
C	3.159822	-2.280938	-1.263331
C	3.279878	-3.705962	-1.049762
C	2.476699	-4.014481	0.007428
C	1.857414	-2.779950	0.435360
H	3.899555	-4.372316	-1.627194
H	2.314574	-4.980916	0.455982
C	0.943713	-2.686506	1.496024
N	0.502521	-0.257966	1.335357
C	0.311446	-1.500664	1.898560
C	-0.654834	-1.421717	2.971369
C	-1.053155	-0.120314	3.047132
C	-0.324519	0.599313	2.026438
H	-0.981904	-2.250462	3.577762
H	-1.765716	0.315603	3.728116
C	-0.443986	1.979237	1.801044
O	0.454412	-0.060817	-1.317244
C	-1.405559	2.746046	2.657446
C	-2.738136	2.960119	2.269227
C	-1.028361	3.294483	3.894174
C	-3.648074	3.668431	3.048030
C	-1.906071	4.009815	4.703062
C	-3.223790	4.194584	4.272425
H	-4.665633	3.806829	2.706694
H	-1.568936	4.414596	5.648366
H	-3.919793	4.748666	4.890766
C	0.619045	-3.941192	2.249328
C	-0.438483	-4.785261	1.873429
C	1.357837	-4.341712	3.374694
C	-0.753948	-5.953010	2.561669
C	1.075944	-5.501060	4.090535
C	0.011422	-6.308352	3.676919
H	-1.579117	-6.571994	2.234469
H	1.673715	-5.768548	4.952048
H	-0.221404	-7.214318	4.223597
C	4.769786	-2.351721	-3.153598
C	4.326283	-2.864043	-4.384208
C	6.107832	-2.616539	-2.820090
C	5.148276	-3.596343	-5.235533
C	6.962261	-3.343751	-3.643197
C	6.473346	-3.835557	-4.857802
H	4.762110	-3.971815	-6.174238
H	7.986748	-3.522084	-3.343636
H	7.125416	-4.404019	-5.510103
C	3.024020	4.396824	-2.499077
C	2.350453	4.856691	-3.643216
C	4.081648	5.197715	-2.039351
C	2.698085	6.035921	-4.295981
C	4.459885	6.382431	-2.663580
C	3.759102	6.799753	-3.799846
H	2.150467	6.351507	-5.174509
H	5.282726	6.966191	-2.272080
H	4.040185	7.719772	-4.298272
Cl	-3.318532	2.287196	0.672894
Cl	0.688227	3.071269	4.479806
Cl	6.773706	-1.982420	-1.240262
Cl	2.604259	-2.557431	-4.901654
Cl	-1.453379	-4.345203	0.420414
Cl	2.753683	-3.305028	3.937300
Cl	5.013712	4.675361	-0.555520
Cl	0.964773	3.878645	-4.312221
C	-5.018048	-2.276341	-0.156429
C	-5.359560	-3.566868	-0.550364
C	-4.989206	-4.057600	-1.796276
C	-4.261000	-3.217847	-2.650836
C	-3.911897	-1.915420	-2.267896
C	-4.297992	-1.446073	-1.004317
H	-5.269124	-5.065171	-2.073185
H	-3.352291	-1.264718	-2.930043
H	-4.042584	-0.444530	-0.680448
I	-3.684734	-3.941588	-4.560982
N	3.245213	0.526661	1.131433
C	4.097552	0.711572	1.890183
C	5.170761	0.944699	2.846027
H	5.650390	1.907360	2.647467
H	4.773593	0.953572	3.864952
H	5.923461	0.154921	2.769140
C	-0.212058	-0.025336	-5.700449
S	-1.873072	0.773352	-5.436618
O	-2.693975	0.162064	-6.500687
O	-2.207751	0.357394	-4.055776
O	-1.570507	2.208984	-5.608105
F	0.286990	0.230961	-6.970127
F	0.733423	0.429682	-4.787706
F	-0.280255	-1.410271	-5.558323
F	-5.407053	-1.829256	1.09866
F	-6.080893	-4.371725	0.320385

$^{6}RC_{(b)}$

Fe	1.610935	0.182375	-0.326637
N	1.185421	2.204042	-0.043749
C	0.280786	2.724281	0.849894
C	0.181763	4.158146	0.652886
C	1.032682	4.480753	-0.365913
C	1.660443	3.247214	-0.800805
H	-0.448814	4.825317	1.218166
H	1.219829	5.457994	-0.780784
C	2.616778	3.141445	-1.836356
N	3.031306	0.699848	-1.763941
C	3.249700	1.956386	-2.274984
C	4.237324	1.878809	-3.334951
C	4.597013	0.566055	-3.450069
C	3.833696	-0.170920	-2.460738
H	4.606049	2.713589	-3.908892
H	5.311626	0.137943	-4.134410
C	3.911809	-1.565382	-2.245729
N	2.304017	-1.783109	-0.373249
C	3.200675	-2.304962	-1.273536
C	3.318998	-3.734877	-1.059277
C	2.488014	-4.053380	-0.022819
C	1.849855	-2.822003	0.402729
H	3.953839	-4.401219	-1.620692
H	2.323425	-5.026113	0.411805
C	0.910625	-2.712115	1.452819
N	0.460552	-0.278256	1.351115
C	0.265269	-1.530232	1.881990
C	-0.706224	-1.449615	2.956512
C	-1.085813	-0.140911	3.054057
C	-0.347361	0.591302	2.042540
H	-1.049839	-2.278975	3.553461
H	-1.793517	0.287946	3.745039
C	-0.437215	1.983437	1.815463
O	0.414400	-0.068894	-1.381505
C	-1.381435	2.752177	2.692201
C	-2.713540	2.994299	2.319219
C	-0.985328	3.273477	3.934741
C	-3.605495	3.703539	3.117872
C	-1.844575	3.988579	4.763426
C	-3.162727	4.201595	4.347477
H	-4.623567	3.863882	2.787796
H	-1.492952	4.371694	5.712496
H	-3.844621	4.755836	4.981204
C	0.572415	-3.974004	2.191258
C	-0.477212	-4.815962	1.790026
C	1.291049	-4.382776	3.326720
C	-0.804143	-5.989307	2.463448
C	0.997265	-5.547696	4.028580
C	-0.058876	-6.352654	3.589656
H	-1.622722	-6.606295	2.116487
H	1.579741	-5.821303	4.898614
H	-0.300715	-7.262940	4.125136
C	4.841703	-2.338282	-3.134436
C	4.421674	-2.860334	-4.369215
C	6.177655	-2.586598	-2.781015
C	5.264142	-3.585569	-5.206460
C	7.052212	-3.306575	-3.589317
C	6.586514	-3.807755	-4.809205
H	4.895726	-3.968906	-6.149105
H	8.074256	-3.472263	-3.274453
H	7.254415	-4.370519	-5.450337
C	2.995148	4.412928	-2.538018
C	2.313949	4.857056	-3.683803
C	4.044988	5.228755	-2.086952
C	2.646739	6.035315	-4.346009
C	4.408582	6.413112	-2.720666
C	3.700364	6.814493	-3.858067
H	2.093627	6.338300	-5.225545
H	5.225948	7.008734	-2.335575
H	3.969985	7.733958	-4.363829
Cl	-3.318835	2.357605	0.716956
Cl	0.733004	3.014780	4.500850
Cl	6.812923	-1.940508	-1.193293
Cl	2.702137	-2.578523	-4.910370
Cl	-1.466348	-4.365402	0.322277
Cl	2.676692	-3.350320	3.921836
Cl	4.987319	4.727113	-0.602196

Cl	0.938730	3.857772	-4.343433
C	-5.047750	-2.182213	-0.108824
C	-5.379378	-3.489656	-0.452422
C	-5.007256	-4.024672	-1.679342
C	-4.287510	-3.212376	-2.566997
C	-3.948467	-1.893422	-2.234974
C	-4.336103	-1.379340	-0.989370
H	-5.279445	-5.044279	-1.917044
H	-3.394563	-1.264005	-2.922090
H	-4.087958	-0.364262	-0.704377
I	-3.709252	-4.004746	-4.449059
N	3.205885	0.515953	1.097793
C	4.054876	0.698074	1.861045
C	5.123664	0.927702	2.822398
H	5.602338	1.892262	2.630818
H	4.722260	0.930250	3.839686
H	5.877808	0.139447	2.743969
C	-0.174933	-0.083031	-5.634193
S	-1.854609	0.699502	-5.452424
O	-2.628527	0.048325	-6.527981
O	-2.234235	0.316720	-4.073644
O	-1.564403	2.133987	-5.652280
F	0.363614	0.140633	-6.893922
F	0.732404	0.414371	-4.705118
F	-0.228519	-1.463735	-5.450778
F	-5.437755	-1.690842	1.129267
F	-6.092555	-4.266430	0.449931

^{2}TS$_{(b)}$

Fe	1.398385	-0.078499	-0.009207
N	0.917959	1.875613	0.204741
C	0.134284	2.434425	1.195678
C	-0.030152	3.851860	0.954676
C	0.656228	4.143324	-0.185812
C	1.245926	2.905777	-0.648498
H	-0.596226	4.526228	1.576691
H	0.756547	5.100214	-0.671941
C	2.052674	2.799692	-1.789453
N	2.454289	0.352671	-1.663362
C	2.623737	1.606854	-2.238843
C	3.541630	1.520629	-3.351693
C	3.967472	0.228027	-3.422514
C	3.309145	-0.495705	-2.359505
H	3.830255	2.346294	-3.981856
H	4.667106	-0.199586	-4.122395
C	3.531866	-1.844450	-2.074063
N	2.044139	-1.989156	-0.102936
C	2.905997	-2.537040	-1.029781
C	3.082847	-3.948742	-0.772351
C	2.318438	-4.251316	0.314762
C	1.681330	-3.023402	0.739245
H	3.703438	-4.613578	-1.351189
H	2.199221	-5.210303	0.792428
C	0.853768	-2.924487	1.864648
N	0.420786	-0.495436	1.733739
C	0.270011	-1.735355	2.315284
C	-0.570206	-1.633059	3.491641
C	-0.924558	-0.323756	3.611749
C	-0.305368	0.382461	2.508322
H	-0.843843	-2.454837	4.133583
H	-1.543951	0.128049	4.369683
C	-0.437007	1.756344	2.278339
O	-0.055979	-0.419794	-0.742766
C	-1.256158	2.551653	3.249858
C	-2.638440	2.742098	3.083777
C	-0.691468	3.153043	4.387207
C	-3.417769	3.474782	3.974407
C	-1.432352	3.893947	5.303428
C	-2.805335	4.052828	5.090785
H	-4.479526	3.591846	3.800843
H	-0.948883	4.337349	6.164141
H	-3.397248	4.626323	5.794135
C	0.603189	-4.170600	2.660831
C	-0.512212	-4.995250	2.436490
C	1.471614	-4.587195	3.684662
C	-0.756421	-6.156834	3.164068
C	1.265614	-5.740452	4.436006
C	0.142067	-6.528803	4.168475
H	-1.630623	-6.758278	2.951295
H	1.965548	-6.016858	5.213757
H	-0.034052	-7.430279	4.743229
C	4.528336	-2.587524	-2.913187
C	4.175210	-3.264968	-4.092357
C	5.888350	-2.649627	-2.561910
C	5.093483	-3.957536	-4.876742
C	6.839966	-3.329221	-3.316372
C	6.434328	-3.986684	-4.481976
H	4.768554	-4.463761	-5.776348
H	7.875199	-3.345232	-3.001460
H	7.161876	-4.520850	-5.081372
C	2.368062	4.059662	-2.539421
C	1.595459	4.502422	-3.626438
C	3.456001	4.878921	-2.191099
C	1.872191	5.674480	-4.325495
C	3.768313	6.056840	-2.863132
C	2.966145	6.453682	-3.937746
H	1.245755	5.972309	-5.156272
H	4.618584	6.651432	-2.555463
H	3.194147	7.368173	-4.472312
Cl	-3.473774	2.000432	1.636013
Cl	1.101255	2.966404	4.698332
Cl	6.460102	-1.801622	-1.045277
Cl	2.432571	-3.254004	-4.641832
Cl	-1.720615	-4.539337	1.144590
Cl	2.947529	-3.577976	4.071681
Cl	4.531719	4.392344	-0.793083
Cl	0.164585	3.509327	-4.169876
C	-4.885740	-1.767133	-2.082026
C	-3.835786	-2.521142	-1.560978
C	-2.517238	-2.223295	-1.871225
C	-2.272229	-1.136172	-2.723164
C	-3.316319	-0.367280	-3.257742
C	-4.637998	-0.695500	-2.930255
H	-1.720283	-2.819562	-1.448624
H	-3.111030	0.453611	-3.934265
H	-5.468890	-0.125895	-3.327059
I	-0.285753	-0.655128	-3.200337
N	3.102063	0.329937	1.138600
C	4.048996	0.555921	1.761624
C	5.244669	0.841550	2.541727
H	5.531403	1.890163	2.421843
H	5.061080	0.646564	3.601971
H	6.072837	0.210671	2.206542
C	-0.231673	0.944968	-7.395644
S	-1.987028	0.598198	-6.880283
O	-1.906717	-0.805080	-6.420439
O	-2.221281	1.600420	-5.816097
O	-2.737294	0.817521	-8.132417
F	0.160335	0.121685	-8.444215
F	-0.066374	2.257857	-7.816390
F	0.670504	0.732021	-6.356096
F	-6.185467	-2.103547	-1.743536
F	-4.120935	-3.584305	-0.714291

^{4}TS$_{(b)}$

Fe	1.537856	-0.066718	-0.119768
N	1.072340	1.887080	0.081411
C	0.099414	2.420101	0.906115
C	-0.040828	3.837398	0.651183
C	0.860917	4.158989	-0.317915
C	1.547728	2.937882	-0.681059
H	-0.730515	4.493466	1.157742
H	1.044611	5.126744	-0.756440
C	2.527417	2.860918	-1.672521
N	2.856775	0.406562	-1.574702
C	3.112018	1.664413	-2.091010
C	4.064885	1.566648	-3.174604
C	4.364120	0.245566	-3.326253
C	3.615449	-0.476716	-2.321543
H	4.443856	2.400455	-3.743604
H	5.036840	-0.202660	-4.039844
C	3.701078	-1.856288	-2.125841
N	2.234096	-1.961248	-0.132180
C	3.054643	-2.530982	-1.089071
C	3.204077	-3.946586	-0.829199
C	2.485257	-4.224513	0.294125
C	1.870939	-2.986119	0.721396
H	3.791916	-4.627082	-1.424230
H	2.370553	-5.175966	0.788372
C	1.025105	-2.874720	1.825956
N	0.462958	-0.477754	1.524679
C	0.359331	-1.697633	2.171525
C	-0.585449	-1.596900	3.260732
C	-1.070361	-0.323080	3.254201
C	-0.410280	0.377049	2.175966
H	-0.845804	-2.400295	3.931084
H	-1.798473	0.110927	3.920621
C	-0.613288	1.726989	1.885242
O	0.296813	-0.376803	-1.187444
C	-1.624300	2.482180	2.693384
C	-2.974968	2.565978	2.312776
C	-1.290715	3.156555	3.881071
C	-3.933729	3.262804	3.042973

C	-2.215027	3.865605	4.643331
C	-3.545618	3.916372	4.216513
H	-4.960802	3.294843	2.703364
H	-1.903714	4.367305	5.550302
H	-4.278369	4.463776	4.797494
C	0.812726	-4.088030	2.680313
C	-0.237845	-4.997459	2.466233
C	1.662677	-4.393341	3.758394
C	-0.439888	-6.128653	3.253046
C	1.498662	-5.511756	4.570582
C	0.437227	-6.384073	4.311099
H	-1.265460	-6.796452	3.043841
H	2.183451	-5.697743	5.387742
H	0.293652	-7.260129	4.932471
C	4.568167	-2.649924	-3.055709
C	4.074976	-3.207831	-4.248066
C	5.929862	-2.887898	-2.798722
C	4.859013	-3.947904	-5.128699
C	6.752119	-3.621354	-3.649665
C	6.207684	-4.153534	-4.822474
H	4.426812	-4.354987	-6.033565
H	7.794761	-3.773821	-3.402933
H	6.833178	-4.726953	-5.496298
C	2.959845	4.133341	-2.336414
C	2.369662	4.611363	-3.519510
C	3.986984	4.935655	-1.808937
C	2.756712	5.795954	-4.140849
C	4.406262	6.126294	-2.395524
C	3.781829	6.556333	-3.570353
H	2.267967	6.117898	-5.051243
H	5.202872	6.704814	-1.946147
H	4.094706	7.480890	-4.040906
Cl	-3.526206	1.723963	0.785036
Cl	0.438555	3.115545	4.479309
Cl	6.686728	-2.209259	-1.276681
Cl	2.315629	-2.963743	-4.687575
Cl	-1.417060	-4.707822	1.100136
Cl	3.063107	-3.277435	4.138739
Cl	4.837029	4.409527	-0.275272
Cl	1.034802	3.644814	-4.309039
C	-4.854736	-2.172063	-1.410653
C	-3.717819	-2.977870	-1.465112
C	-2.536203	-2.512249	-2.020979
C	-2.521839	-1.200474	-2.520067
C	-3.657153	-0.376049	-2.476309
C	-4.837380	-0.878023	-1.917024
H	-1.669837	-3.158921	-2.054533
H	-3.636250	0.623016	-2.891151
H	-5.734298	-0.273890	-1.871452
I	-0.755704	-0.462078	-3.350660
N	3.263708	0.387379	1.310314
C	4.139275	0.650063	2.020546
C	5.242264	0.984143	2.913078
H	5.794229	1.845307	2.525807
H	4.863125	1.230790	3.908833
H	5.929969	0.138230	3.000224
C	-1.321094	1.343962	-7.141237
S	-2.806649	0.599042	-6.306773
O	-2.228233	-0.662741	-5.743509
O	-3.169179	1.610485	-5.298620
O	-3.755046	0.386054	-7.410432
F	-0.861484	0.542752	-8.173799
F	-1.602164	2.593149	-7.667930
F	-0.269785	1.497196	-6.238823
F	-6.007890	-2.682101	-0.847036
F	-3.774864	-4.261511	-0.946272

$^{6}TS_{(b)}$

Fe	1.329316	-0.088414	-0.127427
N	0.932901	1.945384	0.248323
C	0.115707	2.433280	1.233877
C	-0.043530	3.866917	1.064439
C	0.693553	4.222463	-0.030491
C	1.309380	3.009379	-0.539009
H	-0.631640	4.512562	1.696910
H	0.811624	5.209323	-0.448762
C	2.174630	2.937962	-1.653604
N	2.671401	0.508888	-1.652702
C	2.816266	1.777987	-2.155843
C	3.761762	1.755962	-3.256993
C	4.187982	0.462532	-3.389060
C	3.502885	-0.313199	-2.371443
H	4.066718	2.609296	-3.841458
H	4.901412	0.076781	-4.099686
C	3.692269	-1.698260	-2.135074
N	2.213480	-1.997490	-0.168138
C	3.091176	-2.471003	-1.116661
C	3.316452	-3.888722	-0.894697
C	2.569742	-4.246173	0.192705
C	1.882779	-3.049358	0.646040
H	3.957880	-4.522295	-1.486208
H	2.496140	-5.222016	0.645574
C	1.018157	-2.977314	1.766961
N	0.437713	-0.570553	1.694583
C	0.364971	-1.825490	2.255094
C	-0.476274	-1.772904	3.439735
C	-0.890146	-0.479895	3.580275
C	-0.308887	0.276319	2.482977
H	-0.709955	-2.609319	4.078973
H	-1.521564	-0.074114	4.354484
C	-0.469852	1.661617	2.269769
O	-0.141164	-0.478856	-1.045289
C	-1.336639	2.398504	3.248811
C	-2.718530	2.552599	3.049498
C	-0.818788	2.977041	4.419237
C	-3.542611	3.231174	3.942464
C	-1.606208	3.663739	5.338721
C	-2.977427	3.788608	5.093813
H	-4.602463	3.322871	3.743838
H	-1.159326	4.091821	6.226537
H	-3.604880	4.319965	5.799401
C	0.784244	-4.254839	2.518926
C	-0.271237	-5.123352	2.195329
C	1.602819	-4.657602	3.586808
C	-0.510658	-6.313182	2.876311
C	1.399607	-5.838452	4.294972
C	0.333736	-6.668382	3.933035
H	-1.337902	-6.948880	2.588708
H	2.058303	-6.104878	5.111255
H	0.161180	-7.591156	4.473996
C	4.657572	-2.410188	-3.038174
C	4.261041	-2.970733	-4.263493
C	6.014872	-2.558533	-2.707045
C	5.141148	-3.639584	-5.109679
C	6.927804	-3.218465	-3.524104
C	6.481940	-3.762577	-4.732797
H	4.786979	-4.055454	-6.043965
H	7.964125	-3.304999	-3.224569
H	7.179143	-4.280040	-5.380894
C	2.468002	4.228699	-2.362500
C	1.694430	4.675641	-3.446337
C	3.532372	5.063911	-1.984727
C	1.948216	5.867137	-4.119245
C	3.821769	6.262826	-2.629652
C	3.020795	6.662629	-3.704105
H	1.322330	6.167820	-4.949323
H	4.654223	6.871289	-2.301124
H	3.232309	7.593027	-4.217442
Cl	-3.486509	1.836735	1.553320
Cl	0.970098	2.831874	4.768943
Cl	6.633770	-1.851582	-1.138012
Cl	2.521215	-2.818307	-4.794337
Cl	-1.392185	-4.686986	0.818550
Cl	3.004332	-3.594333	4.085291
Cl	4.600334	4.569998	-0.584941
Cl	0.285308	3.658895	-4.011595
C	-5.501134	-0.639146	-1.737995
C	-4.772476	-1.803501	-1.973500
C	-3.449178	-1.747956	-2.388189
C	-2.864154	-0.484029	-2.561871
C	-3.587989	0.695447	-2.330191
C	-4.922056	0.610934	-1.913350
I	-0.864584	-0.364030	-3.178702
N	3.287117	0.398031	1.313408
C	4.220716	0.633143	1.958976
C	5.396879	0.929191	2.769440
H	5.805984	1.907670	2.502182
H	5.134844	0.938975	3.831225
H	6.169654	0.172222	2.607969
C	-0.091844	-1.102675	-7.116686
S	-1.778613	-0.399938	-7.478478
O	-2.430209	-0.451261	-6.149522
O	-1.457665	0.953118	-7.973665
O	-2.310021	-1.344643	-8.479997
F	-0.167616	-2.382262	-6.571876
F	0.693136	-1.186038	-8.256510
F	0.605365	-0.316640	-6.197065
F	-6.818215	-0.745090	-1.326855
H	-5.507102	1.502770	-1.728124
H	-3.131450	1.666624	-2.469973
H	-2.908570	-2.668123	-2.566085
F	-5.386268	-3.031295	-1.789466

^{2}PC$_{(b)}$

Fe	1.331330	0.023241	-0.019328
N	0.893798	1.972532	0.263755
C	0.141783	2.520544	1.285665
C	-0.033467	3.939742	1.061543
C	0.608451	4.241528	-0.101685
C	1.190395	3.010803	-0.597233
H	-0.579103	4.607822	1.708695
H	0.686167	5.203005	-0.583607
C	1.971130	2.930421	-1.755480
N	2.372465	0.479720	-1.700891
C	2.552369	1.751807	-2.230503
C	3.493202	1.698067	-3.325604
C	3.917090	0.405233	-3.431891
C	3.228273	-0.353193	-2.415953
H	3.799310	2.542717	-3.921975
H	4.628854	-0.000991	-4.132791
C	3.391216	-1.723535	-2.204246
N	1.878570	-1.897669	-0.245944
C	2.711067	-2.437407	-1.212342
C	2.807224	-3.868611	-1.035835
C	2.041599	-4.189894	0.045511
C	1.479402	-2.956680	0.552465
H	3.382991	-4.533486	-1.659757
H	1.877296	-5.167106	0.470708
C	0.714326	-2.874871	1.720494
N	0.359779	-0.425460	1.696240
C	0.210573	-1.681458	2.246105
C	-0.541244	-1.593129	3.483358
C	-0.841674	-0.278649	3.672777
C	-0.278095	0.448467	2.552838
H	-0.797353	-2.428462	4.115436
H	-1.390992	0.164378	4.488151
C	-0.391814	1.829619	2.376543
O	-0.257498	-0.182896	-0.872423
C	-1.146821	2.612331	3.407594
C	-2.534453	2.823324	3.326257
C	-0.516698	3.185171	4.525988
C	-3.255714	3.544773	4.273605
C	-1.196148	3.913748	5.498438
C	-2.576680	4.092147	5.366511
H	-4.324008	3.676610	4.161291
H	-0.660133	4.332627	6.340141
H	-3.122108	4.656320	6.113734
C	0.482784	-4.137458	2.497487
C	-0.664034	-4.933732	2.335981
C	1.408280	-4.605964	3.448108
C	-0.886176	-6.109651	3.048257
C	1.228369	-5.774547	4.182740
C	0.070434	-6.530472	3.976245
H	-1.787963	-6.684491	2.881951
H	1.974826	-6.087474	4.901202
H	-0.086664	-7.443327	4.538534
C	4.364986	-2.467354	-3.067661
C	4.012610	-3.023346	-4.309881
C	5.703510	-2.660012	-2.681037
C	4.907630	-3.722005	-5.116103
C	6.632525	-3.350332	-3.454220
C	6.226051	-3.884727	-4.680771
H	4.581930	-4.130311	-6.064033
H	7.650999	-3.467867	-3.107552
H	6.935477	-4.425427	-5.296004
C	2.250784	4.201688	-2.500680
C	1.459374	4.631368	-3.580325
C	3.321940	5.049037	-2.165419
C	1.699492	5.809592	-4.282588
C	3.600300	6.234807	-2.839437
C	2.778976	6.613986	-3.905675
H	1.057310	6.093254	-5.106298
H	4.439689	6.848769	-2.539797
H	2.980236	7.533992	-4.441654
Cl	-3.464358	2.126027	1.912369
Cl	1.289292	2.975159	4.740306
Cl	6.284486	-1.974465	-1.085707
Cl	2.302759	-2.827740	-4.921811
Cl	-1.953691	-4.425399	1.145328
Cl	2.936072	-3.647211	3.763677
Cl	4.428216	4.592013	-0.779970
Cl	0.040185	3.609258	-4.111330
C	-4.974480	-1.812314	-2.282680
C	-3.976739	-2.481171	-1.575893
C	-2.639947	-2.143683	-1.731721
C	-2.332731	-1.104540	-2.618131
C	-3.317679	-0.416735	-3.334857
C	-4.658255	-0.785482	-3.162125
H	-1.884215	-2.675266	-1.169452
H	-3.059643	0.375720	-4.025677
H	-5.449735	-0.278516	-3.699160
I	-0.302451	-0.552582	-2.806579
N	3.044844	0.313368	1.075517
C	4.018484	0.485252	1.674206
C	5.246747	0.704013	2.424934
H	5.513112	1.764733	2.410027
H	5.116711	0.389639	3.464265
H	6.066410	0.130116	1.983495
C	0.539902	0.255437	-7.036498
S	-1.122853	-0.282719	-6.401958
O	-0.734813	-1.214670	-5.286213
O	-1.741374	0.975379	-5.948485
O	-1.735951	-0.959592	-7.551796
F	1.241784	-0.807734	-7.579783
F	0.408437	1.221898	-8.020181
F	1.313669	0.794030	-6.017206
F	-6.292304	-2.187471	-2.094959
F	-4.333305	-3.501528	-0.706565

^{4}PC$_{(b)}$

Fe	1.329057	-0.255569	-0.047584
N	0.712556	1.651126	0.171641
C	-0.136314	2.144374	1.150596
C	-0.434634	3.533178	0.889060
C	0.247785	3.884875	-0.237629
C	0.970474	2.714691	-0.679193
H	-1.077648	4.153248	1.492800
H	0.265963	4.845659	-0.726545
C	1.827241	2.699344	-1.781227
N	2.434203	0.296057	-1.641334
C	2.509803	1.560188	-2.211195
C	3.412589	1.538528	-3.335751
C	3.887271	0.264028	-3.447485
C	3.291139	-0.507124	-2.384334
H	3.649183	2.387355	-3.956980
H	4.583845	-0.118970	-4.175761
C	3.569868	-1.854456	-2.146728
N	2.194935	-2.081756	-0.096195
C	3.045526	-2.574481	-1.072112
C	3.330762	-3.968389	-0.820383
C	2.647334	-4.319402	0.305625
C	1.938789	-3.143359	0.755760
H	3.969583	-4.589943	-1.426989
H	2.623541	-5.281598	0.791547
C	1.133996	-3.108500	1.894999
N	0.446999	-0.732053	1.698063
C	0.459730	-1.966339	2.329311
C	-0.321508	-1.907010	3.541796
C	-0.797892	-0.633713	3.650221
C	-0.321918	0.097380	2.500147
H	-0.475359	-2.730022	4.221111
H	-1.413963	-0.223597	4.434202
C	-0.611833	1.441258	2.258576
O	-0.283821	-0.882994	-1.049523
C	-1.437951	2.181217	3.267322
C	-2.843408	2.181631	3.246742
C	-0.850108	2.925002	4.306670
C	-3.619452	2.869089	4.176518
C	-1.586327	3.626896	5.256634
C	-2.982489	3.596793	5.185777
H	-4.699387	2.836456	4.113583
H	-1.081603	4.183314	6.035648
H	-3.572117	4.137394	5.916666
C	0.999256	-4.361453	2.705590
C	-0.026289	-5.295651	2.478081
C	1.888561	-4.684113	3.745575
C	-0.171868	-6.466315	3.217259
C	1.781742	-5.842082	4.510833
C	0.741815	-6.736900	4.240545
H	-0.980435	-7.151830	2.999401
H	2.494072	-6.041265	5.300847
H	0.643627	-7.643244	4.826233
C	4.490047	-2.565903	-3.091491
C	4.013203	-3.271655	-4.209846
C	5.885218	-2.579112	-2.919743
C	4.845253	-3.941420	-5.102486
C	6.755435	-3.234561	-3.786475
C	6.226287	-3.918890	-4.885025
H	4.425062	-4.469361	-5.948621
H	7.822556	-3.212543	-3.607723
H	6.888896	-4.434525	-5.569950
C	2.064047	3.988447	-2.509421
C	1.321119	4.371952	-3.639366
C	3.051423	4.901983	-2.098138
C	1.528853	5.570752	-4.317198

C	3.293576	6.109998	-2.745499
C	2.521999	6.443219	-3.863026
H	0.927612	5.817199	-5.182730
H	4.067480	6.775876	-2.386442
H	2.696124	7.379768	-4.379462
Cl	-3.722954	1.237596	1.954573
Cl	0.974134	2.983395	4.447740
Cl	6.619777	-1.701886	-1.491768
Cl	2.213192	-3.332730	-4.528756
Cl	-1.243188	-4.982224	1.147746
Cl	3.262861	-3.540464	4.135282
Cl	4.090841	4.505683	-0.644308
Cl	0.024714	3.257536	-4.280820
C	-5.207408	0.693281	-2.277680
C	-4.566960	-0.097194	-1.326126
C	-3.266847	-0.541461	-1.519827
C	-2.629076	-0.167077	-2.706079
C	-3.243329	0.631361	-3.673877
C	-4.559041	1.060329	-3.449118
H	-2.775347	-1.139118	-0.762943
H	-2.730987	0.920554	-4.582326
H	-5.071545	1.682517	-4.171888
I	-0.622868	-0.855517	-2.934829
N	3.353856	0.445536	1.365099
C	4.276463	0.731265	2.007474
C	5.437798	1.089643	2.814739
H	5.684371	2.146465	2.678642
H	5.233464	0.913169	3.874590
H	6.303986	0.489264	2.522269
C	0.643308	-0.343887	-7.040257
S	-1.183435	-0.320590	-6.696051
O	-1.276331	-1.179820	-5.468955
O	-1.468249	1.106515	-6.461032
O	-1.774026	-0.930992	-7.894905
F	1.083005	-1.620105	-7.352160
F	0.963685	0.485366	-8.102631
F	1.364159	0.090286	-5.934778
F	-6.504015	1.114482	-2.036500
F	-5.241831	-0.428662	-0.159458

^{6}PC$_{(b)}$

Fe	1.092496	-0.343098	-0.313254
N	0.717410	1.671825	0.094438
C	-0.107134	2.163728	1.093241
C	-0.377244	3.565342	0.850331
C	0.292813	3.914447	-0.286609
C	0.986362	2.732527	-0.754166
H	-0.992782	4.197453	1.470460
H	0.321896	4.882315	-0.761325
C	1.837825	2.694711	-1.868462
N	2.472926	0.296232	-1.739902
C	2.540314	1.561806	-2.304545
C	3.479075	1.550135	-3.404604
C	3.982150	0.283261	-3.494552
C	3.359854	-0.500452	-2.450704
H	3.726888	2.399784	-4.020748
H	4.713177	-0.084442	-4.196919
C	3.635428	-1.851387	-2.195939
N	2.178882	-2.133424	-0.208760
C	3.075567	-2.603011	-1.152545
C	3.368011	-3.997365	-0.893093
C	2.643602	-4.363020	0.204505
C	1.904353	-3.195083	0.636554
H	4.040458	-4.610779	-1.471488
H	2.619408	-5.328476	0.684512
C	1.072904	-3.149960	1.764553
N	0.414545	-0.761002	1.620731
C	0.407450	-2.005311	2.228435
C	-0.367630	-1.943823	3.448973
C	-0.813942	-0.659825	3.578361
C	-0.329842	0.078729	2.431823
H	-0.536214	-2.769072	4.122469
H	-1.413068	-0.250095	4.375890
C	-0.586607	1.437279	2.192851
O	-0.440736	-0.867126	-1.272221
C	-1.402776	2.177632	3.211129
C	-2.808220	2.187987	3.196190
C	-0.805554	2.909799	4.253108
C	-3.576033	2.874959	4.132983
C	-1.533251	3.611090	5.210187
C	-2.929833	3.591934	5.144191
H	-4.656410	2.850219	4.074264
H	-1.021565	4.158285	5.991193
H	-3.512861	4.132156	5.880629
C	0.905330	-4.415491	2.551833
C	-0.120470	-5.336026	2.275400
C	1.759058	-4.764695	3.612473
C	-0.299314	-6.518322	2.988063
C	1.618159	-5.935292	4.352919
C	0.579470	-6.815524	4.034260
H	-1.106621	-7.192375	2.732919
H	2.303971	-6.155394	5.160677
H	0.455142	-7.731272	4.600033
C	4.625623	-2.538821	-3.088645
C	4.242197	-3.212449	-4.260963
C	6.002716	-2.556652	-2.805716
C	5.145347	-3.859315	-5.100310
C	6.941331	-3.189804	-3.615598
C	6.504030	-3.845099	-4.770854
H	4.795892	-4.363331	-5.992012
H	7.990501	-3.172176	-3.350664
H	7.220600	-4.343361	-5.413010
C	2.056945	3.977856	-2.614606
C	1.317327	4.322274	-3.759124
C	3.018731	4.921206	-2.210913
C	1.501819	5.513744	-4.456065
C	3.236989	6.123702	-2.877003
C	2.468029	6.418736	-4.007016
H	0.903659	5.730010	-5.331759
H	3.991311	6.814302	-2.522997
H	2.623812	7.350533	-4.537722
Cl	-3.700945	1.255345	1.903100
Cl	1.019446	2.950328	4.388312
Cl	6.618610	-1.713045	-1.302981
Cl	2.476490	-3.253798	-4.734047
Cl	-1.293042	-4.986559	0.914362
Cl	3.132284	-3.642241	4.063461
Cl	4.057363	4.571797	-0.744789
Cl	0.055686	3.163055	-4.393996
C	-5.342752	0.809154	-2.138198
C	-4.726870	-0.112505	-1.294044
C	-3.474227	-0.631135	-1.590089
C	-2.857268	-0.186989	-2.763547
C	-3.446501	0.742909	-3.623364
C	-4.716698	1.239206	-3.300254
H	-3.007908	-1.335375	-0.914019
H	-2.948670	1.079972	-4.523133
H	-5.209154	1.962249	-3.937821
I	-0.908468	-0.946300	-3.151515
N	4.142359	0.777662	2.216796
C	5.013080	1.084566	2.921848
C	6.107453	1.470199	3.808529
H	6.361548	2.524637	3.666432
H	5.823447	1.320349	4.854253
H	6.997444	0.868703	3.601796
C	0.209596	-0.743141	-7.091875
S	-1.575389	-0.404085	-6.695391
O	-1.772182	-1.257578	-5.461085
O	-1.607542	1.042192	-6.430453
O	-2.309815	-0.908236	-7.859055
F	0.424328	-2.088079	-7.335562
F	0.616914	-0.033868	-8.206054
F	1.023359	-0.370544	-6.028228
F	-6.591183	1.297427	-1.798063
F	-5.373182	-0.499425	-0.130219

^{2}RC$_{(c)}$

Fe	1.673507	0.195887	-0.266242
N	1.215267	2.157826	-0.039982
C	0.294613	2.697370	0.831327
C	0.191365	4.125595	0.630727
C	1.060553	4.446071	-0.369201
C	1.692024	3.213286	-0.784301
H	-0.454155	4.787548	1.184551
H	1.258654	5.419054	-0.788112
C	2.649494	3.127654	-1.807279
N	3.006848	0.681455	-1.713725
C	3.254722	1.934784	-2.229667
C	4.231191	1.855216	-3.293103
C	4.564981	0.540079	-3.423133
C	3.797387	-0.184797	-2.435218
H	4.605694	2.692725	-3.858604
H	5.265022	0.099242	-4.113922
C	3.872340	-1.573672	-2.248101
N	2.300554	-1.730105	-0.344827
C	3.170921	-2.280200	-1.259586
C	3.289470	-3.705182	-1.044815
C	2.488590	-4.011240	0.014932
C	1.871643	-2.775324	0.442338
H	3.906990	-4.373068	-1.622781
H	2.326446	-4.976847	0.465270
C	0.958448	-2.679620	1.503575
N	0.514932	-0.252055	1.336739

C	0.326274	-1.493052	1.904088
C	-0.639494	-1.412002	2.977218
C	-1.040279	-0.110997	3.048236
C	-0.313458	0.605932	2.024350
H	-0.964602	-2.239040	3.586992
H	-1.753141	0.326219	3.728081
C	-0.436613	1.984852	1.792956
O	0.469763	-0.061200	-1.316807
C	-1.404526	2.751710	2.642175
C	-2.738121	2.952553	2.250382
C	-1.033134	3.313477	3.874615
C	-3.654293	3.661042	3.021641
C	-1.917158	4.029600	4.675930
C	-3.235552	4.201138	4.241854
H	-4.672315	3.789021	2.677646
H	-1.584358	4.444996	5.618152
H	-3.936397	4.755690	4.854277
C	0.632215	-3.933223	2.257948
C	-0.425982	-4.776379	1.881808
C	1.369515	-4.333580	3.384287
C	-0.743575	-5.943095	2.570752
C	1.085444	-5.491882	4.100980
C	0.020297	-6.298232	3.687131
H	-1.569128	-6.561434	2.243301
H	1.682057	-5.759318	4.963310
H	-0.214173	-7.203379	4.234459
C	4.771855	-2.355097	-3.157491
C	4.320888	-2.858148	-4.389264
C	6.108885	-2.631264	-2.829284
C	5.134888	-3.592367	-5.246547
C	6.955414	-3.360887	-3.658407
C	6.459262	-3.843237	-4.873858
H	4.743180	-3.960507	-6.185862
H	7.979471	-3.548120	-3.362841
H	7.105179	-4.413400	-5.530780
C	3.043117	4.396746	-2.501101
C	2.371342	4.853249	-3.647696
C	4.099849	5.199006	-2.041856
C	2.720159	6.030431	-4.303454
C	4.479153	6.381861	-2.668989
C	3.780436	6.795659	-3.807815
H	2.174026	6.343435	-5.183827
H	5.301259	6.966853	-2.277780
H	4.062470	7.714117	-4.308579
Cl	-3.311255	2.261621	0.659150
Cl	0.683871	3.106767	4.465018
Cl	6.784291	-2.008756	-1.248905
Cl	2.599182	-2.536953	-4.899854
Cl	-1.438296	-4.336396	0.426801
Cl	2.766066	-3.297966	3.947011
Cl	5.028963	4.681070	-0.554658
Cl	0.985807	3.873550	-4.314582
C	-5.071173	-2.345676	-0.175626
C	-5.409973	-3.625140	-0.601690
C	-5.007411	-4.052248	-1.863509
C	-4.271394	-3.213614	-2.700427
C	-3.937877	-1.924398	-2.259287
C	-4.340190	-1.490011	-0.989993
H	-3.370361	-1.255837	-2.896979
H	-4.090139	-0.498372	-0.635108
I	-3.682875	-3.898492	-4.603653
N	3.257314	0.532045	1.135078
C	4.107920	0.717874	1.895551
C	5.178249	0.952238	2.854314
H	5.659231	1.914113	2.655206
H	4.777819	0.963614	3.871936
H	5.930594	0.161735	2.781546
C	-0.246376	0.002078	-5.627867
S	-1.913577	0.785429	-5.356705
O	-2.729293	0.180716	-6.428336
O	-2.247323	0.351174	-3.980930
O	-1.621089	2.225081	-5.510000
F	0.250482	0.275673	-6.894801
F	0.695016	0.455460	-4.710356
F	-0.303380	-1.384736	-5.500222
F	-5.479630	-1.940900	1.083925
F	-6.137281	-4.468748	0.214792
F	-5.359833	-5.330362	-2.256719

$^{4}RC_{(c)}$

Fe	1.675355	0.195882	-0.265245
N	1.216521	2.157472	-0.039731
C	0.293600	2.696908	0.829364
C	0.189011	4.124812	0.627254
C	1.059851	4.445540	-0.371085
C	1.693564	3.213233	-0.784205
H	-0.458519	4.786418	1.179143
H	1.257517	5.418415	-0.790458
C	2.652164	3.127785	-1.805766
N	3.008322	0.681296	-1.713015
C	3.256774	1.934710	-2.228693
C	4.231897	1.854834	-3.293352
C	4.564224	0.539508	-3.424739
C	3.797244	-0.185422	-2.436388
H	4.606337	2.692345	-3.858894
H	5.262803	0.098473	-4.116882
C	3.871401	-1.574187	-2.249835
N	2.301593	-1.729759	-0.344683
C	3.169968	-2.280548	-1.261205
C	3.287008	-3.705814	-1.047450
C	2.487533	-4.011602	0.013357
C	1.872591	-2.775331	0.442618
H	3.902670	-4.374101	-1.626936
H	2.324852	-4.977343	0.463220
C	0.960719	-2.679276	1.504625
N	0.516222	-0.251876	1.336374
C	0.328225	-1.492686	1.904692
C	-0.638214	-1.411653	2.977217
C	-1.040564	-0.111128	3.046860
C	-0.313823	0.605999	2.023069
H	-0.962927	-2.238595	3.587329
H	-1.754517	0.325774	3.725765
C	-0.437933	1.984391	1.790857
O	0.472248	-0.060772	-1.316951
C	-1.407331	2.751047	2.638579
C	-2.740701	2.950518	2.245304
C	-1.037674	3.314100	3.870955
C	-3.658268	3.658792	3.015094
C	-1.923137	4.030028	4.670866
C	-3.241239	4.200121	4.235345
H	-4.676042	3.785654	2.669956
H	-1.591637	4.446428	5.613102
H	-3.943178	4.754519	4.846656
C	0.634847	-3.932634	2.259561
C	-0.424461	-4.775179	1.885134
C	1.373573	-4.333332	3.384839
C	-0.741717	-5.941641	2.574665
C	1.089894	-5.491400	4.102073
C	0.023640	-6.297148	3.689908
H	-1.568140	-6.559512	2.248527
H	1.687623	-5.759102	4.963547
H	-0.210550	-7.202105	4.237672
C	4.770166	-2.355896	-3.159752
C	4.318638	-2.858798	-4.391380
C	6.107273	-2.632441	-2.832125
C	5.132114	-3.593154	-5.249049
C	6.953326	-3.362158	-3.661653
C	6.456596	-3.844312	-4.876942
H	4.739934	-3.961140	-6.188227
H	7.977447	-3.549662	-3.366482
H	7.102128	-4.414556	-5.534173
C	3.046654	4.396933	-2.498991
C	2.375184	4.854637	-3.645292
C	4.104053	5.198100	-2.039384
C	2.724873	6.031912	-4.300415
C	4.484330	6.380954	-2.665940
C	3.785873	6.795955	-3.804483
H	2.178849	6.345906	-5.180503
H	5.306937	6.965062	-2.274463
H	4.068617	7.714461	-4.304759
Cl	-3.311585	2.258160	0.653885
Cl	0.678891	3.109357	4.463334
Cl	6.783526	-2.010340	-1.251936
Cl	2.596755	-2.537396	-4.901291
Cl	-1.438803	-4.334759	0.431644
Cl	2.771461	-3.298406	3.945527
Cl	5.032867	4.678640	-0.552530
Cl	0.988343	3.876744	-4.312177
C	-5.070259	-2.348207	-0.172896
C	-5.408425	-3.627701	-0.599368
C	-5.006720	-4.053717	-1.861822
C	-4.272200	-3.214028	-2.698979
C	-3.939252	-1.924809	-2.257405
C	-4.340737	-1.491512	-0.987478
H	-3.372906	-1.255352	-2.895202
H	-4.091182	-0.499879	-0.632232
I	-3.685038	-3.897330	-4.603181
N	3.258625	0.532277	1.135556
C	4.109185	0.718406	1.896008
C	5.179934	0.953137	2.854228
H	5.660725	1.915014	2.654672
H	4.779962	0.964739	3.872028

H	5.932344	0.162707	2.781342
C	-0.248696	0.005230	-5.622340
S	-1.915579	0.789446	-5.351764
O	-2.731194	0.185183	-6.423732
O	-2.250023	0.355203	-3.976137
O	-1.622328	2.228965	-5.504869
F	0.248329	0.277543	-6.889475
F	0.692907	0.458938	-4.705203
F	-0.306355	-1.381441	-5.493488
F	-5.477850	-1.944412	1.087258
F	-6.134314	-4.472331	0.217302
F	-5.358539	-5.331912	-2.255453

^{6}RC$_{(c)}$

Fe	1.621121	0.185441	-0.315385
N	1.195673	2.207650	-0.036191
C	0.290432	2.729128	0.856181
C	0.188597	4.162134	0.654470
C	1.039043	4.483107	-0.365288
C	1.668515	3.249279	-0.796817
H	-0.443193	4.829913	1.217676
H	1.224586	5.459383	-0.783143
C	2.623159	3.141640	-1.833793
N	3.037249	0.699932	-1.757983
C	3.254809	1.955571	-2.271715
C	4.238677	1.875588	-3.334988
C	4.596585	0.562295	-3.449720
C	3.836195	-0.172613	-2.456602
H	4.606100	2.709266	-3.911358
H	5.308300	0.132519	-4.136038
C	3.913469	-1.566957	-2.240300
N	2.314263	-1.780092	-0.359850
C	3.206535	-2.304224	-1.263180
C	3.324828	-3.733820	-1.046771
C	2.498242	-4.049844	-0.006017
C	1.862457	-2.817351	0.419841
H	3.956925	-4.401566	-1.609599
H	2.335074	-5.021616	0.431288
C	0.926451	-2.705220	1.472582
N	0.475427	-0.271622	1.366518
C	0.282599	-1.522278	1.901392
C	-0.686115	-1.439423	2.978238
C	-1.067146	-0.130867	3.072614
C	-0.332204	0.599074	2.056948
H	-1.027184	-2.267341	3.578636
H	-1.773487	0.299335	3.764161
C	-0.425616	1.990114	1.824672
O	0.421440	-0.068583	-1.366130
C	-1.372867	2.759589	2.697407
C	-2.708120	2.986883	2.326414
C	-0.976992	3.296665	3.933209
C	-3.603234	3.697167	3.120577
C	-1.839329	4.013391	4.757293
C	-3.160464	4.211580	4.343435
H	-4.623587	3.845997	2.792164
H	-1.487868	4.408937	5.701306
H	-3.844720	4.766975	4.973600
C	0.587900	-3.965931	2.212762
C	-0.462193	-4.807699	1.812214
C	1.305763	-4.373701	3.348987
C	-0.790486	-5.979808	2.487014
C	1.010691	-5.537434	4.052324
C	-0.045968	-6.342090	3.614115
H	-1.609389	-6.596645	2.140561
H	1.592626	-5.810386	4.922923
H	-0.288799	-7.251406	4.150790
C	4.836484	-2.342505	-3.133772
C	4.407810	-2.863878	-4.365892
C	6.173750	-2.594325	-2.788034
C	5.243341	-3.591933	-5.207615
C	7.041598	-3.317106	-3.601064
C	6.567374	-3.817654	-4.817914
H	4.868392	-3.974704	-6.147914
H	8.064996	-3.485446	-3.292082
H	7.229930	-4.382690	-5.462586
C	2.999411	4.411557	-2.539362
C	2.312188	4.854917	-3.681841
C	4.053054	5.226448	-2.095640
C	2.643000	6.031549	-4.347901
C	4.414887	6.409169	-2.733433
C	3.700751	6.809777	-3.867409
H	2.085289	6.334010	-5.224710
H	5.235360	7.004170	-2.354032
H	3.968936	7.727950	-4.376280
Cl	-3.313096	2.329379	0.732353
Cl	0.744729	3.055950	4.496904
Cl	6.820040	-1.949017	-1.204446
Cl	2.685986	-2.577362	-4.897452
Cl	-1.449705	-4.358104	0.342849
Cl	2.692263	-3.341707	3.942812
Cl	5.002770	4.725970	-0.615204
Cl	0.931477	3.856762	-4.331504
C	-5.087334	-2.251615	-0.148423
C	-5.433519	-3.539525	-0.541797
C	-5.036132	-3.999559	-1.793648
C	-4.297934	-3.185540	-2.652560
C	-3.957126	-1.887205	-2.244520
C	-4.354212	-1.419832	-0.985402
H	-3.388004	-1.238066	-2.900568
H	-4.098861	-0.421009	-0.655099
I	-3.716792	-3.920892	-4.539131
N	3.219426	0.522232	1.103309
C	4.070221	0.705675	1.864222
C	5.141137	0.937141	2.822744
H	5.618865	1.901689	2.628761
H	4.742077	0.940848	3.840957
H	5.895502	0.149166	2.743623
C	-0.194329	-0.082307	-5.609331
S	-1.871991	0.702137	-5.416261
O	-2.653637	0.053940	-6.487853
O	-2.244156	0.317874	-4.035541
O	-1.581123	2.136474	-5.615311
F	0.336406	0.143091	-6.872011
F	0.719115	0.412626	-4.685043
F	-0.248305	-1.463219	-5.428018
F	-5.490248	-1.813559	1.101791
F	-6.162897	-4.358953	0.297027
F	-5.395943	-5.285017	-2.154652

^{2}TS$_{(c)}$

Fe	1.425727	-0.091950	-0.033051
N	0.940615	1.861992	0.157058
C	0.120152	2.421997	1.116971
C	-0.016168	3.843249	0.881949
C	0.728141	4.137184	-0.221065
C	1.318489	2.895941	-0.671674
H	-0.601932	4.519049	1.483868
H	0.864153	5.097547	-0.691405
C	2.153076	2.785286	-1.791196
N	2.497503	0.328872	-1.678504
C	2.700011	1.583059	-2.245329
C	3.614023	1.480385	-3.359493
C	4.004202	0.177043	-3.441386
C	3.333589	-0.536051	-2.378989
H	3.922856	2.302451	-3.984753
H	4.690939	-0.263531	-4.145962
C	3.544431	-1.884604	-2.085840
N	2.082734	-2.001015	-0.093057
C	2.936967	-2.560176	-1.019213
C	3.136017	-3.963138	-0.730556
C	2.394327	-4.248236	0.376714
C	1.741347	-3.020490	0.776306
H	3.756922	-4.633775	-1.302265
H	2.296092	-5.196169	0.880593
C	0.899606	-2.913824	1.889592
N	0.412693	-0.499804	1.692931
C	0.271822	-1.730649	2.294994
C	-0.617244	-1.627248	3.434830
C	-1.011835	-0.326292	3.511800
C	-0.364150	0.374857	2.421534
H	-0.895314	-2.443106	4.082352
H	-1.673338	0.123522	4.234521
C	-0.501503	1.744122	2.172126
O	-0.016993	-0.456475	-0.782801
C	-1.373515	2.538203	3.097451
C	-2.745929	2.720958	2.857581
C	-0.872992	3.145307	4.261492
C	-3.575280	3.451528	3.703653
C	-1.665352	3.884405	5.135132
C	-3.025941	4.035393	4.849466
H	-4.626943	3.562454	3.473759
H	-1.230509	4.332527	6.019043
H	-3.657340	4.607386	5.518883
C	0.662382	-4.145078	2.712699
C	-0.405965	-5.022664	2.460241
C	1.492127	-4.489903	3.793210
C	-0.643531	-6.165745	3.218641
C	1.291225	-5.622830	4.576317
C	0.213454	-6.463978	4.282304
H	-1.480794	-6.809927	2.983471
H	1.960197	-5.843715	5.397851
H	0.041529	-7.350180	4.881616
C	4.515815	-2.646710	-2.937258

C	4.127440	-3.331908	-4.100756
C	5.882475	-2.721952	-2.616182
C	5.018802	-4.044138	-4.898374
C	6.808106	-3.421482	-3.384720
C	6.367859	-4.085987	-4.533669
H	4.667263	-4.555621	-5.784916
H	7.849976	-3.447282	-3.093209
H	7.075014	-4.635473	-5.143539
C	2.511539	4.044823	-2.522008
C	1.752921	4.530759	-3.600444
C	3.627871	4.819891	-2.163258
C	2.070738	5.701867	-4.283358
C	3.981348	5.995343	-2.819118
C	3.192830	6.435447	-3.887003
H	1.453958	6.033918	-5.108361
H	4.852146	6.555237	-2.503852
H	3.452780	7.348524	-4.409251
Cl	-3.499023	1.970560	1.369697
Cl	0.901991	2.970333	4.666979
Cl	6.498938	-1.865215	-1.122216
Cl	2.372589	-3.303304	-4.609343
Cl	-1.545712	-4.665977	1.079963
Cl	2.909753	-3.411604	4.211297
Cl	4.683711	4.277541	-0.770700
Cl	0.284492	3.598800	-4.151228
C	-4.741685	-1.937498	-1.975998
C	-3.654953	-2.772576	-1.731331
C	-2.383609	-2.360972	-2.110970
C	-2.190831	-1.121084	-2.722648
C	-3.294700	-0.291641	-2.973082
C	-4.577521	-0.705076	-2.598295
H	-3.153840	0.653508	-3.482153
H	-5.442098	-0.081397	-2.783888
I	-0.259342	-0.523953	-3.226516
N	3.104382	0.330017	1.139541
C	4.034427	0.563551	1.784768
C	5.208175	0.857953	2.594179
H	5.613982	1.838016	2.327878
H	4.944414	0.863328	3.655468
H	5.980201	0.101350	2.427743
C	-0.566011	1.224243	-7.316455
S	-2.246566	0.862792	-6.601585
O	-2.112730	-0.554559	-6.198458
O	-2.344246	1.830152	-5.485585
O	-3.145004	1.118954	-7.744117
F	-0.312321	0.442713	-8.436849
F	-0.441650	2.552261	-7.701746
F	0.453695	0.965134	-6.403398
F	-5.996908	-2.364737	-1.588531
F	-3.830902	-3.993760	-1.110837
F	-1.321881	-3.211116	-1.868662

^{4}TS$_{(c)}$

Fe	1.491279	-0.059270	-0.057891
N	1.041688	1.898745	0.167720
C	0.150401	2.441027	1.074150
C	-0.001287	3.858845	0.830658
C	0.800605	4.169505	-0.225492
C	1.446680	2.943881	-0.643165
H	-0.635419	4.520895	1.398240
H	0.945312	5.133670	-0.685830
C	2.340731	2.861914	-1.711178
N	2.741665	0.419146	-1.575951
C	2.930056	1.670594	-2.137033
C	3.839783	1.576055	-3.256300
C	4.192003	0.264483	-3.376196
C	3.508387	-0.455751	-2.325915
H	4.162019	2.405787	-3.864760
H	4.857051	-0.178151	-4.100289
C	3.640045	-1.828286	-2.109251
N	2.179103	-1.957970	-0.110784
C	3.010450	-2.511426	-1.068714
C	3.160692	-3.930450	-0.829629
C	2.417955	-4.230972	0.271623
C	1.799558	-3.000304	0.713973
H	3.759515	-4.598991	-1.427117
H	2.293011	-5.191917	0.744412
C	0.943161	-2.908747	1.811274
N	0.471138	-0.480739	1.612896
C	0.324672	-1.723297	2.208980
C	-0.585366	-1.627522	3.326506
C	-0.996315	-0.329915	3.399663
C	-0.338441	0.385458	2.331345
H	-0.870010	-2.448205	3.965215
H	-1.678528	0.108417	4.110238
C	-0.504403	1.749853	2.093778
O	0.194482	-0.363875	-1.073103
C	-1.429359	2.517233	2.988683
C	-2.799066	2.661362	2.707040
C	-0.987380	3.143280	4.167274
C	-3.676799	3.370153	3.522664
C	-1.828115	3.861690	5.012873
C	-3.182462	3.973062	4.683401
H	-4.723201	3.449869	3.258243
H	-1.435033	4.324154	5.908895
H	-3.851326	4.528443	5.330123
C	0.668095	-4.151709	2.602158
C	-0.396560	-5.018768	2.299217
C	1.460052	-4.529598	3.700660
C	-0.666843	-6.176384	3.024266
C	1.227069	-5.677302	4.453140
C	0.153391	-6.503905	4.108029
H	-1.500387	-6.809228	2.748551
H	1.868669	-5.920932	5.289951
H	-0.043615	-7.401307	4.682503
C	4.514649	-2.610154	-3.041938
C	4.019343	-3.197819	-4.219077
C	5.885705	-2.806684	-2.801469
C	4.811244	-3.927400	-5.101383
C	6.715845	-3.528352	-3.654806
C	6.169520	-4.090997	-4.812451
H	4.377721	-4.358675	-5.994320
H	7.765737	-3.648739	-3.421475
H	6.801016	-4.655748	-5.487990
C	2.684505	4.123829	-2.443426
C	1.976078	4.555367	-3.578675
C	3.739815	4.959331	-2.037106
C	2.280210	5.727216	-4.266682
C	4.078787	6.138729	-2.694227
C	3.339131	6.521702	-3.817385
H	1.702036	6.013445	-5.135659
H	4.901752	6.744715	-2.338241
H	3.588167	7.436606	-4.341862
Cl	-3.487769	1.886525	1.199419
Cl	0.777291	3.022439	4.637240
Cl	6.643187	-2.087491	-1.298626
Cl	2.247562	-3.009046	-4.634584
Cl	-1.495130	-4.633398	0.890271
Cl	2.875250	-3.476071	4.188588
Cl	4.737632	4.494863	-0.574167
Cl	0.587813	3.547773	-4.209527
C	-4.937406	-1.844328	-1.385709
C	-3.867574	-2.726981	-1.514944
C	-2.673862	-2.272975	-2.058836
C	-2.541194	-0.942262	-2.467087
C	-3.626296	-0.060887	-2.328675
C	-4.832325	-0.517631	-1.789616
I	-0.739976	-0.302230	-3.268943
N	3.272032	0.374340	1.291043
C	4.179348	0.604220	1.972028
C	5.322190	0.895334	2.828488
H	5.862097	1.769940	2.454798
H	4.988117	1.100265	3.849553
H	6.007625	0.043300	2.848796
C	-0.273079	0.598353	-7.220520
S	-2.037920	0.775144	-6.660176
O	-2.167949	-0.382928	-5.720705
O	-2.051967	2.098545	-6.014946
O	-2.809441	0.629822	-7.904323
F	-0.060866	-0.603972	-7.875477
F	0.098042	1.618998	-8.078496
F	0.601453	0.633053	-6.132022
F	-6.112533	-2.316730	-0.842449
F	-3.981145	-4.035734	-1.097872
F	-1.626846	-3.162719	-2.176568
H	-5.680745	0.144178	-1.678100
H	-3.534699	0.970542	-2.641735

^{6}TS$_{(c)}$

Fe	1.364039	-0.107255	-0.155538
N	1.009303	1.946779	0.143151
C	0.162560	2.482415	1.077461
C	0.042319	3.912975	0.857288
C	0.834303	4.218442	-0.214312
C	1.442277	2.976903	-0.659724
H	-0.558409	4.590405	1.442974
H	0.991677	5.188820	-0.657457
C	2.344396	2.850329	-1.740107
N	2.750763	0.405613	-1.668654
C	2.955818	1.656377	-2.197345
C	3.916021	1.569640	-3.282194
C	4.282691	0.255294	-3.384849
C	3.552416	-0.467373	-2.359571

H	4.267940	2.396504	-3.878225
H	4.986079	-0.176383	-4.078872
C	3.679140	-1.853849	-2.089323
N	2.185226	-2.042179	-0.120270
C	3.053042	-2.573028	-1.047840
C	3.237191	-3.987909	-0.775141
C	2.477927	-4.285377	0.321538
C	1.819689	-3.055600	0.727138
H	3.864000	-4.659253	-1.340141
H	2.376127	-5.241921	0.808819
C	0.940297	-2.923329	1.831053
N	0.406194	-0.511008	1.650431
C	0.296170	-1.742040	2.256863
C	-0.578868	-1.629672	3.412421
C	-0.978110	-0.326649	3.488049
C	-0.350587	0.377437	2.381620
H	-0.845044	-2.436455	4.076562
H	-1.627327	0.118270	4.225175
C	-0.480330	1.756183	2.112208
O	-0.087602	-0.486825	-1.111379
C	-1.378889	2.539213	3.024170
C	-2.749131	2.697810	2.758680
C	-0.906068	3.158108	4.192882
C	-3.603863	3.418450	3.587526
C	-1.725267	3.887273	5.049826
C	-3.083041	4.015199	4.740155
H	-4.653057	3.511993	3.339337
H	-1.312992	4.345331	5.939426
H	-3.734717	4.579444	5.396528
C	0.677959	-4.162709	2.636276
C	-0.385975	-5.031705	2.341515
C	1.479604	-4.524625	3.731490
C	-0.647462	-6.183917	3.077502
C	1.253396	-5.667142	4.493306
C	0.180157	-6.499341	4.159547
H	-1.480023	-6.822050	2.811255
H	1.899917	-5.902468	5.328672
H	-0.010864	-7.392767	4.742026
C	4.589994	-2.632759	-2.993273
C	4.125161	-3.231745	-4.175690
C	5.955260	-2.807561	-2.714058
C	4.947264	-3.957512	-5.032452
C	6.812931	-3.525169	-3.542719
C	6.300131	-4.102164	-4.708881
H	4.540892	-4.400417	-5.932394
H	7.858422	-3.631138	-3.284141
H	6.954266	-4.663833	-5.365005
C	2.710271	4.114627	-2.462575
C	2.017177	4.549911	-3.604246
C	3.766367	4.936875	-2.035734
C	2.339162	5.722111	-4.282753
C	4.121343	6.115406	-2.685153
C	3.398054	6.506937	-3.816286
H	1.774165	6.015848	-5.157834
H	4.944252	6.714134	-2.317063
H	3.660179	7.421822	-4.334166
Cl	-3.460040	1.929052	1.259949
Cl	0.864194	3.009492	4.625958
Cl	6.657900	-2.063209	-1.198998
Cl	2.361233	-3.061282	-4.623783
Cl	-1.483819	-4.652235	0.932782
Cl	2.890063	-3.456812	4.195192
Cl	4.736833	4.451128	-0.563434
Cl	0.632899	3.548876	-4.247856
C	-5.053162	-2.026832	-1.576779
C	-3.932598	-2.852510	-1.586126
C	-2.730214	-2.362438	-2.080386
C	-2.637237	-1.053380	-2.555744
C	-3.774598	-0.232651	-2.544861
C	-4.990004	-0.723429	-2.055364
I	-0.796289	-0.342963	-3.230356
N	3.286727	0.369319	1.314365
C	4.194896	0.616376	1.990853
C	5.337980	0.929047	2.841321
H	5.878982	1.794030	2.447228
H	5.004082	1.159570	3.857017
H	6.024108	0.078378	2.884306
C	-0.574031	0.721649	-7.291563
S	-2.316859	1.138189	-6.787952
O	-2.645242	0.032102	-5.856748
O	-2.162889	2.465999	-6.160394
O	-3.037073	1.113287	-8.075291
F	-0.493513	-0.536222	-7.874727
F	-0.066416	1.635807	-8.203020
F	0.293008	0.715620	-6.196499
F	-6.237905	-2.533341	-1.079024
F	-4.003185	-4.142322	-1.099102
F	-1.635051	-3.204442	-2.081825
H	-5.876873	-0.103960	-2.038775
H	-3.716528	0.780397	-2.919275

$^{2}PC_{(c)}$

Fe	1.344850	0.053649	-0.018607
N	0.919284	2.005729	0.259628
C	0.188601	2.564233	1.291026
C	0.025290	3.984830	1.065820
C	0.647248	4.275444	-0.110970
C	1.209927	3.037358	-0.611096
H	-0.502158	4.660685	1.719949
H	0.724916	5.234130	-0.598421
C	1.973708	2.946300	-1.779952
N	2.388688	0.498093	-1.701463
C	2.558943	1.765994	-2.246181
C	3.504108	1.706678	-3.336670
C	3.944677	0.417306	-3.421615
C	3.258168	-0.335584	-2.400776
H	3.804872	2.546258	-3.942838
H	4.666091	0.010568	-4.112277
C	3.428165	-1.702593	-2.173299
N	1.881759	-1.870429	-0.240672
C	2.735901	-2.412592	-1.186608
C	2.826324	-3.843659	-1.005006
C	2.030458	-4.162851	0.055092
C	1.456627	-2.928277	0.545421
H	3.417242	-4.510118	-1.612873
H	1.852856	-5.139367	0.476602
C	0.655908	-2.843925	1.688820
N	0.356823	-0.386475	1.686683
C	0.162773	-1.645739	2.214583
C	-0.611444	-1.554041	3.437850
C	-0.871994	-0.233776	3.645470
C	-0.269681	0.493056	2.545789
H	-0.905872	-2.390889	4.050897
H	-1.421295	0.212953	4.458831
C	-0.349685	1.878355	2.382857
O	-0.236298	-0.142136	-0.883471
C	-1.082296	2.670268	3.422959
C	-2.465311	2.912932	3.351543
C	-0.432566	3.221510	4.540947
C	-3.164248	3.644480	4.307893
C	-1.089366	3.959220	5.521988
C	-2.466286	4.169541	5.399819
H	-4.229957	3.801090	4.203071
H	-0.538872	4.360709	6.362811
H	-2.994165	4.741270	6.153869
C	0.369664	-4.108122	2.445154
C	-0.755964	-4.910335	2.189133
C	1.212010	-4.567784	3.473860
C	-1.037902	-6.079450	2.891343
C	0.970232	-5.729431	4.201727
C	-0.166159	-6.487921	3.904600
H	-1.920012	-6.658919	2.651699
H	1.653378	-6.035682	4.983252
H	-0.371041	-7.394997	4.460836
C	4.411257	-2.449244	-3.023325
C	4.075048	-2.998316	-4.273292
C	5.742269	-2.651178	-2.616395
C	4.978373	-3.699895	-5.067526
C	6.679023	-3.344797	-3.377181
C	6.288640	-3.872588	-4.611771
H	4.665251	-4.103038	-6.021872
H	7.691213	-3.469643	-3.015034
H	7.004275	-4.415857	-5.217476
C	2.235282	4.209045	-2.545611
C	1.420678	4.622119	-3.614399
C	3.310489	5.063523	-2.243240
C	1.643673	5.790810	-4.337889
C	3.572219	6.240303	-2.939302
C	2.728935	6.602445	-3.994234
H	0.984141	6.061799	-5.152098
H	4.415677	6.860524	-2.665081
H	2.917345	7.515150	-4.547101
Cl	-3.419391	2.246055	1.939178
Cl	1.369388	2.969299	4.742627
Cl	6.302423	-1.972621	-1.010812
Cl	2.375939	-2.790083	-4.911920
Cl	-1.922637	-4.427600	0.868735
Cl	2.712549	-3.609380	3.901868
Cl	4.443891	4.629154	-0.872761
Cl	-0.009207	3.591038	-4.099382
C	-4.841314	-2.029925	-2.220859
C	-3.799375	-2.947548	-2.112025

C	-2.495515	-2.519526	-2.325038
C	-2.230768	-1.184367	-2.626515
C	-3.285762	-0.269726	-2.741135
C	-4.602518	-0.698049	-2.539119
H	-3.088562	0.763618	-2.992294
H	-5.433498	-0.010169	-2.621455
I	-0.240925	-0.561825	-2.808212
N	3.056290	0.333850	1.083691
C	4.028175	0.498457	1.687285
C	5.254130	0.707630	2.444445
H	5.518629	1.768910	2.447095
H	5.121887	0.376524	3.478298
H	6.075920	0.142146	1.996184
C	0.393741	0.270805	-6.991399
S	-1.199875	-0.397635	-6.306708
O	-0.688062	-1.326437	-5.236218
O	-1.884415	0.796226	-5.786753
O	-1.811865	-1.092139	-7.445973
F	1.151924	-0.728913	-7.577690
F	0.161464	1.243180	-7.949617
F	1.161668	0.844847	-5.985502
F	-6.128661	-2.475557	-2.005283
F	-4.048075	-4.261793	-1.778561
F	-1.475847	-3.444649	-2.227726

^{4}PC$_{(c)}$

Fe	1.360803	-0.303236	-0.074914
N	0.691388	1.586426	0.100183
C	-0.244512	2.051306	1.012340
C	-0.578670	3.424640	0.715059
C	0.182287	3.801176	-0.352311
C	0.976893	2.656697	-0.732915
H	-1.291451	4.021515	1.261188
H	0.204307	4.761504	-0.842093
C	1.903473	2.661820	-1.778036
N	2.474306	0.249793	-1.659024
C	2.591245	1.522742	-2.199983
C	3.514083	1.501577	-3.308825
C	3.942879	0.213977	-3.451942
C	3.312826	-0.562111	-2.411521
H	3.789011	2.358218	-3.902963
H	4.635441	-0.173520	-4.181772
C	3.564279	-1.917321	-2.187569
N	2.265035	-2.109068	-0.085623
C	3.071205	-2.622080	-1.088170
C	3.378959	-4.006935	-0.813619
C	2.765657	-4.327461	0.361007
C	2.064931	-3.146243	0.809981
H	3.989768	-4.641549	-1.435403
H	2.779537	-5.273917	0.877330
C	1.299980	-3.090197	1.975629
N	0.483807	-0.766580	1.678135
C	0.574804	-1.964435	2.369184
C	-0.221021	-1.899992	3.572126
C	-0.800695	-0.665861	3.603766
C	-0.361377	0.040053	2.423193
H	-0.320333	-2.695755	4.292854
H	-1.460225	-0.264956	4.356573
C	-0.740045	1.347432	2.111696
O	-0.222042	-1.001500	-1.058801
C	-1.673372	2.054345	3.048286
C	-3.070845	1.924281	2.968953
C	-1.205475	2.891137	4.078118
C	-3.949841	2.576554	3.829513
C	-2.046771	3.562475	4.960719
C	-3.429538	3.402576	4.829882
H	-5.018116	2.441476	3.721433
H	-1.631923	4.194127	5.735392
H	-4.099608	3.917617	5.507963
C	1.240943	-4.310415	2.843278
C	0.245567	-5.292079	2.694485
C	2.178811	-4.552185	3.862202
C	0.172998	-6.433063	3.488848
C	2.145305	-5.677741	4.680568
C	1.132470	-6.622388	4.488314
H	-0.614645	-7.158275	3.330935
H	2.892652	-5.814201	5.451299
H	1.091138	-7.504600	5.116035
C	4.439398	-2.647185	-3.160197
C	3.911699	-3.329712	-4.270066
C	5.837805	-2.702807	-3.027127
C	4.698650	-4.016410	-5.190243
C	6.664202	-3.376112	-3.922548
C	6.085229	-4.035823	-5.011029
H	4.239916	-4.525289	-6.027984
H	7.736046	-3.386536	-3.773491
H	6.713315	-4.565006	-5.717818
C	2.190688	3.964611	-2.462219
C	1.565848	4.354372	-3.659604
C	3.114022	4.886812	-1.936394
C	1.821249	5.568583	-4.292291
C	3.400139	6.110083	-2.535473
C	2.743608	6.450436	-3.722121
H	1.310158	5.819504	-5.212735
H	4.120739	6.781598	-2.087107
H	2.952744	7.398995	-4.202345
Cl	-3.804026	0.844575	1.689095
Cl	0.596743	3.116682	4.303874
Cl	6.636934	-1.858482	-1.613954
Cl	2.101870	-3.337581	-4.540041
Cl	-1.027959	-5.085090	1.396884
Cl	3.518631	-3.339609	4.149816
Cl	4.010429	4.480324	-0.392893
Cl	0.368621	3.229922	-4.455189
C	-5.045477	1.165642	-2.113216
C	-4.729130	-0.045536	-1.504592
C	-3.498428	-0.635952	-1.763965
C	-2.584579	-0.013087	-2.613572
C	-2.909588	1.205841	-3.221304
C	-4.155110	1.794694	-2.974604
H	-2.216491	1.682074	-3.901411
H	-4.429434	2.734281	-3.435623
I	-0.711001	-0.933485	-2.905337
N	3.368775	0.471726	1.347484
C	4.290133	0.761799	1.989855
C	5.450220	1.125640	2.796583
H	5.687866	2.185136	2.665472
H	5.249743	0.941918	3.855940
H	6.320712	0.533987	2.499091
C	0.298296	-0.477650	-7.014973
S	-1.471469	-0.174716	-6.534235
O	-1.624252	-1.093555	-5.356338
O	-1.492935	1.258873	-6.197089
O	-2.233712	-0.596768	-7.716697
F	0.505752	-1.798241	-7.378797
F	0.674564	0.319650	-8.083070
F	1.155062	-0.194541	-5.957313
F	-6.270831	1.736375	-1.835166
F	-5.610602	-0.643794	-0.628780
F	-3.208277	-1.844010	-1.162154

^{6}PC$_{(c)}$

Fe	1.103954	-0.375866	-0.327009
N	0.708875	1.636222	0.071889
C	-0.155033	2.115088	1.043790
C	-0.438713	3.512398	0.791698
C	0.265784	3.873066	-0.320648
C	0.988390	2.700806	-0.768153
H	-1.084254	4.134741	1.390883
H	0.297235	4.842030	-0.793003
C	1.861379	2.671037	-1.866127
N	2.479788	0.267336	-1.754113
C	2.560278	1.537609	-2.306171
C	3.496824	1.526317	-3.408301
C	3.979306	0.253107	-3.517182
C	3.353308	-0.532974	-2.477206
H	3.755012	2.379909	-4.014638
H	4.701407	-0.116805	-4.227575
C	3.623760	-1.886141	-2.228980
N	2.202058	-2.158344	-0.215644
C	3.083919	-2.632283	-1.171106
C	3.397609	-4.019157	-0.897608
C	2.706207	-4.374187	0.224477
C	1.961180	-3.208993	0.653638
H	4.063188	-4.634203	-1.482159
H	2.706228	-5.331376	0.721318
C	1.148955	-3.158607	1.795198
N	0.425284	-0.791602	1.608871
C	0.453582	-2.024076	2.239069
C	-0.333728	-1.966146	3.452047
C	-0.830487	-0.698063	3.549509
C	-0.357728	0.035762	2.394939
H	-0.479152	-2.783873	4.139943
H	-1.454300	-0.295213	4.331466
C	-0.650466	1.382870	2.132495
O	-0.436836	-0.903637	-1.263378
C	-1.523133	2.104178	3.116891
C	-2.926931	2.059756	3.060413
C	-0.986872	2.869187	4.168408
C	-3.749501	2.725827	3.965088
C	-1.770250	3.551429	5.094829
C	-3.162322	3.477657	4.986969
H	-4.825777	2.658357	3.874256

H	-1.304289	4.125702	5.884964
H	-3.787841	4.002266	5.699427
C	1.038408	-4.405963	2.620650
C	0.034208	-5.364829	2.402857
C	1.934199	-4.696970	3.664343
C	-0.085542	-6.530497	3.154642
C	1.853058	-5.848703	4.441957
C	0.833593	-6.769509	4.180968
H	-0.878429	-7.236279	2.943878
H	2.569518	-6.023367	5.234035
H	0.755683	-7.671541	4.776254
C	4.593683	-2.579926	-3.138925
C	4.180897	-3.271330	-4.290802
C	5.978156	-2.588204	-2.894163
C	5.063319	-3.925142	-5.146597
C	6.896843	-3.227718	-3.721769
C	6.430610	-3.900023	-4.855699
H	4.691594	-4.442737	-6.021352
H	7.952861	-3.202293	-3.486333
H	7.131412	-4.403382	-5.511137
C	2.099146	3.960562	-2.595381
C	1.401292	4.310220	-3.764362
C	3.040454	4.905699	-2.149437
C	1.604224	5.508548	-4.444100
C	3.276039	6.115018	-2.797055
C	2.547412	6.415444	-3.952035
H	1.037903	5.728539	-5.339790
H	4.013238	6.806422	-2.410074
H	2.716975	7.352577	-4.468920
Cl	-3.745879	1.079267	1.751687
Cl	0.829887	2.979868	4.360280
Cl	6.631818	-1.724285	-1.419197
Cl	2.402495	-3.328935	-4.712196
Cl	-1.189013	-5.091681	1.069183
Cl	3.282451	-3.518392	4.040397
Cl	4.029422	4.548610	-0.651147
Cl	0.173474	3.148627	-4.458245
C	-5.205686	1.174139	-2.084759
C	-4.842744	0.004031	-1.423537
C	-3.653130	-0.628492	-1.763036
C	-2.824060	-0.079362	-2.741716
C	-3.193079	1.098362	-3.402423
C	-4.401462	1.723650	-3.075811
H	-2.561959	1.516969	-4.175272
H	-4.711211	2.633039	-3.573295
I	-0.982652	-1.023065	-3.115583
N	4.121507	0.792471	2.235598
C	4.983940	1.101751	2.949722
C	6.068887	1.489448	3.847001
H	6.315730	2.546847	3.714478
H	5.778517	1.329688	4.889514
H	6.965034	0.896429	3.642355
C	0.064824	-0.829463	-7.062042
S	-1.686508	-0.396017	-6.612427
O	-1.908650	-1.282067	-5.404955
O	-1.617642	1.038464	-6.296953
O	-2.477526	-0.809825	-7.774163
F	0.200979	-2.180598	-7.326226
F	0.481969	-0.129568	-8.178512
F	0.924143	-0.514077	-6.015566
F	-6.389557	1.784872	-1.728272
F	-5.637587	-0.513517	-0.423388
F	-3.316533	-1.796744	-1.112210

$^{2}RC_{(d)}$

Fe	1.930865	0.027873	-0.202020
N	1.244962	1.928835	-0.037691
C	0.312222	2.399149	0.859208
C	0.005173	3.785035	0.583466
C	0.766463	4.151256	-0.486337
C	1.539817	2.989636	-0.865265
H	-0.694667	4.389967	1.136423
H	0.806790	5.112088	-0.972793
C	2.470542	2.974145	-1.914821
N	3.162121	0.608112	-1.704853
C	3.228397	1.853330	-2.288391
C	4.203928	1.856330	-3.355846
C	4.725890	0.598550	-3.415189
C	4.069308	-0.174822	-2.384865
H	4.452092	2.705982	-3.970669
H	5.482102	0.225811	-4.086524
C	4.330384	-1.529692	-2.133784
N	2.774822	-1.815618	-0.232017
C	3.707948	-2.285787	-1.127953
C	3.974408	-3.686468	-0.886877
C	3.191284	-4.060566	0.164340
C	2.447588	-2.888203	0.568280
H	4.666887	-4.294237	-1.445938
H	3.123975	-5.031402	0.627494
C	1.540277	-2.863401	1.637277
N	0.882404	-0.485976	1.456210
C	0.829760	-1.726069	2.051706
C	-0.072736	-1.702742	3.181209
C	-0.568189	-0.435381	3.262376
C	0.025420	0.314952	2.178393
H	-0.290182	-2.540933	3.822829
H	-1.267791	-0.042503	3.981860
C	-0.258602	1.661755	1.908212
O	0.738249	-0.406976	-1.205128
C	-1.234671	2.364020	2.802981
C	-2.619324	2.325200	2.569615
C	-0.817200	3.102952	3.921960
C	-3.538956	2.978414	3.385037
C	-1.704056	3.769039	4.762100
C	-3.073569	3.704232	4.485960
H	-4.597010	2.921848	3.164835
H	-1.334724	4.325565	5.613561
H	-3.777674	4.217980	5.129504
C	1.313725	-4.139289	2.390262
C	0.311377	-5.049896	2.017465
C	2.085874	-4.495857	3.507637
C	0.079304	-6.239734	2.700490
C	1.886729	-5.675409	4.218736
C	0.875122	-6.549501	3.808075
H	-0.705503	-6.910279	2.375609
H	2.507350	-5.907065	5.074465
H	0.706964	-7.471857	4.351044
C	5.344930	-2.219390	-2.994615
C	4.996122	-2.827166	-4.212007
C	6.698221	-2.300731	-2.628603
C	5.922122	-3.479185	-5.020952
C	7.655123	-2.942026	-3.409106
C	7.258457	-3.534751	-4.612284
H	5.606588	-3.934259	-5.950759
H	8.687247	-2.977764	-3.085792
H	7.990784	-4.038758	-5.231579
C	2.684785	4.248181	-2.674990
C	1.960155	4.551479	-3.839445
C	3.621703	5.209093	-2.260944
C	2.144724	5.732588	-4.552945
C	3.836461	6.400448	-2.946587
C	3.088809	6.659280	-4.100007
H	1.562717	5.924441	-5.445028
H	4.570755	7.110570	-2.589305
H	3.243215	7.582466	-4.645737
Cl	-3.255645	1.380280	1.144221
Cl	0.966158	3.198940	4.311024
Cl	7.244442	-1.531530	-1.062973
Cl	3.260717	-2.760637	-4.770573
Cl	-0.742456	-4.669750	0.574362
Cl	3.413996	-3.371816	4.066814
Cl	4.615533	4.894683	-0.758919
Cl	0.728523	3.357329	-4.458049
C	-7.735036	-1.571227	-0.681214
C	-8.073469	-1.920011	-1.984591
C	-7.121565	-1.790075	-2.991353
C	-5.833295	-1.319391	-2.732483
C	-5.547431	-0.984067	-1.405383
C	-6.467788	-1.097635	-0.369408
I	-4.402391	-1.125497	-4.262827
N	3.504852	0.607107	1.132311
C	4.352927	0.929745	1.848616
C	5.420785	1.338167	2.750039
H	5.761267	2.346813	2.499415
H	5.064301	1.334640	3.783967
H	6.267845	0.651289	2.668263
C	-0.119943	-0.803901	-5.207738
S	-1.296231	0.008555	-6.400396
O	-2.463279	-0.913338	-6.359617
O	-1.522974	1.331143	-5.786874
O	-0.543928	-0.004527	-7.667235
F	0.232703	-2.082821	-5.628321
F	1.057118	-0.077910	-5.071693
F	-0.678658	-0.926623	-3.942785
F	-8.687686	-1.704102	0.309809
F	-9.337288	-2.389281	-2.278501
F	-7.490222	-2.145017	-4.274361
F	-4.279690	-0.511089	-1.093229
H	-6.207845	-0.827126	0.644376

$^{4}RC_{(d)}$

Fe	1.932366	0.029062	-0.201224
N	1.245998	1.929351	-0.037931

C	0.311759	2.399739	0.857983
C	0.003578	3.785045	0.580634
C	0.765378	4.151145	-0.488747
C	1.540326	2.990122	-0.866217
H	-0.697537	4.389664	1.132322
H	0.804939	5.111554	-0.976108
C	2.472087	2.974901	-1.914766
N	3.163254	0.608757	-1.704087
C	3.229704	1.854128	-2.288154
C	4.204746	1.856467	-3.356038
C	4.726174	0.598534	-3.415468
C	4.069998	-0.174547	-2.384689
H	4.452736	2.705849	-3.971307
H	5.481721	0.225369	-4.087317
C	4.330649	-1.529515	-2.133708
N	2.775368	-1.814420	-0.231446
C	3.707647	-2.285449	-1.128479
C	3.971782	-3.686815	-0.888797
C	3.188469	-4.060707	0.162245
C	2.446654	-2.887688	0.567711
H	4.662916	-4.295199	-1.448857
H	3.119607	-5.031972	0.624271
C	1.539342	-2.862716	1.636666
N	0.882550	-0.484896	1.455374
C	0.828866	-1.725514	2.050674
C	-0.074808	-1.702116	3.179228
C	-0.569950	-0.434720	3.260317
C	0.024824	0.315939	2.177199
H	-0.293281	-2.540495	3.820257
H	-1.270261	-0.041927	3.979156
C	-0.258992	1.662758	1.907001
O	0.740534	-0.406127	-1.205505
C	-1.235182	2.365120	2.801565
C	-2.619906	2.325579	2.568712
C	-0.817689	3.104905	3.919991
C	-3.539553	2.978878	3.384083
C	-1.704529	3.771136	4.760012
C	-3.074121	3.705566	4.484388
H	-4.597655	2.921671	3.164273
H	-1.335164	4.328362	5.610999
H	-3.778213	4.219400	5.127877
C	1.312371	-4.138638	2.389485
C	0.309428	-5.048720	2.016965
C	2.084803	-4.495795	3.506472
C	0.077039	-6.238553	2.699899
C	1.885358	-5.675345	4.217492
C	0.873148	-6.548873	3.807121
H	-0.708218	-6.908669	2.375223
H	2.506206	-5.907433	5.072939
H	0.704754	-7.471224	4.350027
C	5.344611	-2.219583	-2.994934
C	4.995278	-2.826594	-4.212570
C	6.697869	-2.302068	-2.629078
C	5.920740	-3.478946	-5.021866
C	7.654253	-2.943727	-3.409922
C	7.257067	-3.535652	-4.613322
H	5.604810	-3.933401	-5.951841
H	8.686375	-2.980352	-3.086700
H	7.988986	-4.039923	-5.232885
C	2.687147	4.249147	-2.674373
C	1.963149	4.553315	-3.839014
C	3.624288	5.209476	-2.259520
C	2.148603	5.734606	-4.551977
C	3.839939	6.401004	-2.944592
C	3.092951	6.660650	-4.098256
H	1.567073	5.927108	-5.444232
H	4.574390	7.110643	-2.586679
H	3.248058	7.583973	-4.643555
Cl	-3.256441	1.379594	1.144120
Cl	0.965743	3.201811	4.308514
Cl	7.244809	-1.533901	-1.063183
Cl	3.259868	-2.758612	-4.770967
Cl	-0.744776	-4.667966	0.574265
Cl	3.413700	-3.372501	4.065317
Cl	4.617165	4.894107	-0.757066
Cl	0.731051	3.360098	-4.458517
C	-7.732522	-1.576696	-0.677521
C	-8.071247	-1.926052	-1.980619
C	-7.120136	-1.795098	-2.988036
C	-5.832422	-1.322813	-2.729904
C	-5.546031	-0.986919	-1.402921
C	-6.465649	-1.101472	-0.366429
I	-4.402452	-1.126672	-4.260894
N	3.505335	0.608292	1.133126
C	4.353102	0.931209	1.849675
C	5.420350	1.338560	2.752318
H	5.761137	2.347418	2.502953
H	5.063098	1.334090	3.785978
H	6.267407	0.651687	2.670508
C	-0.119022	-0.802759	-5.207127
S	-1.296762	0.010058	-6.398147
O	-2.462887	-0.912981	-6.357812
O	-1.524486	1.331702	-5.782954
O	-0.545011	-0.000822	-7.665344
F	0.233856	-2.081077	-5.629476
F	1.057768	-0.076345	-5.071368
F	-0.676488	-0.927136	-3.941761
F	-8.684389	-1.710615	0.313962
F	-9.334777	-2.396983	-2.273904
F	-7.489164	-2.150604	-4.270777
F	-4.278789	-0.512427	-1.092081
H	-6.205610	-0.830551	0.647339

$^{6}RC_{(d)}$

Fe	1.893760	0.009095	-0.241689
N	1.236080	1.976694	-0.035084
C	0.302982	2.429376	0.866019
C	0.009791	3.823830	0.593369
C	0.780376	4.192908	-0.472589
C	1.551062	3.027234	-0.862552
H	-0.686679	4.435691	1.143584
H	0.824970	5.159632	-0.947595
C	2.490889	2.987896	-1.917462
N	3.198068	0.619129	-1.751132
C	3.253118	1.867977	-2.320604
C	4.225019	1.862161	-3.397888
C	4.741715	0.599265	-3.462502
C	4.091149	-0.178625	-2.424960
H	4.477474	2.707671	-4.017219
H	5.492419	0.230199	-4.142514
C	4.343120	-1.541326	-2.149470
N	2.812106	-1.862563	-0.227967
C	3.740549	-2.316810	-1.132519
C	4.015100	-3.718088	-0.876010
C	3.239601	-4.089096	0.185798
C	2.484391	-2.917900	0.588817
H	4.707098	-4.331618	-1.430008
H	3.186786	-5.059037	0.653429
C	1.564252	-2.870716	1.660046
N	0.860193	-0.501166	1.496973
C	0.824100	-1.743191	2.082612
C	-0.093840	-1.717800	3.205828
C	-0.601500	-0.451517	3.277731
C	-0.002526	0.307512	2.196228
H	-0.314742	-2.551606	3.852505
H	-1.311223	-0.067896	3.992791
C	-0.270063	1.664805	1.907620
O	0.703396	-0.430984	-1.239785
C	-1.252462	2.366528	2.798696
C	-2.635659	2.329625	2.556845
C	-0.841691	3.102330	3.922211
C	-3.559912	2.981873	3.367938
C	-1.733108	3.767513	4.758282
C	-3.100919	3.704850	4.473365
H	-4.616607	2.926650	3.140930
H	-1.368540	4.321610	5.613379
H	-3.808574	4.217877	5.113589
C	1.346800	-4.145413	2.421127
C	0.356486	-5.069412	2.049029
C	2.116550	-4.486700	3.544780
C	0.133639	-6.257415	2.738360
C	1.926632	-5.663896	4.262385
C	0.926858	-6.551621	3.852032
H	-0.642121	-6.938466	2.413584
H	2.545316	-5.883320	5.122737
H	0.765868	-7.472368	4.399898
C	5.351217	-2.234567	-3.017966
C	4.991056	-2.845991	-4.230209
C	6.707930	-2.314707	-2.664893
C	5.909207	-3.500604	-5.046021
C	7.657448	-2.958491	-3.452462
C	7.249378	-3.555010	-4.649928
H	5.584810	-3.958470	-5.971406
H	8.692627	-2.993122	-3.138900
H	7.975793	-4.060954	-5.274595
C	2.712087	4.265693	-2.672623
C	1.983962	4.581417	-3.831557
C	3.659087	5.216484	-2.258563
C	2.174967	5.764540	-4.540055
C	3.880586	6.409599	-2.939098
C	3.129344	6.680770	-4.087333
H	1.589983	5.965992	-5.428078

H	4.622701	7.111578	-2.581858
H	3.288858	7.605412	-4.629125
Cl	-3.265280	1.387916	1.126042
Cl	0.939262	3.194988	4.323922
Cl	7.269400	-1.540011	-1.107188
Cl	3.250250	-2.780817	-4.772800
Cl	-0.694386	-4.710315	0.598092
Cl	3.430056	-3.345114	4.103554
Cl	4.657731	4.885947	-0.762967
Cl	0.738219	3.401045	-4.449198
C	-7.802981	-1.584557	-0.721200
C	-8.125358	-1.920877	-2.031893
C	-7.161124	-1.781559	-3.025599
C	-5.876211	-1.313480	-2.746367
C	-5.606553	-0.990779	-1.412725
C	-6.539645	-1.114117	-0.389316
I	-4.427083	-1.104636	-4.257384
N	3.483665	0.600071	1.104654
C	4.330818	0.926083	1.820606
C	5.396740	1.337817	2.722513
H	5.745384	2.341017	2.461468
H	5.034729	1.349085	3.754465
H	6.239276	0.644043	2.653242
C	-0.139356	-0.800135	-5.147596
S	-1.291369	0.039631	-6.345232
O	-2.467571	-0.871483	-6.333719
O	-1.514526	1.355643	-5.716402
O	-0.521263	0.036900	-7.601368
F	0.208918	-2.075678	-5.581455
F	1.041411	-0.086036	-4.983211
F	-0.718166	-0.936519	-3.892994
F	-8.767728	-1.726675	0.256718
F	-9.385553	-2.387200	-2.345888
F	-7.513877	-2.124335	-4.316382
F	-4.342813	-0.521307	-1.080736
H	-6.292259	-0.853398	0.630197

^{2}TS$_{(d)}$

Fe	1.393499	0.018692	-0.012950
N	0.935225	1.968378	0.260913
C	0.154564	2.499808	1.269563
C	0.011862	3.927630	1.083109
C	0.707987	4.253440	-0.042246
C	1.280575	3.026660	-0.551093
H	-0.547112	4.585664	1.728549
H	0.824651	5.227056	-0.490016
C	2.082391	2.951507	-1.697802
N	2.432758	0.493559	-1.668359
C	2.629947	1.767297	-2.194838
C	3.545587	1.705584	-3.310496
C	3.946495	0.408522	-3.430207
C	3.273171	-0.343124	-2.396754
H	3.851661	2.548778	-3.908364
H	4.639863	-0.004670	-4.144747
C	3.475184	-1.704722	-2.161202
N	2.017838	-1.895866	-0.170945
C	2.853916	-2.423708	-1.131351
C	3.016286	-3.845638	-0.923937
C	2.271122	-4.173361	0.169126
C	1.654790	-2.952779	0.641919
H	3.615070	-4.499265	-1.537322
H	2.149288	-5.145414	0.618955
C	0.830515	-2.883810	1.771632
N	0.414647	-0.449417	1.715554
C	0.250386	-1.706346	2.255880
C	-0.604439	-1.636569	3.423971
C	-0.953390	-0.329712	3.581035
C	-0.316124	0.407625	2.508549
H	-0.891584	-2.476809	4.035365
H	-1.580182	0.101241	4.344995
C	-0.434289	1.789353	2.321991
O	-0.075340	-0.304184	-0.736493
C	-1.259573	2.558175	3.309553
C	-2.637958	2.764925	3.131246
C	-0.705640	3.116282	4.473816
C	-3.423746	3.473541	4.035495
C	-1.453342	3.832226	5.404245
C	-2.822067	4.009151	5.178624
H	-4.482137	3.604808	3.851873
H	-0.978336	4.242802	6.285707
H	-3.419116	4.563621	5.892803
C	0.565591	-4.152442	2.526137
C	-0.515946	-4.995965	2.220229
C	1.382077	-4.569789	3.591053
C	-0.779877	-6.172971	2.915360
C	1.154928	-5.738571	4.311672
C	0.063730	-6.542492	3.967318
H	-1.626737	-6.788447	2.641010
H	1.814450	-6.015629	5.123739
H	-0.128600	-7.455620	4.517974
C	4.449827	-2.436477	-3.034833
C	4.090141	-2.991964	-4.274438
C	5.791982	-2.614415	-2.655028
C	4.986624	-3.683024	-5.085344
C	6.720493	-3.296848	-3.435081
C	6.308897	-3.835433	-4.658191
H	4.658526	-4.093601	-6.031400
H	7.742761	-3.404378	-3.096626
H	7.018228	-4.370589	-5.278202
C	2.405927	4.229730	-2.411963
C	1.626224	4.712409	-3.476483
C	3.510026	5.024115	-2.057714
C	1.909378	5.896448	-4.151179
C	3.830442	6.213830	-2.705057
C	3.020724	6.648836	-3.759009
H	1.275877	6.224363	-4.964990
H	4.693156	6.788464	-2.394156
H	3.255528	7.572715	-4.274046
Cl	-3.458497	2.078121	1.648283
Cl	1.081130	2.904307	4.801938
Cl	6.374340	-1.914411	-1.068132
Cl	2.378097	-2.803666	-4.878932
Cl	-1.638570	-4.549564	0.850989
Cl	2.818919	-3.544069	4.070661
Cl	4.594858	4.486855	-0.686514
Cl	0.165030	3.756872	-4.015355
C	-4.822266	-1.689337	-1.824376
C	-3.751228	-2.578841	-1.787791
C	-2.493749	-2.141897	-2.184258
C	-2.280918	-0.828764	-2.609487
C	-3.385721	0.029019	-2.630152
C	-4.658720	-0.376190	-2.247730
I	-0.387175	-0.193436	-3.158626
N	3.105424	0.371399	1.127739
C	4.057059	0.570869	1.752563
C	5.258163	0.824536	2.535174
H	5.562126	1.869924	2.430581
H	5.072448	0.616548	3.592584
H	6.075309	0.185062	2.189440
C	-0.037081	-0.618384	-7.288732
S	-1.786007	0.015931	-7.196651
O	-2.236804	-0.497560	-5.881684
O	-1.599981	1.478486	-7.273755
O	-2.418809	-0.617456	-8.369562
F	0.024199	-1.993808	-7.090138
F	0.546298	-0.351694	-8.518895
F	0.776642	-0.032077	-6.318696
F	-6.063199	-2.136160	-1.428214
F	-3.927310	-3.874911	-1.350922
F	-1.448181	-3.039309	-2.144523
F	-3.210995	1.337403	-3.038971
H	-5.494854	0.308395	-2.273631

^{4}TS$_{(d)}$

Fe	1.524412	-0.056174	-0.053081
N	1.100819	1.908973	0.147008
C	0.182736	2.468482	1.015205
C	0.103001	3.895673	0.797164
C	0.976286	4.195018	-0.204885
C	1.586661	2.951327	-0.621804
H	-0.532258	4.572126	1.346124
H	1.186848	5.162152	-0.632441
C	2.495742	2.845784	-1.675136
N	2.789467	0.386834	-1.566785
C	3.021993	1.633062	-2.122900
C	3.893649	1.504672	-3.268923
C	4.174230	0.177967	-3.412204
C	3.493899	-0.516467	-2.343134
H	4.237804	2.323267	-3.880447
H	4.793763	-0.289984	-4.160322
C	3.597027	-1.889428	-2.113640
N	2.191220	-1.954756	-0.071855
C	3.003027	-2.537430	-1.030948
C	3.178465	-3.942518	-0.738041
C	2.475010	-4.205322	0.398408
C	1.843095	-2.968522	0.801704
H	3.769545	-4.627850	-1.324062
H	2.379178	-5.146829	0.914997
C	0.972928	-2.855548	1.886231
N	0.465283	-0.445505	1.599263
C	0.308942	-1.674427	2.218623
C	-0.674211	-1.571477	3.272140
C	-1.124120	-0.284656	3.277478

C	-0.407173	0.421213	2.241315
H	-0.981056	-2.381866	3.913715
H	-1.864745	0.153875	3.926797
C	-0.555422	1.783355	1.981448
O	0.225022	-0.358487	-1.075301
C	-1.547587	2.558292	2.793755
C	-2.864626	2.776268	2.351988
C	-1.229230	3.118531	4.043025
C	-3.807699	3.489169	3.087062
C	-2.139593	3.838368	4.811873
C	-3.438081	4.020914	4.326322
H	-4.809169	3.626655	2.700523
H	-1.841658	4.249075	5.767785
H	-4.159801	4.578159	4.911740
C	0.714397	-4.073469	2.720113
C	-0.277598	-5.016370	2.397487
C	1.452785	-4.349584	3.884425
C	-0.530156	-6.150276	3.165127
C	1.234879	-5.469923	4.681279
C	0.233391	-6.374122	4.314643
H	-1.306983	-6.844314	2.871712
H	1.833690	-5.633987	5.567720
H	0.048944	-7.251764	4.922819
C	4.408851	-2.707544	-3.071249
C	3.836133	-3.320295	-4.199613
C	5.789492	-2.914659	-2.907887
C	4.565447	-4.082560	-5.107770
C	6.558516	-3.668952	-3.789833
C	5.936998	-4.254865	-4.896932
H	4.074204	-4.532028	-5.960947
H	7.619158	-3.796623	-3.616777
H	6.520371	-4.844874	-5.593821
C	2.905801	4.100593	-2.384411
C	2.206769	4.603760	-3.495536
C	4.019980	4.856269	-1.979334
C	2.574851	5.768578	-4.163803
C	4.423860	6.025860	-2.616948
C	3.691666	6.481475	-3.717653
H	2.001315	6.111854	-5.014973
H	5.290298	6.569038	-2.262771
H	3.990965	7.389842	-4.226902
Cl	-3.386141	2.106532	0.732450
Cl	0.462033	2.913754	4.711924
Cl	6.643052	-2.167977	-1.471538
Cl	2.044323	-3.120846	-4.509680
Cl	-1.300574	-4.772781	0.901781
Cl	2.777822	-3.196236	4.398206
Cl	5.006549	4.296159	-0.542891
Cl	0.740816	3.707141	-4.120875
C	-4.526969	-2.564699	-1.501295
C	-3.325286	-3.188885	-1.830716
C	-2.271636	-2.423307	-2.310815
C	-2.395804	-1.038039	-2.460972
C	-3.619139	-0.452347	-2.112043
C	-4.694091	-1.192244	-1.638337
I	-0.814066	0.086812	-3.161739
N	3.286196	0.386661	1.310271
C	4.184393	0.639215	1.995220
C	5.315326	0.960586	2.856466
H	5.866848	1.814504	2.452919
H	4.966167	1.212897	3.861756
H	5.994607	0.106270	2.925917
C	-0.824601	1.106003	-7.146571
S	-2.458840	1.391401	-6.306571
O	-2.542822	0.198222	-5.406277
O	-2.254267	2.673547	-5.611903
O	-3.424793	1.376959	-7.415680
F	-0.811976	-0.085361	-7.853767
F	-0.517095	2.125942	-8.030427
F	0.209519	1.040863	-6.211053
F	-5.559282	-3.338660	-1.026671
F	-3.172080	-4.547354	-1.662209
F	-1.090881	-3.054393	-2.627522
F	-3.766057	0.915963	-2.233951
H	-5.628708	-0.715954	-1.377614

$^{6}TS_{(d)}$

Fe	1.450889	-0.113463	-0.188043
N	1.073804	1.943568	0.071822
C	0.206938	2.488535	0.980673
C	0.118674	3.921904	0.766168
C	0.946704	4.218836	-0.280943
C	1.545914	2.969221	-0.713876
H	-0.485818	4.607132	1.338708
H	1.134046	5.188579	-0.713706
C	2.471605	2.830638	-1.773314
N	2.875147	0.386793	-1.665758
C	3.088450	1.631874	-2.206663
C	4.061430	1.530262	-3.278658
C	4.426350	0.214059	-3.361493
C	3.681419	-0.494916	-2.337285
H	4.421813	2.349280	-3.880431
H	5.136928	-0.227301	-4.041965
C	3.799839	-1.879416	-2.049879
N	2.258277	-2.044968	-0.116009
C	3.153656	-2.584995	-1.012885
C	3.334817	-3.995652	-0.715567
C	2.546251	-4.281965	0.362398
C	1.869087	-3.050648	0.732486
H	3.980252	-4.671554	-1.253514
H	2.435314	-5.232369	0.859572
C	0.943281	-2.913567	1.794797
N	0.429409	-0.500209	1.589140
C	0.277680	-1.730126	2.184690
C	-0.673778	-1.618800	3.278375
C	-1.079130	-0.316073	3.325758
C	-0.377044	0.389046	2.265652
H	-0.985681	-2.426124	3.921614
H	-1.780333	0.127412	4.014531
C	-0.488663	1.767074	1.986014
O	0.035164	-0.562205	-1.175791
C	-1.432578	2.556783	2.844732
C	-2.756550	2.811273	2.448714
C	-1.051690	3.088516	4.087587
C	-3.653846	3.535908	3.227586
C	-1.916414	3.819279	4.897108
C	-3.226368	4.039888	4.460103
H	-4.664818	3.703674	2.879681
H	-1.574743	4.209494	5.846934
H	-3.912676	4.605940	5.078542
C	0.640450	-4.151529	2.587230
C	-0.369699	-5.051904	2.209133
C	1.351461	-4.483307	3.752480
C	-0.665566	-6.204484	2.931404
C	1.088796	-5.625192	4.503382
C	0.071013	-6.488433	4.085585
H	-1.454599	-6.866852	2.599926
H	1.665934	-5.836892	5.394043
H	-0.147503	-7.381734	4.658461
C	4.720371	-2.670753	-2.932577
C	4.269647	-3.276358	-4.117199
C	6.080180	-2.851139	-2.631574
C	5.100068	-4.014131	-4.955457
C	6.945768	-3.581010	-3.441110
C	6.446925	-4.164565	-4.610060
H	4.704741	-4.461826	-5.857939
H	7.986599	-3.691135	-3.165970
H	7.107294	-4.735720	-5.251588
C	2.848921	4.085994	-2.505131
C	2.156627	4.518739	-3.648218
C	3.913433	4.901930	-2.087772
C	2.487471	5.681630	-4.338037
C	4.277518	6.071662	-2.748116
C	3.555192	6.460141	-3.880892
H	1.923025	5.973279	-5.214142
H	5.106412	6.666257	-2.386819
H	3.824551	7.368022	-4.407295
Cl	-3.341953	2.174471	0.839507
Cl	0.658416	2.830943	4.682061
Cl	6.764332	-2.097527	-1.112625
Cl	2.513739	-3.098607	-4.594278
Cl	-1.352952	-4.717530	0.705564
Cl	2.692712	-3.378704	4.322794
Cl	4.879777	4.421165	-0.611388
Cl	0.759831	3.525560	-4.279852
C	-4.873800	-2.319624	-1.385223
C	-3.742098	-3.058011	-1.721683
C	-2.627606	-2.400803	-2.226941
C	-2.617436	-1.014197	-2.397452
C	-3.773541	-0.313383	-2.039619
C	-4.908831	-0.939736	-1.539868
I	-0.922104	-0.055158	-3.110768
N	3.316734	0.383379	1.328392
C	4.200644	0.646714	2.030260
C	5.313072	0.979991	2.912768
H	5.875559	1.827518	2.510914
H	4.942649	1.246851	3.906654
H	5.990108	0.126583	3.010320
C	-1.154401	0.998749	-7.167603
S	-2.809644	1.380666	-6.407664
O	-3.003553	0.228287	-5.493582
O	-2.566098	2.676747	-5.744043

O	-3.705011	1.410936	-7.579195
F	-1.152462	-0.233303	-7.807392
F	-0.779977	1.953564	-8.101048
F	-0.144649	0.955149	-6.202519
F	-5.970515	-2.985526	-0.884930
F	-3.711580	-4.423880	-1.536001
F	-1.518558	-3.153227	-2.547442
F	-3.792049	1.064601	-2.167346
H	-5.788202	-0.371336	-1.271462

^{2}PC$_{(d)}$

Fe	1.356386	0.088532	-0.006441
N	0.943826	2.039307	0.279609
C	0.249549	2.603586	1.332369
C	0.086066	4.024522	1.108474
C	0.665841	4.307654	-0.091511
C	1.209714	3.066031	-0.604334
H	-0.415926	4.704924	1.777752
H	0.729119	5.263911	-0.585773
C	1.946426	2.969849	-1.790419
N	2.388542	0.526451	-1.696710
C	2.539481	1.792024	-2.253894
C	3.486981	1.735738	-3.341929
C	3.954185	0.454039	-3.407962
C	3.277072	-0.300037	-2.382860
H	3.774392	2.573010	-3.957680
H	4.686389	0.053257	-4.090723
C	3.459260	-1.663812	-2.145656
N	1.874261	-1.836937	-0.245617
C	2.747771	-2.377168	-1.175116
C	2.816416	-3.811081	-1.009558
C	1.981056	-4.135080	0.018505
C	1.411976	-2.899383	0.511783
H	3.417348	-4.476640	-1.608540
H	1.777440	-5.115368	0.418902
C	0.590370	-2.816049	1.640237
N	0.372956	-0.350873	1.695857
C	0.136574	-1.614977	2.194028
C	-0.625063	-1.524428	3.425093
C	-0.831288	-0.200522	3.669132
C	-0.215857	0.530367	2.579621
H	-0.945401	-2.364645	4.020341
H	-1.355630	0.246075	4.498865
C	-0.267053	1.919393	2.435948
O	-0.230897	-0.088322	-0.870880
C	-0.955580	2.715745	3.502244
C	-2.335635	2.983004	3.473903
C	-0.262599	3.247477	4.603523
C	-2.992343	3.719783	4.455871
C	-0.876385	3.989711	5.608630
C	-2.252463	4.224712	5.529575
H	-4.057778	3.895887	4.384429
H	-0.293908	4.375677	6.435044
H	-2.747214	4.800125	6.303045
C	0.235745	-4.091067	2.345501
C	-0.914904	-4.833713	2.030137
C	1.033083	-4.626978	3.372795
C	-1.262626	-6.018470	2.673609
C	0.725806	-5.807004	4.044006
C	-0.432453	-6.504780	3.687951
H	-2.161677	-6.549658	2.389393
H	1.375954	-6.173936	4.827522
H	-0.687184	-7.425128	4.199969
C	4.462009	-2.405439	-2.976463
C	4.150446	-2.964179	-4.228503
C	5.787840	-2.593041	-2.546955
C	5.072997	-3.661098	-5.004500
C	6.743133	-3.281383	-3.289178
C	6.377492	-3.818861	-4.527144
H	4.778866	-4.072224	-5.961469
H	7.750416	-3.395014	-2.910100
H	7.107776	-4.358357	-5.118567
C	2.179906	4.226556	-2.574453
C	1.343674	4.613998	-3.635982
C	3.247906	5.099374	-2.300124
C	1.539331	5.775443	-4.378669
C	3.482470	6.270069	-3.015847
C	2.618438	6.606309	-4.062538
H	0.863768	6.026256	-5.186164
H	4.321318	6.905415	-2.763023
H	2.785918	7.513907	-4.630343
Cl	-3.343048	2.343820	2.086063
Cl	1.539682	2.962068	4.748214
Cl	6.314834	-1.902685	-0.935492
Cl	2.459321	-2.775968	-4.892910
Cl	-2.032029	-4.237264	0.709694
Cl	2.558955	-3.748745	3.874071
Cl	4.408634	4.698783	-0.942415
Cl	-0.081139	3.558216	-4.082152
C	-4.797762	-2.133773	-2.299676
C	-3.772827	-3.067480	-2.439260
C	-2.465694	-2.619470	-2.584600
C	-2.169280	-1.256613	-2.591655
C	-3.226313	-0.354511	-2.446011
C	-4.545018	-0.767864	-2.301570
I	-0.201622	-0.588265	-2.769760
N	3.073499	0.354664	1.086076
C	4.044213	0.516198	1.692356
C	5.267392	0.721987	2.454706
H	5.483309	1.790831	2.539322
H	5.160802	0.305019	3.460091
H	6.109392	0.231774	1.958032
C	0.340169	0.128996	-6.960390
S	-1.202796	-0.636167	-6.260527
O	-0.629899	-1.476996	-5.147678
O	-1.984940	0.518524	-5.795007
O	-1.744763	-1.426098	-7.372173
F	1.168108	-0.826710	-7.524622
F	0.039817	1.061050	-7.939113
F	1.063730	0.778288	-5.966963
F	-6.086237	-2.592938	-2.154462
F	-4.043548	-4.416768	-2.416678
F	-1.462906	-3.553488	-2.719219
F	-2.956335	1.000028	-2.443199
H	-5.347657	-0.052160	-2.191174

^{4}PC$_{(d)}$

Fe	1.273445	0.151086	0.006564
N	1.018426	2.128506	0.331511
C	0.264455	2.712080	1.335865
C	0.176480	4.138119	1.121374
C	0.877071	4.416011	-0.014624
C	1.403883	3.163250	-0.505410
H	-0.351497	4.829519	1.758366
H	1.028503	5.376965	-0.479397
C	2.207600	3.048594	-1.641219
N	2.430530	0.574975	-1.596381
C	2.710437	1.835005	-2.113345
C	3.622659	1.717797	-3.223771
C	3.911077	0.391558	-3.370763
C	3.171947	-0.320162	-2.357762
H	4.000431	2.543454	-3.805227
H	4.565987	-0.064669	-4.095645
C	3.207964	-1.705814	-2.192571
N	1.774315	-1.791777	-0.169336
C	2.522925	-2.377965	-1.178505
C	2.541625	-3.811980	-1.007442
C	1.813988	-4.092351	0.110484
C	1.343955	-2.833043	0.638600
H	3.047030	-4.506972	-1.658585
H	1.615053	-5.059248	0.544080
C	0.610517	-2.709614	1.819552
N	0.355326	-0.243121	1.752185
C	0.171621	-1.487862	2.332890
C	-0.558190	-1.349748	3.571004
C	-0.820434	-0.021433	3.736066
C	-0.251048	0.667970	2.602514
H	-0.829587	-2.162800	4.224983
H	-1.346296	0.452079	4.549562
C	-0.322584	2.048883	2.414224
O	-0.467910	0.020046	-0.963435
C	-1.068555	2.863663	3.426450
C	-2.447649	3.114493	3.318566
C	-0.438957	3.428935	4.549019
C	-3.162146	3.867396	4.246212
C	-1.112699	4.187866	5.501980
C	-2.484880	4.405891	5.344638
H	-4.223920	4.030157	4.114581
H	-0.578558	4.599659	6.348333
H	-3.025318	4.994266	6.076635
C	0.302595	-3.953636	2.597004
C	-0.895423	-4.669610	2.430907
C	1.193970	-4.483053	3.547108
C	-1.198866	-5.827834	3.141318
C	0.932853	-5.637049	4.280532
C	-0.273845	-6.311747	4.071278
H	-2.136751	-6.340891	2.972881
H	1.654650	-6.001129	5.000043
H	-0.493573	-7.211906	4.633018
C	4.061266	-2.510343	-3.126674
C	3.601782	-2.966204	-4.374891
C	5.385859	-2.860935	-2.808175
C	4.383530	-3.718207	-5.247984

C	6.202608	-3.610644	-3.649724
C	5.692199	-4.041690	-4.877962
H	3.978730	-4.044272	-6.197289
H	7.215444	-3.851380	-3.354057
H	6.313658	-4.626377	-5.545807
C	2.563322	4.300357	-2.384777
C	1.814886	4.753382	-3.485631
C	3.661228	5.102890	-2.028799
C	2.119916	5.916461	-4.187411
C	4.003044	6.272449	-2.702149
C	3.222008	6.678657	-3.788582
H	1.509948	6.221015	-5.027956
H	4.860179	6.853011	-2.386665
H	3.472822	7.586600	-4.324203
Cl	-3.372488	2.430429	1.895649
Cl	1.355350	3.166239	4.795280
Cl	6.102325	-2.309405	-1.216682
Cl	1.900807	-2.562313	-4.906732
Cl	-2.136614	-4.068891	1.230658
Cl	2.781308	-3.627962	3.860610
Cl	4.715583	4.604812	-0.617859
Cl	0.372435	3.783337	-4.049134
C	-4.227219	-3.523757	-2.661525
C	-2.921483	-3.886813	-2.338896
C	-1.918385	-2.926487	-2.399064
C	-2.201132	-1.612922	-2.775218
C	-3.523452	-1.294568	-3.095850
C	-4.550374	-2.228743	-3.046565
I	-0.683176	-0.171079	-2.854323
N	3.411501	0.386480	1.379586
C	4.382376	0.518264	2.000349
C	5.604126	0.684747	2.780174
H	6.054189	1.660744	2.577482
H	5.385307	0.617100	3.849608
H	6.328513	-0.093189	2.522828
C	0.078493	0.593532	-7.253021
S	-1.536634	0.430233	-6.347889
O	-1.203154	-0.646505	-5.351612
O	-1.738773	1.761167	-5.754856
O	-2.479532	0.002904	-7.389376
F	0.430406	-0.592427	-7.877271
F	0.008140	1.578016	-8.225443
F	1.108126	0.932096	-6.385911
F	-5.209706	-4.484253	-2.593530
F	-2.626638	-5.177952	-1.964950
F	-0.630474	-3.299361	-2.085282
F	-3.827666	-0.004705	-3.487289
H	-5.566705	-1.959242	-3.298230

^{6}PC$_{(d)}$

Fe	1.251405	0.118554	-0.150452
N	1.027527	2.137046	0.277218
C	0.260818	2.672912	1.292352
C	0.177146	4.110095	1.118612
C	0.888847	4.423283	-0.004695
C	1.425441	3.183536	-0.531522
H	-0.355934	4.787037	1.767389
H	1.039899	5.401010	-0.434186
C	2.243882	3.079620	-1.669729
N	2.586423	0.616270	-1.670390
C	2.803796	1.890497	-2.168924
C	3.746306	1.816968	-3.265237
C	4.109073	0.505558	-3.402616
C	3.385073	-0.247804	-2.401095
H	4.097376	2.657152	-3.843253
H	4.804549	0.088930	-4.113933
C	3.485070	-1.636105	-2.205462
N	1.937968	-1.841461	-0.273191
C	2.797893	-2.366898	-1.220678
C	2.904390	-3.798799	-1.026651
C	2.118675	-4.121758	0.043536
C	1.521128	-2.892513	0.524602
H	3.502976	-4.466292	-1.626180
H	1.965266	-5.099211	0.472796
C	0.688401	-2.794342	1.652791
N	0.355372	-0.333690	1.657879
C	0.156213	-1.601153	2.172525
C	-0.667874	-1.507560	3.360557
C	-0.949485	-0.184328	3.554741
C	-0.305786	0.553139	2.486360
H	-0.985165	-2.340867	3.967363
H	-1.536668	0.251260	4.347708
C	-0.357279	1.948534	2.326240
O	-0.339921	-0.016269	-1.194180
C	-1.146085	2.727739	3.336806
C	-2.517922	2.991403	3.178194
C	-0.566084	3.244243	4.508536
C	-3.270686	3.710571	4.102405
C	-1.278676	3.968709	5.460205
C	-2.641509	4.200918	5.250805
H	-4.324882	3.884273	3.929975
H	-0.781300	4.343370	6.345357
H	-3.211987	4.762681	5.980942
C	0.384461	-4.061584	2.398179
C	-0.697729	-4.895437	2.067119
C	1.165501	-4.494874	3.484883
C	-0.998954	-6.068107	2.754845
C	0.902374	-5.659001	4.201313
C	-0.190908	-6.447731	3.830512
H	-1.846216	-6.672078	2.457147
H	1.537203	-5.944667	5.029938
H	-0.411219	-7.356918	4.377286
C	4.421621	-2.393631	-3.100370
C	4.033602	-2.890347	-4.357132
C	5.754620	-2.654978	-2.735916
C	4.889897	-3.597371	-5.197122
C	6.645129	-3.357839	-3.542638
C	6.204161	-3.831412	-4.782155
H	4.537951	-3.957872	-6.155012
H	7.661029	-3.530592	-3.211861
H	6.883628	-4.380178	-5.423467
C	2.566755	4.349345	-2.401292
C	1.793784	4.802788	-3.484808
C	3.656382	5.167008	-2.054779
C	2.068007	5.976497	-4.181242
C	3.968903	6.348127	-2.722466
C	3.165049	6.751682	-3.793057
H	1.439338	6.279418	-5.008465
H	4.821197	6.939800	-2.414538
H	3.393342	7.668188	-4.324151
Cl	-3.382665	2.369523	1.689886
Cl	1.214898	2.962916	4.824202
Cl	6.380499	-2.046814	-1.126505
Cl	2.325897	-2.606355	-4.944545
Cl	-1.778896	-4.449290	0.661427
Cl	2.612147	-3.500348	4.003419
Cl	4.738376	4.675055	-0.662725
Cl	0.350885	3.817743	-4.027901
C	-4.976301	-2.353427	-2.158821
C	-3.909644	-3.246463	-2.239293
C	-2.637426	-2.757356	-2.506612
C	-2.417352	-1.391670	-2.685828
C	-3.513342	-0.528935	-2.594968
C	-4.798999	-0.986813	-2.336092
I	-0.497202	-0.650705	-3.013489
N	3.398486	0.399307	1.359695
C	4.335178	0.540767	2.029493
C	5.513443	0.719384	2.872010
H	5.772105	1.779608	2.945091
H	5.323033	0.337425	3.879013
H	6.367495	0.180895	2.451360
C	-0.365736	0.121065	-7.088870
S	-1.658667	-1.015730	-6.386542
O	-0.885919	-1.665586	-5.257455
O	-2.719186	-0.107142	-5.932613
O	-1.960002	-1.943561	-7.480067
F	0.716895	-0.586118	-7.580399
F	-0.880080	0.886876	-8.119253
F	0.106952	0.987817	-6.109522
F	-6.229018	-2.853225	-1.892626
F	-4.103109	-4.593767	-2.036948
F	-1.592737	-3.650081	-2.584317
F	-3.314377	0.826397	-2.760467
H	-5.633999	-0.303648	-2.270084

^{2}RC$_{(e)}$

Fe	1.657544	0.187191	-0.298061
N	1.150891	2.132876	-0.064020
C	0.309933	2.664500	0.878595
C	0.123073	4.080514	0.647782
C	0.851045	4.398034	-0.459973
C	1.504385	3.182360	-0.893128
H	-0.488276	4.734295	1.247954
H	0.951075	5.361377	-0.932752
C	2.407837	3.109128	-1.955504
N	2.986717	0.714780	-1.729606
C	3.125702	1.948170	-2.310304
C	4.154439	1.915682	-3.327039
C	4.647450	0.645101	-3.347091
C	3.906143	-0.106538	-2.358365
H	4.460351	2.754326	-3.930807
H	5.429673	0.247730	-3.973067
C	4.076088	-1.471236	-2.117246

N	2.325794	-1.720545	-0.386485
C	3.302152	-2.221459	-1.207705
C	3.420577	-3.653067	-1.037252
C	2.489716	-4.017134	-0.110336
C	1.815472	-2.805888	0.302597
H	4.116705	-4.287382	-1.561198
H	2.285343	-5.004407	0.270743
C	0.831929	-2.750947	1.292766
N	0.507780	-0.299156	1.296473
C	0.251349	-1.558723	1.772670
C	-0.676806	-1.500699	2.880937
C	-0.967134	-0.184097	3.082341
C	-0.236917	0.562801	2.081739
H	-1.043517	-2.351172	3.432079
H	-1.618686	0.244440	3.826334
C	-0.321873	1.947012	1.915251
O	0.467719	-0.085465	-1.360551
C	-1.160834	2.724367	2.884289
C	-2.534004	2.940335	2.680784
C	-0.613482	3.287574	4.048426
C	-3.322604	3.666333	3.568444
C	-1.366875	4.019039	4.961353
C	-2.730533	4.207153	4.714208
H	-4.377155	3.806208	3.369698
H	-0.900207	4.433003	5.845658
H	-3.331465	4.774604	5.414738
C	0.387798	-4.041184	1.912005
C	-0.666655	-4.794278	1.370124
C	0.994615	-4.570491	3.062689
C	-1.101415	-5.994352	1.923827
C	0.590789	-5.766632	3.648277
C	-0.465261	-6.479168	3.070997
H	-1.918897	-6.538951	1.469772
H	1.090071	-6.134865	4.535005
H	-0.791980	-7.412042	3.514674
C	5.136981	-2.196644	-2.888440
C	4.890880	-2.766878	-4.148326
C	6.439266	-2.350430	-2.385402
C	5.866044	-3.448991	-4.870227
C	7.442575	-3.023276	-3.075542
C	7.148045	-3.575589	-4.326205
H	5.629178	-3.872539	-5.837504
H	8.431983	-3.114317	-2.646813
H	7.917464	-4.103662	-4.876619
C	2.670505	4.357479	-2.742254
C	1.955981	4.656452	-3.914321
C	3.642867	5.293999	-2.354582
C	2.179425	5.812383	-4.657053
C	3.897074	6.460021	-3.069896
C	3.155626	6.716820	-4.227690
H	1.603077	6.002135	-5.553230
H	4.657210	7.152251	-2.732089
H	3.340558	7.620630	-4.795891
Cl	-3.329179	2.236244	1.198367
Cl	1.166203	3.057120	4.395608
Cl	6.852810	-1.637434	-0.754048
Cl	3.230102	-2.611495	-4.887981
Cl	-1.514987	-4.184291	-0.127831
Cl	2.380461	-3.663592	3.835692
Cl	4.633785	4.979623	-0.850824
Cl	0.685642	3.488104	-4.506563
C	-5.644803	-2.754135	0.416283
C	-5.956923	-3.456347	-0.742090
C	-5.343266	-3.113383	-1.943105
C	-4.413113	-2.075785	-2.024877
C	-4.119838	-1.387331	-0.846204
C	-4.721934	-1.715742	0.364113
I	-3.486606	-1.568873	-3.845402
N	3.230366	0.550290	1.112476
C	4.082665	0.743778	1.869170
C	5.157150	0.985958	2.821286
H	5.628663	1.952220	2.620917
H	4.763555	0.991818	3.841621
H	5.915576	0.201901	2.741492
C	0.248014	-0.524888	-5.925049
S	-1.336599	0.136658	-6.643957
O	-2.299668	-0.953081	-6.324480
O	-1.539756	1.390548	-5.894197
O	-1.018210	0.272625	-8.075678
F	0.584842	-1.757945	-6.475082
F	1.313645	0.333924	-6.156176
F	0.151215	-0.704108	-4.550803
F	-3.208687	-0.348768	-0.852924
F	-4.407042	-1.024439	1.512945
F	-6.243930	-3.086196	1.608554
F	-6.869452	-4.486580	-0.693886
F	-5.682573	-3.837338	-3.068087

$^4RC_{(e)}$

Fe	1.900390	0.025932	-0.189373
N	1.215156	1.925879	-0.021508
C	0.298514	2.399682	0.889026
C	-0.021226	3.781576	0.607381
C	0.715153	4.141776	-0.481633
C	1.489598	2.982022	-0.864145
H	-0.713328	4.387619	1.168788
H	0.739511	5.098084	-0.978002
C	2.410000	2.965594	-1.921275
N	3.123690	0.607178	-1.697868
C	3.178376	1.848705	-2.288697
C	4.157733	1.856515	-3.352673
C	4.695759	0.605120	-3.401366
C	4.042990	-0.170500	-2.370355
H	4.398310	2.705342	-3.971640
H	5.459401	0.237511	-4.067106
C	4.310785	-1.522380	-2.116371
N	2.741102	-1.818095	-0.227482
C	3.678753	-2.284390	-1.119828
C	3.936951	-3.688513	-0.889963
C	3.142323	-4.069623	0.150002
C	2.402765	-2.897290	0.561308
H	4.630917	-4.294131	-1.449505
H	3.066040	-5.044904	0.602337
C	1.497537	-2.874347	1.630710
N	0.862791	-0.488829	1.473702
C	0.802355	-1.732203	2.060316
C	-0.083633	-1.706436	3.202751
C	-0.559306	-0.432952	3.302819
C	0.026492	0.318313	2.215234
H	-0.303525	-2.547232	3.840113
H	-1.242524	-0.036967	4.036202
C	-0.250892	1.667239	1.953968
O	0.701360	-0.406573	-1.186421
C	-1.196862	2.378607	2.873512
C	-2.588223	2.346456	2.683143
C	-0.740632	3.120572	3.975366
C	-3.478200	3.008998	3.523823
C	-1.597042	3.795758	4.839341
C	-2.974813	3.737424	4.606047
H	-4.542893	2.957212	3.337025
H	-1.198330	4.353964	5.676332
H	-3.655722	4.258129	5.268670
C	1.261055	-4.154216	2.373781
C	0.247337	-5.050809	1.997946
C	2.034133	-4.528288	3.484827
C	0.005295	-6.243696	2.672157
C	1.825216	-5.711434	4.187088
C	0.802428	-6.571101	3.773710
H	-0.788094	-6.903046	2.345216
H	2.446900	-5.956843	5.038198
H	0.626626	-7.496009	4.309869
C	5.340528	-2.205488	-2.964343
C	5.014296	-2.812108	-4.188526
C	6.688228	-2.281822	-2.576851
C	5.956299	-3.457925	-4.983971
C	7.660524	-2.916796	-3.343262
C	7.286103	-3.508405	-4.554091
H	5.657744	-3.912298	-5.919703
H	8.687440	-2.948542	-3.003403
H	8.030587	-4.007606	-5.162685
C	2.609293	4.235502	-2.692343
C	1.888125	4.516703	-3.864497
C	3.528580	5.214914	-2.281601
C	2.057995	5.694425	-4.587255
C	3.728430	6.403479	-2.976510
C	2.983812	6.640365	-4.136571
H	1.478731	5.868869	-5.484672
H	4.449412	7.128171	-2.621394
H	3.126698	7.561198	-4.689371
Cl	-3.275694	1.398543	1.284533
Cl	1.054507	3.207183	4.308959
Cl	7.206196	-1.513607	-1.001200
Cl	3.288015	-2.753889	-4.775726
Cl	-0.808337	-4.647263	0.562517
Cl	3.376500	-3.423224	4.047787
Cl	4.520626	4.929153	-0.772693
Cl	0.680909	3.297667	-4.482900
C	-7.597230	-1.516476	-0.682739
C	-7.935926	-1.919039	-1.969544
C	-7.002033	-1.809162	-2.995495
C	-5.720075	-1.303641	-2.773014
C	-5.408075	-0.906768	-1.471236

C	-6.327468	-1.008335	-0.432336
I	-4.311512	-1.145705	-4.329328
N	3.482034	0.601949	1.135567
C	4.335860	0.919267	1.847392
C	5.410798	1.319591	2.744035
H	5.779299	2.312718	2.472056
H	5.050382	1.349297	3.776172
H	6.239367	0.608512	2.681722
C	-0.061148	-0.833386	-5.350325
S	-1.282686	-0.056091	-6.520196
O	-2.432170	-0.998888	-6.436573
O	-1.518106	1.268980	-5.916635
O	-0.566299	-0.073301	-7.807116
F	0.299170	-2.112655	-5.761855
F	1.106968	-0.087038	-5.259208
F	-0.582320	-0.945211	-4.068168
F	-8.512934	-1.620334	0.337453
F	-9.192496	-2.422701	-2.220922
F	-7.381046	-2.220534	-4.257084
F	-5.990390	-0.605935	0.841101
F	-4.157854	-0.394687	-1.179590

$^{6}RC_{(e)}$

Fe	1.863222	-0.001874	-0.239242
N	1.202206	1.964233	-0.031620
C	0.274543	2.416923	0.874659
C	-0.028862	3.808070	0.596539
C	0.730805	4.175491	-0.477822
C	1.505856	3.012456	-0.866809
H	-0.724592	4.418971	1.148739
H	0.765784	5.139684	-0.958754
C	2.443050	2.974491	-1.923773
N	3.162671	0.609802	-1.752088
C	3.212093	1.857606	-2.323613
C	4.187563	1.855906	-3.397644
C	4.713285	0.596487	-3.457336
C	4.063739	-0.183696	-2.420975
H	4.436652	2.701841	-4.017761
H	5.469085	0.230993	-4.133620
C	4.322187	-1.544308	-2.142757
N	2.786067	-1.871554	-0.226351
C	3.716641	-2.323080	-1.129656
C	3.991603	-3.724759	-0.876065
C	3.213989	-4.098937	0.183111
C	2.458135	-2.928944	0.588165
H	4.685031	-4.336456	-1.430305
H	3.160759	-5.070056	0.648259
C	1.541674	-2.882658	1.662201
N	0.838030	-0.512619	1.504387
C	0.805949	-1.754127	2.090721
C	-0.099382	-1.726872	3.224038
C	-0.602268	-0.459110	3.302508
C	-0.014764	0.298364	2.213687
H	-0.315003	-2.560315	3.872958
H	-1.302287	-0.073674	4.026089
C	-0.284234	1.655409	1.926804
O	0.670043	-0.443385	-1.233442
C	-1.248668	2.361996	2.833623
C	-2.637386	2.316633	2.627325
C	-0.812808	3.111325	3.938853
C	-3.543348	2.974365	3.454680
C	-1.685519	3.782062	4.789974
C	-3.059775	3.711275	4.540113
H	-4.605189	2.912316	3.255142
H	-1.301856	4.346160	5.630048
H	-3.753233	4.228428	5.192438
C	1.325793	-4.158068	2.422455
C	0.331992	-5.079636	2.053635
C	2.100194	-4.502544	3.541964
C	0.110152	-6.268290	2.742158
C	1.911355	-5.680466	4.258675
C	0.907994	-6.565678	3.851670
H	-0.668403	-6.947387	2.419987
H	2.533593	-5.902342	5.115829
H	0.747810	-7.486940	4.398906
C	5.343225	-2.231418	-3.000917
C	5.001210	-2.845384	-4.217023
C	6.696403	-2.302948	-2.632242
C	5.932912	-3.494270	-5.022048
C	7.659038	-2.940680	-3.408643
C	7.268721	-3.540058	-4.610601
H	5.622013	-3.954442	-5.950913
H	8.690732	-2.968511	-3.083168
H	8.005500	-4.041487	-5.226704
C	2.657338	4.251426	-2.682367
C	1.935218	4.556055	-3.848036
C	3.592073	5.212888	-2.264722
C	2.119656	5.738841	-4.558879
C	3.806744	6.405955	-2.947503
C	3.061263	6.666110	-4.102009
H	1.539398	5.931539	-5.451930
H	4.539462	7.116234	-2.587288
H	3.215521	7.590605	-4.645570
Cl	-3.300407	1.356453	1.225219
Cl	0.977040	3.212831	4.296895
Cl	7.235442	-1.524095	-1.068706
Cl	3.266574	-2.792218	-4.780043
Cl	-0.724847	-4.716324	0.608107
Cl	3.418290	-3.364231	4.096559
Cl	4.584414	4.896675	-0.761853
Cl	0.706875	3.361357	-4.472800
C	-7.678333	-1.503379	-0.706420
C	-8.022796	-1.844794	-2.009338
C	-7.078922	-1.730801	-3.025707
C	-5.781163	-1.281013	-2.777372
C	-5.463390	-0.946778	-1.459665
C	-6.392392	-1.052658	-0.429832
I	-4.356659	-1.107121	-4.317119
N	3.457486	0.592412	1.101862
C	4.307855	0.918133	1.814125
C	5.378026	1.329335	2.711250
H	5.718053	2.336979	2.456014
H	5.023986	1.329560	3.746026
H	6.224514	0.641733	2.629574
C	-0.097543	-0.797841	-5.245371
S	-1.284428	0.006296	-6.433101
O	-2.443736	-0.927146	-6.388273
O	-1.522662	1.325823	-5.818325
O	-0.538575	-0.001100	-7.703266
F	0.257284	-2.075943	-5.665472
F	1.076584	-0.066249	-5.118084
F	-0.648685	-0.919777	-3.976822
F	-8.604345	-1.611719	0.303949
F	-9.295246	-2.292306	-2.285896
F	-7.464411	-2.079692	-4.304018
F	-6.048152	-0.712406	0.859630
F	-4.195974	-0.495933	-1.142012

$^{2}TS_{(e)}$

Fe	1.390656	0.090153	0.014644
N	0.982233	2.043542	0.339099
C	0.232473	2.574005	1.371165
C	0.120167	4.008103	1.213416
C	0.796491	4.337088	0.077072
C	1.331388	3.106480	-0.463930
H	-0.409547	4.667214	1.882016
H	0.924459	5.315255	-0.357439
C	2.108833	3.034504	-1.628121
N	2.441189	0.573533	-1.632813
C	2.643545	1.852814	-2.145322
C	3.554572	1.798185	-3.264657
C	3.952497	0.500810	-3.397546
C	3.278635	-0.259400	-2.371778
H	3.861817	2.645819	-3.855555
H	4.642576	0.092847	-4.118274
C	3.462962	-1.626876	-2.155913
N	1.967143	-1.832629	-0.194718
C	2.815789	-2.354820	-1.148881
C	2.952796	-3.782420	-0.966018
C	2.179282	-4.120212	0.104161
C	1.573483	-2.899667	0.590380
H	3.555064	-4.432857	-1.579401
H	2.033481	-5.099036	0.531564
C	0.738890	-2.839033	1.713663
N	0.394072	-0.392770	1.726349
C	0.188072	-1.659792	2.227367
C	-0.661671	-1.597623	3.399808
C	-0.960132	-0.284617	3.602564
C	-0.299322	0.463900	2.552270
H	-0.978176	-2.446516	3.984103
H	-1.567646	0.143548	4.383444
C	-0.365994	1.854804	2.412038
O	-0.090379	-0.157512	-0.726643
C	-1.150243	2.622363	3.433373
C	-2.522818	2.882323	3.282053
C	-0.560368	3.125728	4.604904
C	-3.270120	3.590540	4.218634
C	-1.269031	3.839300	5.567144
C	-2.633716	4.070505	5.367661
H	-4.325744	3.763847	4.055107
H	-0.767375	4.206432	6.452986
H	-3.200617	4.623822	6.106857
C	0.446593	-4.117696	2.441373

C	-0.648522	-4.936052	2.116598
C	1.251499	-4.569068	3.501525
C	-0.936157	-6.120607	2.789246
C	1.000805	-5.746529	4.199685
C	-0.103345	-6.524328	3.837132
H	-1.792803	-6.715652	2.500613
H	1.652374	-6.050145	5.008649
H	-0.313886	-7.443723	4.370397
C	4.436203	-2.354718	-3.034629
C	4.069543	-2.923360	-4.266406
C	5.784629	-2.511379	-2.668857
C	4.967399	-3.603347	-5.085014
C	6.714536	-3.182552	-3.456994
C	6.297252	-3.731627	-4.673496
H	4.634440	-4.024382	-6.024748
H	7.741877	-3.274182	-3.129404
H	7.007701	-4.257751	-5.299922
C	2.420089	4.316006	-2.341583
C	1.604910	4.812262	-3.372727
C	3.542464	5.098905	-2.022045
C	1.872468	5.998591	-4.049505
C	3.848515	6.290394	-2.673166
C	3.004197	6.738873	-3.693809
H	1.211905	6.337780	-4.836748
H	4.726410	6.856392	-2.390149
H	3.227606	7.664377	-4.210990
Cl	-3.387779	2.269851	1.791932
Cl	1.221971	2.840709	4.899473
Cl	6.370931	-1.802080	-1.087756
Cl	2.343827	-2.775610	-4.843436
Cl	-1.756204	-4.446613	0.750386
Cl	2.704903	-3.578849	4.005228
Cl	4.669461	4.544684	-0.692563
Cl	0.115520	3.871516	-3.859415
C	-4.798110	-1.605373	-2.195847
C	-3.748402	-2.507758	-2.052715
C	-2.450129	-2.104771	-2.339412
C	-2.171306	-0.803606	-2.760999
C	-3.237980	0.086854	-2.897956
C	-4.543725	-0.306087	-2.624550
I	-0.224003	-0.217127	-3.149324
N	3.105774	0.365266	1.165622
C	4.060103	0.505815	1.802225
C	5.264330	0.681084	2.601143
H	5.354080	1.721373	2.926392
H	5.227616	0.038532	3.485273
H	6.148301	0.419236	2.012684
C	-0.238601	-0.601164	-7.478958
S	-1.748593	-1.455633	-6.804498
O	-1.191994	-2.228264	-5.670024
O	-2.617073	-0.321130	-6.428503
O	-2.203495	-2.259018	-7.955789
F	0.741132	-1.509758	-7.858135
F	-0.539339	0.172129	-8.592237
F	0.340282	0.250431	-6.538076
F	-6.082215	-1.996202	-1.914429
F	-3.995431	-3.788270	-1.613500
F	-5.581588	0.583743	-2.766319
F	-1.434157	-3.022120	-2.192382
F	-3.017097	1.382509	-3.306478

$^{4}TS_{(e)}$

Fe	1.490240	-0.059883	-0.070845
N	1.038041	1.900315	0.140927
C	0.150248	2.449012	1.046588
C	0.027648	3.871911	0.819335
C	0.838829	4.178827	-0.230810
C	1.463892	2.946326	-0.659055
H	-0.596578	4.539299	1.391515
H	1.003096	5.144921	-0.680375
C	2.355219	2.858654	-1.728276
N	2.746499	0.414126	-1.586412
C	2.935156	1.662947	-2.155082
C	3.841453	1.561300	-3.275496
C	4.195208	0.248895	-3.386875
C	3.515180	-0.464377	-2.330759
H	4.162738	2.387077	-3.889803
H	4.860159	-0.197712	-4.108554
C	3.655619	-1.833953	-2.100131
N	2.180693	-1.955121	-0.110363
C	3.027732	-2.510130	-1.054959
C	3.187978	-3.924951	-0.800311
C	2.433421	-4.222531	0.293588
C	1.796017	-2.994543	0.715177
H	3.800793	-4.593161	-1.383710
H	2.310484	-5.180393	0.772972
C	0.908209	-2.905515	1.787333
N	0.441144	-0.477425	1.576345
C	0.270999	-1.723057	2.162038
C	-0.681477	-1.630640	3.243061
C	-1.092209	-0.332317	3.307619
C	-0.391904	0.388484	2.271349
H	-0.993056	-2.454015	3.865471
H	-1.801103	0.103313	3.993242
C	-0.535418	1.756900	2.045481
O	0.190202	-0.384577	-1.090465
C	-1.460562	2.529926	2.935596
C	-2.806315	2.765538	2.604091
C	-1.037805	3.071912	4.162306
C	-3.679638	3.479615	3.420113
C	-1.875394	3.791951	5.009359
C	-3.206276	3.993696	4.631058
H	-4.707354	3.631468	3.116851
H	-1.497646	4.187607	5.943194
H	-3.872776	4.551496	5.278132
C	0.616776	-4.148741	2.571981
C	-0.416129	-5.036947	2.224019
C	1.362794	-4.506718	3.708745
C	-0.700635	-6.194982	2.942790
C	1.114270	-5.654184	4.456541
C	0.072588	-6.501386	4.066545
H	-1.508654	-6.844367	2.631925
H	1.720215	-5.882078	5.323793
H	-0.135730	-7.398836	4.636900
C	4.534351	-2.619162	-3.026199
C	4.042463	-3.211831	-4.202363
C	5.905027	-2.812258	-2.781453
C	4.837702	-3.943724	-5.079626
C	6.738237	-3.536269	-3.629772
C	6.195409	-4.104416	-4.786386
H	4.407211	-4.378875	-5.972163
H	7.787798	-3.653995	-3.393591
H	6.829320	-4.671072	-5.458056
C	2.702629	4.117165	-2.465090
C	1.976633	4.558993	-3.585220
C	3.777305	4.937636	-2.080132
C	2.282819	5.726308	-4.279657
C	4.119012	6.112293	-2.744453
C	3.361988	6.505517	-3.852402
H	1.690970	6.020893	-5.136546
H	4.957210	6.706956	-2.405269
H	3.613056	7.416874	-4.382053
Cl	-3.469020	2.119915	1.026653
Cl	0.697954	2.838502	4.693434
Cl	6.657174	-2.084293	-1.280336
Cl	2.272034	-3.025187	-4.623704
Cl	-1.454290	-4.682608	0.761128
Cl	2.737040	-3.427830	4.253762
Cl	4.796024	4.459995	-0.636142
Cl	0.561298	3.571750	-4.187121
C	-4.716321	-1.972133	-1.189191
C	-3.700350	-2.833169	-1.594200
C	-2.559134	-2.320856	-2.198329
C	-2.412315	-0.947373	-2.414702
C	-3.444365	-0.099204	-2.003001
C	-4.588285	-0.601473	-1.395090
I	-0.694541	-0.189718	-3.272027
N	3.246586	0.388641	1.283065
C	4.145632	0.638844	1.967611
C	5.277745	0.955572	2.828861
H	5.818184	1.822900	2.439359
H	4.931354	1.184317	3.840718
H	5.966112	0.107102	2.877713
C	-0.407042	0.623625	-7.195716
S	-2.154690	0.862907	-6.602120
O	-2.292767	-0.262486	-5.624757
O	-2.119446	2.204770	-5.997685
O	-2.956923	0.699754	-7.824195
F	-0.235997	-0.606661	-7.808524
F	-0.031398	1.602751	-8.097762
F	0.494473	0.677940	-6.127480
F	-5.837647	-2.473051	-0.584312
F	-3.815090	-4.184273	-1.370800
F	-1.564425	-3.195774	-2.565746
F	-3.339862	1.261538	-2.173948
F	-5.578218	0.253501	-0.976479

$^{6}TS_{(e)}$

Fe	1.430247	-0.104518	-0.180746
N	1.036037	1.945649	0.093342
C	0.176169	2.478596	1.016328
C	0.070836	3.911737	0.807999
C	0.879003	4.220348	-0.250966

C	1.486005	2.978895	-0.696411
H	-0.532625	4.588854	1.391201
H	1.048741	5.193161	-0.684087
C	2.400878	2.854288	-1.766204
N	2.830969	0.414058	-1.673858
C	3.028947	1.664047	-2.208692
C	4.001367	1.579584	-3.282394
C	4.381513	0.268017	-3.372741
C	3.646564	-0.455075	-2.351652
H	4.352093	2.405878	-3.879925
H	5.096535	-0.161424	-4.056205
C	3.779085	-1.840366	-2.075346
N	2.250532	-2.033117	-0.134108
C	3.141803	-2.560054	-1.042614
C	3.324158	-3.974590	-0.766413
C	2.537167	-4.276966	0.308714
C	1.861651	-3.051047	0.698395
H	3.968175	-4.642540	-1.315874
H	2.426199	-5.234892	0.791218
C	0.935097	-2.929999	1.763198
N	0.414974	-0.515016	1.590095
C	0.270266	-1.753649	2.171920
C	-0.672298	-1.656772	3.274737
C	-1.076836	-0.355005	3.343538
C	-0.385610	0.364674	2.285982
H	-0.978521	-2.472455	3.910148
H	-1.771741	0.079146	4.044519
C	-0.502013	1.745923	2.025188
O	-0.002373	-0.546800	-1.153793
C	-1.425202	2.525872	2.915087
C	-2.756711	2.794648	2.555813
C	-1.012300	3.034082	4.158032
C	-3.630866	3.511113	3.368006
C	-1.852983	3.755674	5.000291
C	-3.171481	3.991396	4.598396
H	-4.648697	3.690591	3.047054
H	-1.486522	4.127261	5.948370
H	-3.839624	4.550618	5.242392
C	0.628996	-4.181437	2.533309
C	-0.394427	-5.062921	2.146325
C	1.348362	-4.545440	3.683541
C	-0.695877	-6.227299	2.846885
C	1.080563	-5.700170	4.412752
C	0.049220	-6.543267	3.987279
H	-1.495079	-6.874285	2.509433
H	1.664153	-5.936870	5.292847
H	-0.173085	-7.446122	4.543494
C	4.698869	-2.617766	-2.971197
C	4.243878	-3.213496	-4.159237
C	6.061050	-2.795131	-2.679663
C	5.072646	-3.939367	-5.009361
C	6.925255	-3.512947	-3.501399
C	6.422130	-4.087220	-4.673101
H	4.674223	-4.379898	-5.914033
H	7.968156	-3.621117	-3.233364
H	7.081252	-4.649177	-5.323982
C	2.753219	4.115174	-2.501253
C	2.055726	4.526364	-3.649340
C	3.797187	4.957007	-2.083826
C	2.362167	5.693649	-4.342933
C	4.136547	6.132047	-2.748033
C	3.409548	6.498832	-3.885028
H	1.794666	5.968395	-5.222544
H	4.950440	6.747001	-2.386663
H	3.659818	7.410550	-4.414251
Cl	-3.387952	2.191216	0.950529
Cl	0.709539	2.756686	4.707869
Cl	6.750026	-2.053837	-1.156781
Cl	2.484582	-3.037984	-4.624335
Cl	-1.386743	-4.684995	0.658843
Cl	2.705842	-3.466433	4.263850
Cl	4.771482	4.503292	-0.603825
Cl	0.686295	3.497213	-4.282009
C	-4.959529	-1.967881	-1.180330
C	-3.927508	-2.827493	-1.543785
C	-2.774322	-2.315781	-2.126484
C	-2.625194	-0.946485	-2.357402
C	-3.672505	-0.101549	-1.986254
C	-4.831686	-0.600398	-1.402448
I	-0.862566	-0.192783	-3.151448
N	3.293308	0.394231	1.319500
C	4.181693	0.660487	2.014462
C	5.299918	0.996324	2.888509
H	5.841178	1.862120	2.496672
H	4.938504	1.235782	3.892630
H	5.993599	0.153680	2.959000
C	-0.749692	0.570741	-7.175619
S	-2.469614	1.070259	-6.665818
O	-2.790627	0.062728	-5.624297
O	-2.269983	2.446333	-6.170635
O	-3.229983	0.936535	-7.922165
F	-0.703950	-0.742416	-7.623311
F	-0.256579	1.375896	-8.190398
F	0.150934	0.665363	-6.109240
F	-6.096587	-2.467249	-0.599162
F	-4.038606	-4.177162	-1.303468
F	-1.767173	-3.195709	-2.454860
F	-3.570028	1.261024	-2.164866
F	-5.838778	0.255575	-1.025308

$^{2}PC_{(e)}$

Fe	1.357237	0.080996	-0.004262
N	0.940800	2.030679	0.277780
C	0.248777	2.596198	1.331442
C	0.084001	4.016617	1.105669
C	0.660079	4.297995	-0.096513
C	1.203044	3.055812	-0.608963
H	-0.416521	4.697844	1.775184
H	0.721321	5.253417	-0.592599
C	1.935195	2.958505	-1.798024
N	2.379857	0.514873	-1.702922
C	2.528876	1.781286	-2.261823
C	3.476679	1.725132	-3.348762
C	3.949352	0.444868	-3.411058
C	3.274982	-0.309656	-2.385465
H	3.761850	2.561768	-3.966381
H	4.684202	0.045860	-4.092001
C	3.463238	-1.671468	-2.142765
N	1.878745	-1.843946	-0.241820
C	2.754781	-2.383991	-1.169182
C	2.828335	-3.817080	-0.999236
C	1.992826	-4.141029	0.028729
C	1.419078	-2.905963	0.517965
H	3.432092	-4.482281	-1.595743
H	1.792040	-5.120871	0.431601
C	0.595416	-2.822433	1.644807
N	0.375007	-0.357407	1.697970
C	0.139174	-1.621340	2.196734
C	-0.624040	-1.530493	3.426795
C	-0.830694	-0.206536	3.670234
C	-0.214788	0.524043	2.580867
H	-0.944637	-2.370548	4.022099
H	-1.355854	0.240279	4.499311
C	-0.266408	1.912976	2.436233
O	-0.229660	-0.100631	-0.869387
C	-0.955645	2.709870	3.501659
C	-2.335884	2.976110	3.472304
C	-0.263460	3.243020	4.602684
C	-2.993462	3.713432	4.453244
C	-0.878224	3.985853	5.606761
C	-2.254407	4.219903	5.526791
H	-4.058985	3.888738	4.381144
H	-0.296391	4.373029	6.433052
H	-2.749906	4.795771	6.299435
C	0.241093	-4.097201	2.350732
C	-0.905039	-4.844468	2.030007
C	1.034332	-4.628079	3.383813
C	-1.252726	-6.028771	2.674338
C	0.726926	-5.807518	4.055945
C	-0.427041	-6.509810	3.694833
H	-2.148259	-6.563667	2.386016
H	1.373722	-6.170640	4.843991
H	-0.681798	-7.429736	4.207587
C	4.468190	-2.412102	-2.971632
C	4.157673	-2.975556	-4.221821
C	5.794811	-2.593852	-2.542186
C	5.082040	-3.671708	-4.996268
C	6.751921	-3.281210	-3.282969
C	6.387335	-3.823621	-4.519097
H	4.788799	-4.086737	-5.951815
H	7.759806	-3.390328	-2.904179
H	7.119081	-4.362452	-5.109308
C	2.163514	4.214427	-2.584973
C	1.319049	4.601008	-3.640269
C	3.233845	5.087113	-2.319596
C	1.509721	5.761323	-4.386003
C	3.463539	6.256678	-3.038733
C	2.591813	6.591865	-4.079373
H	0.828015	6.011543	-5.188500
H	4.304456	6.892073	-2.793027
H	2.755526	7.498556	-4.649719
Cl	-3.342196	2.334667	2.084858

Cl	1.538915	2.958827	4.748339
Cl	6.319971	-1.896723	-0.933193
Cl	2.465194	-2.795145	-4.885515
Cl	-2.015706	-4.255528	0.700685
Cl	2.554819	-3.744150	3.891076
Cl	4.403560	4.688508	-0.969125
Cl	-0.110223	3.545908	-4.072997
C	-4.805638	-2.082601	-2.315563
C	-3.787137	-3.021719	-2.449069
C	-2.471706	-2.594067	-2.591295
C	-2.156784	-1.236341	-2.602134
C	-3.188737	-0.308446	-2.465453
C	-4.509035	-0.723014	-2.325134
I	-0.176122	-0.591441	-2.769071
N	3.073454	0.352922	1.083485
C	4.043594	0.517590	1.689825
C	5.265919	0.727005	2.452435
H	5.477911	1.796545	2.538162
H	5.160644	0.308628	3.457383
H	6.109707	0.240321	1.955330
C	0.340314	0.150161	-6.931849
S	-1.198704	-0.633187	-6.243010
O	-0.621395	-1.480573	-5.136164
O	-1.991114	0.509466	-5.765624
O	-1.731846	-1.417509	-7.362424
F	1.173778	-0.793674	-7.507309
F	0.034946	1.092866	-7.898338
F	1.059329	0.790390	-5.929151
F	-6.103194	-2.497685	-2.171197
F	-4.080326	-4.363416	-2.420188
F	-5.517081	0.199968	-2.193941
F	-1.483305	-3.542946	-2.717459
F	-2.920792	1.040522	-2.468848

$^{4}PC_{(e)}$

Fe	1.279687	0.150239	0.007790
N	1.020624	2.127125	0.330610
C	0.263535	2.710109	1.333067
C	0.173619	4.135747	1.117496
C	0.876217	4.414163	-0.017184
C	1.406215	3.162139	-0.506096
H	-0.356983	4.826609	1.752875
H	1.026901	5.375079	-0.482261
C	2.212271	3.048207	-1.640289
N	2.433496	0.574237	-1.597132
C	2.715794	1.834817	-2.112130
C	3.629644	1.717826	-3.221025
C	3.916651	0.391349	-3.369360
C	3.175480	-0.320823	-2.358378
H	4.009278	2.543752	-3.800868
H	4.572145	-0.064655	-4.093842
C	3.209944	-1.706656	-2.194559
N	1.776900	-1.792726	-0.170713
C	2.524421	-2.378890	-1.180954
C	2.541268	-3.812979	-1.011396
C	1.814090	-4.093587	0.106845
C	1.346024	-2.834398	0.636638
H	3.045428	-4.507959	-1.663506
H	1.614268	-5.060723	0.539478
C	0.613741	-2.711246	1.818295
N	0.356668	-0.244880	1.749776
C	0.174714	-1.489559	2.331495
C	-0.554472	-1.351460	3.569830
C	-0.818658	-0.023388	3.733960
C	-0.250501	0.666075	2.599977
H	-0.824410	-2.164409	4.224528
H	-1.344912	0.449932	4.547300
C	-0.324050	2.046707	2.410960
O	-0.465844	0.022688	-0.967823
C	-1.073009	2.860683	3.421607
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C	-2.495430	4.400663	5.336947
H	-4.231843	4.020737	4.104460
H	-0.591043	4.598924	6.343438
H	-3.038227	4.988159	6.067901
C	0.307236	-3.955317	2.596152
C	-0.892847	-4.669024	2.435479
C	1.202428	-4.487162	3.541351
C	-1.194665	-5.827552	3.146033
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C	-0.265709	-6.314132	4.070675
H	-2.134318	-6.338755	2.981897
H	1.667822	-6.007624	4.990254
H	-0.484107	-7.214597	4.632436
C	4.061628	-2.511215	-3.130024
C	3.599383	-2.967448	-4.377031
C	5.387019	-2.861260	-2.814383
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C	5.689131	-4.041780	-4.884942
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H	7.215802	-3.850796	-3.364545
H	6.309354	-4.626113	-5.554241
C	2.568306	4.300159	-2.383283
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C	3.664034	5.104395	-2.024487
C	2.127254	5.915027	-4.187511
C	4.005851	6.274290	-2.697236
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Cl	0.382419	3.779412	-4.053311
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C	-2.923625	-3.872653	-2.323270
C	-1.916609	-2.915081	-2.388510
C	-2.196604	-1.605680	-2.777492
C	-3.510603	-1.272883	-3.106173
C	-4.526567	-2.220266	-3.045509
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N	3.407769	0.384692	1.377198
C	4.374697	0.518688	2.003505
C	5.591850	0.688300	2.789672
H	6.038184	1.667104	2.592349
H	5.368154	0.616044	3.857791
H	6.321101	-0.085354	2.533181
C	0.068413	0.583121	-7.247348
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O	-1.214216	-0.645726	-5.338904
O	-1.739635	1.762835	-5.746534
O	-2.493352	0.003339	-7.374881
F	0.413528	-0.606441	-7.868053
F	-0.000250	1.564616	-8.222622
F	1.100770	0.920167	-6.383053
F	-5.226066	-4.459188	-2.584301
F	-2.636919	-5.159816	-1.939728
F	-0.631609	-3.288597	-2.068740
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$^{6}PC_{(e)}$

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C	2.811214	1.884071	-2.164508
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C	3.390062	-0.255461	-2.395860
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H	3.503085	-4.474004	-1.618090
H	1.963155	-5.103847	0.480124
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C	0.153860	-1.603428	2.175291
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C	-0.309264	0.551605	2.486077
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H	-1.544678	0.251082	4.344403

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C	1.162448	-4.494856	3.492609
C	-1.000409	-6.070038	2.761855
C	0.898764	-5.658054	4.210351
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H	-1.847012	-6.674792	2.463891
H	1.532580	-5.942276	5.040243
H	-0.414403	-7.356235	4.386970
C	4.425387	-2.402531	-3.093065
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C	5.757820	-2.665353	-2.727602
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C	6.207618	-3.842070	-4.773661
H	4.542212	-3.966986	-6.147676
H	7.663635	-3.542917	-3.202304
H	6.886988	-4.391493	-5.414506
C	2.579839	4.343785	-2.395605
C	1.811348	4.799824	-3.481213
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C	-2.611878	-2.755665	-2.512335
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C	-3.483687	-0.520636	-2.622439
C	-4.764269	-1.001730	-2.372286
I	-0.473049	-0.641462	-3.011954
N	3.389704	0.394894	1.351001
C	4.334446	0.544451	2.007364
C	5.523693	0.734008	2.831664
H	5.770691	1.797007	2.904606
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H	6.377192	0.207277	2.395313
C	-0.455705	0.178477	-7.080183
S	-1.691055	-1.007989	-6.357397
O	-0.868046	-1.642651	-5.254027
O	-2.767958	-0.139969	-5.864509
O	-1.990083	-1.935944	-7.450920
F	0.638593	-0.486370	-7.603223
F	-1.021491	0.934177	-8.090535
F	0.008903	1.052259	-6.103575
F	-6.219003	-2.845074	-1.926763
F	-4.080181	-4.590038	-2.043410
F	-5.829521	-0.138814	-2.304343
F	-1.565435	-3.645697	-2.576564
F	-3.308914	0.831505	-2.791738