Supporting Information

Computational Study of Fluorinated Diglyoxime-Iron Complexes: Tuning the Electrocatalytic Pathways for Hydrogen Evolution

Aparna Karippara Harshan,[†] Brian H. Solis,[†‡] Jay R. Winkler,[§] Harry B. Gray,[§] and Sharon Hammes-Schiffer[†]*

[†]*Department of Chemistry, 600 South Mathews Avenue, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801*

[‡]Current address: *Institut für Chemie, Humboldt Universität zu Berlin, Unter den Linden 6, 10099 Berlin, Germany*

[§]*Beckman Institute, California Institute of Technology, Pasadena, California 91125, United States*

*corresponding author; e-mail: shs3@illinois.edu

Table S1. Comparison of Bond Lengths and Angles for Intermediates of **B** Optimized in Gas Phase and Dichloromethane Solution [a]

	$[Fe^{II}py_2]^0$		$[Fe^{I}py]^-$		$[Fe^{0}py]^{2-}$	
Bond length or angle	Solution	Gas	Solution	Gas	Solution	Gas
Fe-N1(py)	1.99	2.00	1.99	1.99	1.90	1.90
Fe-N2(py)	2.01	2.02	-	-	-	-
Fe-N(1)	1.88	1.89	1.87	1.87	1.85	1.85
Fe-N(2)	1.89	1.89	1.87	1.88	1.85	1.86
Fe-N(3)	1.89	1.89	1.86	1.87	1.86	1.86
Fe-N(4)	1.90	1.90	1.87	1.88	1.86	1.87
N(1)-Fe-N(2)	97.3	96.8	92.4	92.1	93.8	93.1
N(2)-Fe-N(3)	81.9	82.2	81.4	81.7	82.0	82.4
N(3)-Fe-N(4)	97.8	97.6	93.1	93.0	94.5	94.3
N(4)-Fe-N(1)	82.7	83.1	81.9	82.4	82.4	83.0
N(3)-N(4)-N(1)-Fe	–2.7	–2.6	–17.0	–17.5	–13.8	–13.8

[a] Calculations performed with BP86 functional with 6-31+G(d,p) basis set for central part of molecule and 6-31G basis set for C_6F_6 groups and axial pyridine ligands. Bond lengths are given in angstroms and angles are given in degrees.

Table S2. Spin Density at the Fe Center, ρ_{Fe}, and Relative Free Energies for Different Spin States of Intermediates [a]

Catalyst	#pyridines	Charge	S	$<S^2>$	ρ_{Fe}	ΔG (kcal/mol)
A	2	0	0	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)
	2	0	1	2.01 (2.02)	0.70 (0.98)	19.90 (23.83)
	1	0	0	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)
	1	0	1	2.03 (2.04)	1.68 (1.93)	–4.17 (–7.07)
	2	−1	1/2	0.75 (0.79)	–0.07 (0.18)	0.00 (0.00)
	2	−1	3/2	3.76 (3.78)	0.91 (1.00)	26.70 (22.61)
	1	−1	1/2	0.80 (1.32)	1.08 (1.82)	0 (0)
	1	−1	3/2	3.78 (3.77)	1.80 (1.91)	17.76 (12.04)
	2	−2	0	0.00	0.00	0.00
	2	−2	1	2.01	0.12	9.25
	1	−2	0	0.00	0.00	0.00
	1	−2	1	2.05	1.59	15.42
	0	−2	0	0.00	0.00	0.00
	0	−2	1	2.04	1.55	–8.97
B	2	0	2	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)
	2	0	2	2.01(2.03)	0.63 (0.99)	17.84 (23.27)
	1	0	1	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)
	1	0	1	2.04 (2.04)	1.73 (1.96)	–4.84 (–8.00)
	1[b]	1	0	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)
	1[b]	1	1	2.04 (2.04)	1.71 (1.95)	–3.26 (–7.18)
	2	−1	1/2	0.75	–0.06	0.00
	2	−1	3/2	3.79	1.73	21.15
	1	−1	1/2	0.79	1.02	0.00
	1	−1	3/2	3.78	1.84	17.81
	2	−2	0	0.00	0.00	0.00
	2	−2	1	2.01	0.05	9.26
	1	−2	0	0.00	0.00	0.00
	1	−2	1	2.07	1.54	16.32
	0	−2	0	0.00	0.00	0.00
	0	−2	1	2.04	1.58	–7.78

[a] Calculations performed with BP86 functional with 6-31+G(d,p) basis set for central part of molecule and 6-31G basis set for C_6F_6 groups and axial pyridine ligands. B3P86 results for selected intermediates are given in parentheses.
[b] Ligand-protonated species.

Table S3. Estimated Relative Free Energies for Pyridine Dissociation for Relevant States of **A** and **B** in Dichloromethane Solution [a]

Complex	Charge	Reactant	*S*	Product	*S*	Δ*G*
A	0	$Fe^{II}py_2$	0	$Fe^{II}py$	1	9.60
	–1	$Fe^{I}(gly)^{\bullet}py_2$	1/2	$Fe^{I}py$	1/2	–11.43
	–2	$Fe^{0}py_2$	0	$Fe^{0}py$	0	–23.63
	–2	$Fe^{0}py$	0	Fe^{0}	1	7.97
B	0	$Fe^{II}py_2$	0	$Fe^{II}py$	1	9.46
	–1	$Fe^{I}(gly)^{\bullet}py_2$	1/2	$Fe^{I}py$	1/2	–10.62
	–2	$Fe^{0}py_2$	0	$Fe^{0}py$	0	–24.61
	–2	$Fe^{0}py_2$	0	Fe^{0}	1	8.24

[a] Calculations performed with BP86 functional with 6-31+G(d,p) basis set for central part of molecule and 6-31G basis set for C_6F_6 groups and axial pyridine ligands. Free energies are given in kcal/mol, and the product free energy is the sum of the free energy of the complex and a solvated py ligand. Basis set superposition error (BSSE) corrections were not included.

Table S4. Difference in pK_a Associated with Protonation at the Ligand versus Protonation at the Metal Center for **B** with Different Functionals[a]

Functional	BP86	B3P86	M06L	ωB97XD[b]
ΔpK_a [c]	2.70	6.34	4.24	−1.08

[a] Calculations presented in this table were performed with the 6-311+G(d,p) basis set with Cl atoms substituted for C_6F_5 groups, which have similar Hammett constant.[1]
[b] The trends in relative pK_a's for all functionals except ωB97XD agree well. Severe spin contamination observed for the doublet state with the ωB97XD functional is most likely responsible for this discrepancy.
[c] ΔpK_a = pK_a of $[Fe^{I}py..\mathbf{H}]^0$ − pK_a of $[Fe^{III}\mathbf{H}py]^0$

Table S5. Relative pK_a Values for **A** and **B** [a]

A	Relative pK_a
$[Fe^{III}\mathbf{H}py]^0$	−10.03
$[Fe^{II}\mathbf{H}py]^-$	9.43
B	
$[Fe^{II}py_2\ldots\mathbf{H}]^+$	−11.35
$[Fe^{I}py\ldots\mathbf{H}]^0$	0.00
$[Fe^{III}\mathbf{H}py]^0$	−3.81
$[Fe^{II}\mathbf{H}py]^-$	15.25
$[Fe^{0}py\ldots\mathbf{H}]^-$	12.16
$[Fe^{III}\mathbf{H}py\ldots H]^+$	−18.49
$Fe^{III}Hpy\ldots\mathbf{H}]^+$	−14.68
$[Fe^{II}\mathbf{H}py\ldots H]^0$	1.55
$[Fe^{II}Hpy\ldots\mathbf{H}]^0$	−1.54

[a] Calculations were performed with BP86 functional with 6-31+G(d,p) basis set for central part of molecule and 6-31G basis set for C_6F_6 groups and axial pyridine ligands. These pK_a values are plotted in Figure 4 of the main paper. The bold **H** indicates the acidic proton, '…H' indicates a protonated ligand, and FeH indicates a metal hydride. $[Fe^{I}py\ldots\mathbf{H}]^0$ for **B** is the reference pK_a, and all other values are calculated relative to this value.

Table S6. Spin Properties for Protonated Species of **A** and **B** [a]

Complex	Protonated	S	$\langle S^2 \rangle$	ρ_{Fe}
A	$[Fe^{III}Hpy]^0$	1/2	0.76	0.87
	$[Fe^{II}Hpy]^-$	0	0.00	0.00
B	$[Fe^{III}Hpy]^0$	1/2	0.76	0.87
	$[Fe^{II}Hpy]^-$	0	0.00	0.00
	$[Fe^{II}py_2\ldots H]^+$	0	0.00	0.00
	$[Fe^{II}py\ldots H]^+$	1	2.04	1.72
	$[Fe^{II}(gly)^{\bullet}py_2\ldots H]^0$	1/2	0.76	–0.06
	$[Fe^{I}py\ldots H]^0$	1/2	0.81	1.16
	$[Fe^{0}py\ldots H]^-$	0	0.00	0.00
	$[Fe^{III}Hpy\ldots H]^+$	1/2	0.77	0.89
	$[Fe^{II}Hpy\ldots H]^0$	0	0.00	0.00

[a] Calculations were performed with BP86 functional with 6-31+G(d,p) basis set for central part of molecule and 6-31G basis set for C_6F_6 groups and axial pyridine ligands. Fe…H indicates a protonated ligand, and FeH indicates a metal hydride.

Because the formation of an Fe^0 intermediate in the catalytic cycle is unusual, we analyzed the structures of the $[Fe^Ipy]^-$ and $[Fe^0py]^{2-}$ species in more detail. Table S7 provides the relative free energies of the optimized doublet and quartet states of $[Fe^Ipy]^-$ and the relative free energies of the optimized singlet and triplet states of the square pyramidal and trigonal bipyramidal $[Fe^0py]^{2-}$. The doublet $[Fe^Ipy]^-$ state, in which the unpaired spin is localized on the Fe center, is much more thermodynamically stable than the quartet state. For $[Fe^0py]^{2-}$, the singlet square pyramidal state is more thermodynamically stable than the triplet square pyramidal state and both trigonal bipyramidal states. In the doublet and triplet square pyramidal states, the unpaired electrons are primarily localized on the Fe center, without significant delocalization onto the ligands. Moreover, the trigonal bipyramidal structure is highly unfavorable for the $[Fe^0py]^{2-}$ species.

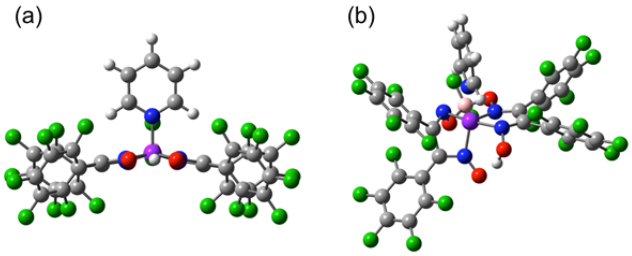

Figure S1. DFT/BP86 optimized structures for (a) square pyramidal and (b) trigonal bipyramidal $[Fe^0py]^{2-}$.

Table S7. Spin Densities and Relative Free Energies for Fe^I and Fe^0 States of **B** [a]

Species	S	ρ_{Fe}	ΔG
$[Fe^Ipy]^-$	1/2	1.02	0.00 [b]
	3/2	1.84	17.81
$[Fe^0py]^{2-}$	0	0.00	0.00 [c]
	1	1.46	16.32
tbp-$[Fe^0py]^{2-}$ [d]	0	0.00	50.78
	1	1.23	50.56

[a] Calculations performed with BP86 functional. Free energies given in kcal/mol.
[b] Reference free energy for Fe^I species.
[c] Reference free energy for Fe^0 species.
[d] *tbp*=trigonal bipyramidal. All other species in this table are square pyramidal.

Table S8. Parameters Used for CV Simulations of **A** using DigiElch7 [a]

#	Charge Transfer Reaction	E^o (V vs SCE)	α	K_S (cm/s)
1	$[Fe^{II}py_2]^0 + e = [Fe^{II}(gly)^{\bullet}py_2]^-$	−0.71	0.5	10000
2	$[Fe^{I}py]^- + e = [Fe^{0}py]^{2-}$	−0.94	0.5	10000
3	$[Fe^{II}py]^0 + e = [Fe^{II}py]^-$	*0.29*	0.5	10000
4	$[Fe^{III}Hpy]^0 + e = [Fe^{II}Hpy]^-$	*0.21*	0.5	10000
	Chemical Reaction	K_{eq}	k_f	k_b
5	$[Fe^{II}py_2]^0 = [Fe^{II}py]^0 + py$	*9.1689E−08*	0.2 [b]	2.1813E+06
6	$[Fe^{II}(gly)^{\bullet}py_2]^- = [Fe^{I}py]^- + py$	7.29E+09 (2.41E+08)	5 [b]	6.8591E−10
8	$py + HA = pyH^+ + A^-$	0.003	1E+07 [c]	3.33E+09
9	$[Fe^{0}py]^{2-} + HA = [Fe^{II}Hpy]^- + A^-$	1	500 [c]	500
10	$[Fe^{II}Hpy]^- + HA = [Fe^{II}H_2py]^0 + A^-$	1000	1E+07 [c]	10000
11	$[Fe^{II}H_2py]^0 + py = [Fe^{II}py_2]^0 + H_2$	1000	1E+07 [c]	10000
12	$[Fe^{I}py]^- + HA = [Fe^{III}Hpy]^0 + A^-$	3.50E−20 (2.88E−19)	0.1 [c]	2.8558E+18

[a] Parameters that were fixed to the DFT/BP86 calculated values are given in italics. All other parameters except the reduction potentials of the first two charge transfer reactions were free to fit to the experimental CVs. When available, the DFT/BP86 calculated values are given in parentheses. The trend in the magnitudes of the forward rate constants was constrained to be the same as the trend in the magnitudes of the equilibrium constants for the catalyst protonation reactions so that larger forward rate constants are associated with larger equilibrium constants for these reactions. All values are given for dichloromethane solution, with concentrations [**A**] = 0.5 mM and [TFA] = 0–10 mM. The scan rate was 100 mV/s.

[b] Unit of k_f is s^{-1} (first-order reaction), and unit of k_b is $M^{-1}s^{-1}$ (second-order reaction).

[c] Unit of k_f is $M^{-1}s^{-1}$ (second-order reaction), and unit of k_b is $M^{-1}s^{-1}$ (second-order reaction).

Table S9. Parameters Used for CV Simulations of **B** using DigiElch7 [a]

#	Charge Transfer Reaction	E^o (V vs SCE)	α	*K*s (cm/s)
1	$[Fe^{II}py_2]^0 + e = [Fe^{II}(gly)^{\bullet}py_2]^-$	*−0.92*	0.5	10000
2	$[Fe^{II}py]^0 + e = [Fe^{I}py]^-$	*−0.05*	0.5	10000
3	$[Fe^{I}py]^- + e = [Fe^{0}py]^{2-}$	*−1.17*	0.5	10000
4	$[Fe^{II}py\ldots H]^0 + e = [Fe^{I}py\ldots H]^-$	*0.73*	0.5	10000
5	$[Fe^{I}py\ldots H]^0 + e = [Fe^{0}py\ldots H]^-$	*−0.45*	0.5	10000
6	$[Fe^{III}Hpy]^0 + e = [Fe^{II}Hpy]^-$	*−0.04*	0.5	10000
7	$[Fe^{III}Hpy\ldots H]^+ + e = [Fe^{II}Hpy\ldots H]^0$	*0.74*	0.5	10000
	Chemical Reaction	K_{eq}	k_f	k_b
8	$[Fe^{II}py_2]^0 = [Fe^{II}py]^0 + py$	*1.1556E−07*	0.002 [b]	17307
9	$[Fe^{II}(gly)^{\bullet}py_2]^- = [Fe^{I}py]^- + py$	5.84E+007 (6.12E+07)	10 [b]	1.71E−07
10	$[Fe^{I}py]^- + HA = [Fe^{I}py\ldots H]^0 + A^-$	10	10000 [c]	1000
11	$[Fe^{0}py]^{2-} + HA = [Fe^{0}py\ldots H]^- + A^-$	1.47E+013 (1.44E+13)	15000 [c]	1.018E−09
12	$[Fe^{I}py\ldots H]^0 = [Fe^{III}Hpy]^0$	0.00014657 (0.000156)	0.1 [d]	682.27
13	$[Fe^{0}py\ldots H]^- = [Fe^{II}Hpy]^-$	*1245.1*	1 [d]	.0008
14	$py + HA = pyH^+ + A^-$	0.001	5E+06 [c]	5E+09
15	$[Fe^{II}Hpy]^- + HA = [Fe^{II}H_2py]^0 + A^-$	1000	12000 [c]	12
16	$[Fe^{II}H_2py]^0 = [Fe^{II}py]^0 + H_2$	1000	10000 [b]	10
17	$[Fe^{0}py]^{2-} + HA = [Fe^{II}Hpy]^- + A^-$	1.83E+016 (1.79E+16)	16000 [c]	8.72E−13
18	$[Fe^{I}py]^- + HA = [Fe^{III}Hpy]^0 + A^-$	0.0014567 (1.56E−03)	1E−05 [c]	0.006823
19	$[Fe^{I}py\ldots H]^0 + HA = [Fe^{III}Hpy\ldots H]^+ + A^-$	2.7735E−18 (3.24E−18)	1E−10 [c]	3.6056E+07
20	$[Fe^{0}py\ldots H]^- + HA = [Fe^{II}Hpy\ldots H]^0 + A^-$	*358.5*	11000 [c]	30.683
21	$[Fe^{II}Hpy\ldots H]^0 + py = [Fe^{II}py_2]^0 + H_2$	3.0054E+13	20000 [c]	6.6546E−10

[a] Parameters that were fixed to the DFT/BP86 calculated values are given in italics. All other parameters were free to fit to the experimental CVs. When available, the DFT/BP86 calculated values are given in parentheses. The trend in the magnitudes of the forward rate constants was constrained to be the same as the trend in the magnitudes of the equilibrium constants for the catalyst protonation reactions so that larger forward rate constants are associated with larger equilibrium constants for these reactions. All values are given for dichloromethane solution, with concentrations [**B**] = 0.5 mM and [TFA] = 0–10 mM. The scan rate was 100 mV/s.

[b] Unit of k_f is s^{-1} (first-order reaction), and the unit of k_b is $M^{-1}s^{-1}$ (second-order reaction).

[c] Unit of k_f is $M^{-1}s^{-1}$ (second-order reaction), and the unit of k_b is $M^{-1}s^{-1}$ (second-order reaction).

[d] Unit of k_f is s^{-1} (first-order reaction), and the unit of k_b is s^{-1} (first-order reaction).

Reference

(S1) Solis, B. H.; Hammes-Schiffer, S., *J. Am. Chem. Soc.* **2011,** *133*, 19036-19039.

Coordinates and Energies of Optimized Structures

1. $[Fe^{II}py_2]^0$, Complex **A**

E = -5792.67511971 hartrees

Fe	-0.00002800	0.03180500	-0.00551300
N	-1.40904700	-0.08017000	-1.25103700
O	-1.27782300	-0.11044200	-2.59426200
B	-0.00024600	0.51134800	-3.18131800
O	1.27719000	-0.11096300	-2.59451500
N	1.40870400	-0.08068300	-1.25131900
C	2.62137000	-0.26786000	-0.73582500
C	2.62311000	-0.24281400	0.72986100
N	1.41651500	-0.01989900	1.24331800
O	1.27625500	-0.08194100	2.58539500
B	0.00037000	0.55734600	3.16666500
O	-1.27582500	-0.08154800	2.58564800
N	-1.41633700	-0.01941700	1.24360200
C	-2.62311500	-0.24187700	0.73038300
C	-2.62168100	-0.26690200	-0.73530200
F	0.00055700	1.92089400	2.92464700
F	0.00044800	0.18624700	4.49425900
N	0.00031200	2.02851400	-0.03792200
C	-1.17310400	2.73376200	-0.04288000
C	1.17397200	2.73335200	-0.04314800
C	-1.20536200	4.13327800	-0.05262300
H	-2.09775600	2.16079300	-0.03315200
C	1.20671700	4.13285500	-0.05289500
H	2.09842300	2.16005300	-0.03364400
C	0.00080300	4.85410600	-0.05767200
H	-2.17273900	4.64047200	-0.05208900
H	2.17427100	4.63971200	-0.05258400
H	0.00099400	5.94705800	-0.06265300
N	-0.00037800	-2.00161100	0.04582000
C	-0.00071700	-2.72707200	-1.11780800
C	-0.00030700	-2.68053600	1.23845700
C	-0.00097600	-4.12888900	-1.11947100
H	-0.00078300	-2.16458600	-2.05085800
C	-0.00056200	-4.08075700	1.29626600
H	-0.00004500	-2.07778800	2.14684400
C	-0.00089600	-4.82359100	0.10205100
H	-0.00123700	-4.65638700	-2.07571700
H	-0.00049300	-4.57160800	2.27233700
H	-0.00109300	-5.91654900	0.12359500
F	-0.00045800	0.13217400	-4.50577500
F	0.00005800	1.88388000	-2.96352400
C	-3.83101300	-0.42491200	-1.56894600

C	-4.90645500	0.47994900	-1.47738800
C	-3.95289400	-1.46168700	-2.51548200
C	-6.04935500	0.37189200	-2.27781400
C	-5.07915900	-1.58935400	-3.33783100
C	-6.13287500	-0.66987300	-3.21495500
C	-3.81781300	-0.46667200	1.56985000
C	-4.24291600	0.48815500	2.51645700
C	-4.56583300	-1.65683300	1.48644900
C	-5.35027300	0.26992200	3.34513300
C	-5.68186700	-1.89867100	2.29641500
C	-6.07315800	-0.92862300	3.23225500
C	3.83046800	-0.42638600	-1.56970700
C	4.90643500	0.47784900	-1.47819400
C	3.95160300	-1.46309400	-2.51641200
C	6.04915000	0.36924500	-2.27881200
C	5.07766200	-1.59129100	-3.33896000
C	6.13192700	-0.67243700	-3.21611300
C	3.81790000	-0.46800600	1.56909200
C	4.56542500	-1.65847700	1.48565700
C	4.24359300	0.48674600	2.51551200
C	5.68153300	-1.90068100	2.29541100
C	5.35103800	0.26815100	3.34397600
C	6.07341500	-0.93069700	3.23106900
F	-7.17056100	-1.15115300	4.03758600
F	-6.38307100	-3.08549500	2.19298700
F	-4.16194000	-2.65604900	0.59915100
F	-5.74862400	1.22986000	4.25372200
F	-3.57424100	1.69983900	2.60932600
F	-7.25159900	-0.79153400	-4.01214400
F	-5.17182300	-2.62438000	-4.24721700
F	-7.07791600	1.28768400	-2.16545400
F	-4.81824900	1.55405700	-0.58885500
F	-2.95037600	-2.41636400	-2.61728400
F	2.94849600	-2.41714900	-2.61822300
F	5.16957900	-2.62623200	-4.24851800
F	7.25045400	-0.79462400	-4.01349700
F	7.07825900	1.28442500	-2.16647700
F	4.81900000	1.55185200	-0.58945800
F	4.16093400	-2.65763900	0.59857200
F	6.38223000	-3.08780400	2.19196100
F	7.17089700	-1.15359000	4.03619200
F	5.74997200	1.22802400	4.25237700
F	3.57544700	1.69872200	2.60838000

2. $[Fe^{II}py]^{0}$, Complex **A**
E = -5544.39550301

Fe	0.00008500	0.63939900	-0.01798100
N	-1.37254000	0.27871100	-1.26934600
O	-1.25662700	0.26180300	-2.61011000
B	-0.00018100	0.92770100	-3.17890900
O	1.25611400	0.26130100	-2.61036700
N	1.37231000	0.27815700	-1.26962600
C	2.54551900	-0.11126700	-0.75021200
C	2.55230000	-0.10344200	0.69585400
N	1.38070700	0.27726000	1.22520100
O	1.25653100	0.18711400	2.56325800
B	0.00044200	0.83162500	3.16284200
O	-1.25602400	0.18760900	2.56351500
N	-1.38042900	0.27779000	1.22548300
C	-2.55226900	-0.10247900	0.69636900
C	-2.54578400	-0.11028600	-0.74969600
F	0.00068600	2.19787700	2.90391400
F	0.00050900	0.47847300	4.48953100
N	0.00047200	2.65291100	0.02445300
C	-1.17882200	3.34225700	0.04558700
C	1.18002000	3.34182500	0.04555000
C	-1.21153600	4.74167300	0.08475700
H	-2.09263000	2.74699000	0.03781300
C	1.21324600	4.74122800	0.08471800
H	2.09361300	2.74622600	0.03776700
C	0.00098600	5.45535200	0.10359200
H	-2.17441500	5.25652100	0.10351600
H	2.17631300	5.25572400	0.10344900
H	0.00118700	6.54800600	0.13587100
F	-0.00037600	0.64790100	-4.52185200
F	0.00012600	2.28379100	-2.85338100
C	-3.69082300	-0.50443900	-1.59393900
C	-4.91936000	0.18038700	-1.53137800
C	-3.59308000	-1.56677400	-2.51599600
C	-6.00655000	-0.16055200	-2.34402500
C	-4.66246900	-1.92443300	-3.34644600
C	-5.87319200	-1.21848500	-3.25740800
C	-3.69639700	-0.50172000	1.53985700
C	-4.24819800	0.39261100	2.47966000
C	-4.26076600	-1.78965200	1.47225100
C	-5.30780600	0.02742400	3.31741400
C	-5.32518400	-2.18032600	2.29427200
C	-5.84791500	-1.26570600	3.22179200
C	3.69024700	-0.50585900	-1.59467300
C	4.91895000	0.17872300	-1.53258900
C	3.59205100	-1.56839600	-2.51645500
C	6.00585200	-0.16262100	-2.34545000

C	4.66115100	-1.92646500	-3.34710200
C	5.87203800	-1.22073700	-3.25855300
C	3.69642600	-0.50315600	1.53911800
C	4.26031800	-1.79128600	1.47131400
C	4.24871500	0.39090500	2.47888900
C	5.32473800	-2.18240700	2.29312100
C	5.30833500	0.02527200	3.31643300
C	5.84795900	-1.26804600	3.22062000
F	-6.89647000	-1.63521600	4.03650700
F	-5.84815900	-3.45556600	2.20890000
F	-3.72152300	-2.72619000	0.59247900
F	-5.83712600	0.92973800	4.21744600
F	-3.75554400	1.68858300	2.55297300
F	-6.93482100	-1.56725000	-4.06439900
F	-4.54431000	-2.97652200	-4.23088900
F	-7.19309900	0.54243400	-2.26474100
F	-5.05131700	1.26461100	-0.66143600
F	-2.42584900	-2.31050800	-2.57586700
F	2.42470100	-2.31198600	-2.57577400
F	4.54255700	-2.97875800	-4.23124300
F	6.93338400	-1.56990700	-4.06574000
F	7.19255900	0.54015200	-2.26665400
F	5.05135000	1.26316200	-0.66298300
F	3.72059700	-2.72755000	0.59154300
F	5.84724400	-3.45782700	2.20755400
F	6.89652300	-1.63799500	4.03512500
F	5.83814000	0.92732700	4.21643900

3. $[Fe^{II}(gly)^{\bullet}py_2]^{-}$, Complex **A**
E = -5792.77748072 hartrees

Fe	-0.00002700	0.04103200	-0.00799400
N	-1.39868900	-0.07254400	-1.25139600
O	-1.26931100	-0.12411500	-2.61222200
B	-0.00024400	0.48880600	-3.18628000
O	1.26870600	-0.12458000	-2.61246600
N	1.39835600	-0.07303400	-1.25166800
C	2.62587500	-0.27220400	-0.73137600
C	2.63024100	-0.22779400	0.71800600
N	1.40831200	0.00935000	1.23596100
O	1.26626700	-0.11175200	2.59327600
B	0.00036100	0.51378900	3.17032500
O	-1.26586900	-0.11131000	2.59351600
N	-1.40813400	0.00986000	1.23623100
C	-2.63025700	-0.22679500	0.71851500
C	-2.62618900	-0.27125900	-0.73086800
F	0.00058900	1.89590000	2.97372700

F	0.00042400	0.13585700	4.51222400
N	0.00031800	2.03253200	-0.05096800
C	-1.17368800	2.73556500	-0.05796900
C	1.17457200	2.73515000	-0.05815800
C	-1.20579300	4.13562800	-0.07121300
H	-2.09373300	2.15443100	-0.04660500
C	1.20716800	4.13520100	-0.07140800
H	2.09441200	2.15368800	-0.04694900
C	0.00081400	4.85647000	-0.07790100
H	-2.17341600	4.64347800	-0.07194900
H	2.17496900	4.64271000	-0.07230500
H	0.00100700	5.95026600	-0.08538000
N	-0.00037900	-1.98667500	0.04943500
C	-0.00071700	-2.71051200	-1.11403200
C	-0.00031100	-2.66317500	1.24185000
C	-0.00097900	-4.11282200	-1.11540800
H	-0.00078300	-2.14195400	-2.04373600
C	-0.00056900	-4.06428400	1.30001900
H	-0.00004500	-2.05294700	2.14542700
C	-0.00090300	-4.80742100	0.10627300
H	-0.00123900	-4.64064100	-2.07188900
H	-0.00050100	-4.55489800	2.27669200
H	-0.00110200	-5.90117100	0.12793900
F	-0.00044300	0.12017300	-4.52952600
F	0.00003200	1.87837400	-3.00027100
C	-3.82757300	-0.43007300	-1.56729500
C	-4.93558600	0.43778800	-1.45621100
C	-3.93080800	-1.44496800	-2.54498400
C	-6.07756200	0.31488200	-2.25564800
C	-5.05295500	-1.57953600	-3.37046600
C	-6.13578100	-0.69927400	-3.22240800
C	-3.81362900	-0.45133400	1.56440800
C	-4.20156300	0.47706500	2.55829600
C	-4.60772200	-1.61375800	1.45756900
C	-5.29817000	0.25951100	3.39948500
C	-5.71942200	-1.84786000	2.27566000
C	-6.06535100	-0.90729500	3.25624600
C	3.82703800	-0.43142100	-1.56803800
C	4.93566100	0.43561300	-1.45666600
C	3.92941600	-1.44587700	-2.54626500
C	6.07745800	0.31229400	-2.25629800
C	5.05135900	-1.58082300	-3.37196100
C	6.13483600	-0.70141700	-3.22357800
C	3.81370900	-0.45278100	1.56364900
C	4.60724100	-1.61558600	1.45674800
C	4.20231100	0.47554100	2.55735000

C	5.71902200	-1.85012000	2.27460100
C	5.29901800	0.25756600	3.39829900
C	6.06562400	-0.90961200	3.25500300
F	-7.16409300	-1.12433400	4.07380800
F	-6.45956800	-3.01561800	2.14646800
F	-4.25324300	-2.61365400	0.54684900
F	-5.66159500	1.20454800	4.34678700
F	-3.51915000	1.67988700	2.67660500
F	-7.25997500	-0.83598800	-4.02206300
F	-5.12613000	-2.60339800	-4.30293200
F	-7.13426100	1.20529300	-2.12385100
F	-4.88588800	1.50981500	-0.55877600
F	-2.92368300	-2.39389200	-2.66325100
F	2.92149800	-2.39389900	-2.66500900
F	5.12366100	-2.60422700	-4.30499900
F	7.25882700	-0.83851600	-4.02345100
F	7.13481400	1.20187400	-2.12416900
F	4.88685900	1.50715400	-0.55860100
F	4.25206400	-2.61544000	0.54625500
F	6.45858400	-3.01824400	2.14536600
F	7.16445900	-1.12707600	4.07232700
F	5.66311000	1.20253500	4.34541300
F	3.52050000	1.67870200	2.67567900

4. $[Fe^{I}py]^{-}$, Complex **A**

E = -5544.53597378 hartrees

Fe	0.00007900	0.59630400	-0.04133300
N	-1.33489200	0.14562500	-1.26715900
O	-1.24418000	0.11710700	-2.62974500
B	-0.00021600	0.76398500	-3.18736400
O	1.24364000	0.11667700	-2.62999900
N	1.33463200	0.14513300	-1.26743200
C	2.54546200	-0.18417000	-0.75431400
C	2.55330900	-0.15658900	0.66860600
N	1.33935100	0.16835700	1.18270300
O	1.24369600	0.05861200	2.54012800
B	0.00042100	0.66122600	3.15306600
O	-1.24325400	0.05916900	2.54038600
N	-1.33912100	0.16889700	1.18297600
C	-2.55330900	-0.15557000	0.66912500
C	-2.54575000	-0.18319700	-0.75379500
F	0.00072000	2.05732500	2.99779100
F	0.00046800	0.26147200	4.48545900
N	0.00045800	2.58719700	0.09123200
C	-1.17815100	3.27716000	0.11284700
C	1.17931600	3.27672800	0.11308200

C	-1.21083900	4.67733000	0.14908400
H	-2.09005100	2.67752900	0.11051900
C	1.21250600	4.67688700	0.14931800
H	2.09099700	2.67676400	0.11096100
C	0.00096300	5.39205300	0.16587300
H	-2.17460900	5.19162700	0.16838300
H	2.17646000	5.19083100	0.16881000
H	0.00116000	6.48550300	0.19595600
F	-0.00040100	0.50338000	-4.55152600
F	0.00005600	2.14335000	-2.89015100
C	-3.69871200	-0.51879500	-1.60932700
C	-4.89781800	0.21894500	-1.56391200
C	-3.64888200	-1.58425500	-2.53408500
C	-5.99248400	-0.06994200	-2.38786700
C	-4.72349700	-1.88510600	-3.38035700
C	-5.90138900	-1.12685600	-3.30444800
C	-3.70349000	-0.48615300	1.53016700
C	-4.19559600	0.43566700	2.47918700
C	-4.35240600	-1.73571400	1.47627300
C	-5.25911300	0.13199400	3.33604900
C	-5.42879800	-2.06119100	2.31210100
C	-5.88091300	-1.12316800	3.25027800
C	3.69813800	-0.52014400	-1.61008500
C	4.89753400	0.21713700	-1.56481600
C	3.64773100	-1.58548600	-2.53494600
C	5.99193700	-0.07207800	-2.38900400
C	4.72207500	-1.88665200	-3.38145100
C	5.90026900	-1.12885800	-3.30568200
C	3.70352200	-0.48767500	1.52941200
C	4.35189200	-1.73751400	1.47537200
C	4.19622300	0.43392400	2.47834000
C	5.42831600	-2.06346300	2.31097300
C	5.25978800	0.12978400	3.33497800
C	5.88102800	-1.12564500	3.24906700
F	-6.94394600	-1.43053800	4.08426700
F	-6.03305100	-3.30737900	2.23467300
F	-3.89497900	-2.71493700	0.59423700
F	-5.72680500	1.06832700	4.24482600
F	-3.64708000	1.71011400	2.54333400
F	-6.97516700	-1.42592700	-4.12746000
F	-4.64978900	-2.94659700	-4.26746500
F	-7.15080500	0.69117000	-2.32106500
F	-5.00301000	1.31323400	-0.70027100
F	-2.53069900	-2.40026100	-2.58253100
F	2.52923300	-2.40106600	-2.58327500
F	4.64779800	-2.94802000	-4.26866000

F	6.97377900	-1.42824600	-4.12892900
F	7.15056000	0.68858600	-2.32233400
F	5.00330500	1.31129200	-0.70107700
F	3.89385200	-2.71654300	0.59343900
F	6.03201300	-3.30991300	2.23341100
F	6.94409900	-1.43348200	4.08283500
F	5.72807700	1.06590800	4.24366300
F	3.64829600	1.70861900	2.54259500

5. $[Fe^{0}py]^{2-}$, Complex **A**

E = -5544.55116669 hartrees

Fe	0.00003600	0.38533300	-0.00466100
N	-1.33790300	-0.00962800	-1.22503100
O	-1.25025500	-0.05725000	-2.59794400
B	-0.00025200	0.53004600	-3.18519300
O	1.24966700	-0.05767600	-2.59818800
N	1.33759200	-0.01011200	-1.22529200
C	2.58240000	-0.23112000	-0.71883300
C	2.59131600	-0.17751200	0.71598100
N	1.35281700	0.07065700	1.22144300
O	1.24896200	-0.07276600	2.58801100
B	0.00037300	0.50731200	3.19358100
O	-1.24856900	-0.07226400	2.58825700
N	-1.35262300	0.07116000	1.22170300
C	-2.59131500	-0.17654400	0.71648400
C	-2.58269300	-0.23018400	-0.71833000
F	0.00064900	1.91397800	3.09378600
F	0.00041800	0.08026200	4.53419200
N	0.00038400	2.28941100	-0.04311500
C	-1.18021900	2.99562000	-0.05235900
C	1.18123500	2.99520400	-0.05246000
C	-1.20739400	4.39355600	-0.07505600
H	-2.09512300	2.40082000	-0.03373100
C	1.20889800	4.39313000	-0.07515900
H	2.09593200	2.40008100	-0.03390400
C	0.00087900	5.11846400	-0.08823600
H	-2.17547600	4.90308000	-0.07898800
H	2.17715800	4.90231500	-0.07917300
H	0.00107200	6.21279900	-0.10474400
F	-0.00045000	0.15348100	-4.53923500
F	0.00000500	1.94039300	-3.05130900
C	-3.75374500	-0.45530000	-1.56906100
C	-4.92696000	0.32822700	-1.46600000
C	-3.78054600	-1.46923000	-2.56017600
C	-6.04514400	0.13792800	-2.28521800
C	-4.87761800	-1.66270000	-3.40666100

C	-6.02118700	-0.86130100	-3.26819800
C	-3.74823900	-0.45693200	1.57333200
C	-4.14447800	0.43237700	2.60447200
C	-4.53431600	-1.62615100	1.44388000
C	-5.22501500	0.17032700	3.45224000
C	-5.63422600	-1.89951800	2.26589900
C	-5.98109200	-1.00022400	3.28287800
C	3.75321400	-0.45662000	-1.56979100
C	4.92672100	0.32649600	-1.46692900
C	3.77947400	-1.47052700	-2.56094500
C	6.04467900	0.13584300	-2.28637300
C	4.87631400	-1.66434400	-3.40765000
C	6.02018400	-0.86334200	-3.26938600
C	3.74828800	-0.45843800	1.57258900
C	4.53379300	-1.62802000	1.44293400
C	4.14516200	0.43065700	2.60366800
C	5.63375900	-1.90191900	2.26469900
C	5.22576800	0.16808300	3.45118700
C	5.98126800	-1.00281300	3.28162400
F	-7.07120500	-1.25985300	4.11084200
F	-6.36058200	-3.07946600	2.11324300
F	-4.18311000	-2.60354200	0.50678400
F	-5.60091300	1.08678900	4.43079800
F	-3.50043100	1.65465000	2.74517100
F	-7.12566600	-1.06147000	-4.09385700
F	-4.87872700	-2.69004800	-4.34611400
F	-7.16493400	0.96024500	-2.16564800
F	-4.97195600	1.39921400	-0.56306700
F	-2.73245400	-2.37361900	-2.65355400
F	2.73105800	-2.37455900	-2.65414600
F	4.87688700	-2.69166200	-4.34713700
F	7.12443100	-1.06385800	-4.09527200
F	7.16477700	0.95776800	-2.16699100
F	4.97226700	1.39742800	-0.56395700
F	4.18191600	-2.60523100	0.50590300
F	6.35953300	-3.08220100	2.11185100
F	7.07144600	-1.26296800	4.10933600
F	5.60231000	1.08434300	4.42968700
F	3.50172600	1.65323200	2.74453300

6. $[Fe^{III}Hpy]^{0}$, Complex **A**

E = -5544.98440599 hartrees

Fe	0.00003100	0.35305700	-0.01780800
N	-1.38624300	0.10550800	-1.26312500
O	-1.26329100	0.06677200	-2.59798400
B	-0.00022600	0.71407600	-3.18062000

O	1.26272400	0.06631400	-2.59824600
N	1.38595900	0.10498400	-1.26341200
C	2.59170600	-0.17100800	-0.74532500
C	2.59658200	-0.16465100	0.69754900
N	1.39312100	0.10664600	1.22278700
O	1.26411800	-0.00240000	2.55364300
B	0.00041500	0.62749600	3.16224200
O	-1.26368500	-0.00186200	2.55390600
N	-1.39290400	0.10720000	1.22307400
C	-2.59657800	-0.16363300	0.69808200
C	-2.59199000	-0.17002300	-0.74479400
F	0.00068200	1.99564500	2.92449100
F	0.00047100	0.24946100	4.48113100
N	0.00041600	2.39192400	0.01236300
C	-1.17641900	3.08461100	0.02701100
C	1.17751100	3.08417000	0.02702500
C	-1.21058000	4.48427700	0.05361700
H	-2.09326400	2.49377800	0.02423000
C	1.21219400	4.48382200	0.05362600
H	2.09413400	2.49299200	0.02427500
C	0.00094100	5.19923800	0.06633500
H	-2.17416600	4.99796700	0.06763800
H	2.17597200	4.99715200	0.06765900
H	0.00114600	6.29214500	0.08905700
F	-0.00042400	0.39762000	-4.51476100
F	0.00005500	2.07628600	-2.88987900
C	-3.76674900	-0.45733200	-1.59166500
C	-4.92335700	0.34300400	-1.53743500
C	-3.76796100	-1.52949800	-2.50720400
C	-6.03594100	0.10297300	-2.35182800
C	-4.86439500	-1.78807700	-3.33935300
C	-6.00201700	-0.96890700	-3.25823400
C	-3.76735900	-0.47312500	1.54450600
C	-4.24866900	0.45822500	2.48632600
C	-4.42603200	-1.71537000	1.47650100
C	-5.33052800	0.17176900	3.32659800
C	-5.51452700	-2.02699200	2.30085700
C	-5.96562100	-1.07735300	3.23082300
C	3.76619900	-0.45871300	-1.59243100
C	4.92308500	0.34123800	-1.53841400
C	3.76687600	-1.53086100	-2.50799200
C	6.03542500	0.10086300	-2.35303800
C	4.86305800	-1.78978000	-3.34036700
C	6.00096400	-0.97098400	-3.25946300
C	3.76740200	-0.47465200	1.54373400
C	4.42556000	-1.71716000	1.47554000

C	4.24926300	0.45645200	2.48551500
C	5.51408100	-2.02926700	2.29967800
C	5.33116000	0.16951200	3.32557300
C	5.96572700	-1.07986300	3.22961500
F	-7.03673200	-1.36901000	4.04767500
F	-6.13164200	-3.25923200	2.21452700
F	-3.96155900	-2.68681700	0.59248400
F	-5.78704900	1.10924600	4.23045200
F	-3.65731000	1.71203400	2.56314400
F	-7.08996800	-1.21924500	-4.06655300
F	-4.84434900	-2.85077100	-4.21858100
F	-7.14989300	0.91669500	-2.28070000
F	-4.95263900	1.43906900	-0.67254100
F	-2.67501400	-2.37855100	-2.56166400
F	2.67365100	-2.37957000	-2.56223900
F	4.84249000	-2.85245300	-4.21960800
F	7.08866900	-1.22166100	-4.06800900
F	7.14966000	0.91421500	-2.28211300
F	4.95290300	1.43727200	-0.67349900
F	3.96053100	-2.68837000	0.59155500
F	6.13068100	-3.26175200	2.21316700
F	7.03686800	-1.37200000	4.04625700
F	5.78822900	1.10675500	4.22939300
F	3.65843500	1.71050100	2.56250400
H	-0.00025700	-1.16269100	-0.01169400

7. $[Fe^{II}Hpy]^{-}$, Complex **A**

E= -5545.12033375 hartrees

Fe	0.00000300	0.25088900	-0.01457300
N	-1.38154400	0.02528300	-1.25159100
O	-1.26751900	-0.01978400	-2.60030900
B	-0.00026300	0.58390300	-3.18549300
O	1.26690200	-0.02023200	-2.60057200
N	1.38121900	0.02477300	-1.25187700
C	2.60064100	-0.18605700	-0.74100600
C	2.60448000	-0.16269500	0.71344800
N	1.39101800	0.06601300	1.22644900
O	1.26763600	-0.04185700	2.57182900
B	0.00039100	0.56027100	3.16773800
O	-1.26722100	-0.04134500	2.57209100
N	-1.39082700	0.06654200	1.22673400
C	-2.60447800	-0.16171600	0.71398000
C	-2.60094000	-0.18508700	-0.74047400
F	0.00065600	1.94696400	2.99621900
F	0.00044700	0.15949700	4.49805800
N	0.00037800	2.25533900	-0.02388300

C	-1.17431100	2.95789600	-0.02240500
C	1.17533400	2.95745200	-0.02254300
C	-1.20742100	4.35778900	-0.02068500
H	-2.09234000	2.36895100	-0.01670500
C	1.20897300	4.35733100	-0.02082800
H	2.09313800	2.36815400	-0.01694600
C	0.00091200	5.07832200	-0.02033600
H	-2.17394600	4.86812600	-0.01626300
H	2.17569100	4.86730300	-0.01651900
H	0.00112000	6.17206000	-0.01701000
F	-0.00046900	0.21360300	-4.52357900
F	0.00000500	1.97320400	-2.99702400
C	-3.78655500	-0.42548800	-1.58235800
C	-4.93279400	0.39036700	-1.50070400
C	-3.82758600	-1.47543100	-2.52614600
C	-6.05884800	0.19271100	-2.30834300
C	-4.93434500	-1.68433600	-3.35870800
C	-6.05647300	-0.84990900	-3.24631300
C	-3.77793700	-0.45019300	1.56200300
C	-4.22503500	0.46893800	2.53522200
C	-4.49311800	-1.66051600	1.46620400
C	-5.31237700	0.19795400	3.37420600
C	-5.59312700	-1.95144600	2.28317600
C	-6.00181000	-1.01727900	3.24523900
C	3.78601000	-0.42687600	-1.58311800
C	4.93247400	0.38869900	-1.50181600
C	3.82659200	-1.47698300	-2.52674700
C	6.05830400	0.19065500	-2.30967200
C	4.93312400	-1.68627900	-3.35951200
C	6.05547200	-0.85210000	-3.24749200
C	3.77798900	-0.45168300	1.56122900
C	4.49263200	-1.66230900	1.46525300
C	4.22568000	0.46723200	2.53438100
C	5.59267800	-1.95373700	2.28199700
C	5.31307200	0.19575500	3.37314100
C	6.00195300	-1.01977300	3.24400600
F	-7.08726100	-1.29021600	4.06130500
F	-6.26303300	-3.15985000	2.16442900
F	-4.07803700	-2.63680400	0.56038200
F	-5.73398700	1.12934900	4.30925000
F	-3.60554200	1.70530100	2.64623600
F	-7.16190000	-1.05768400	-4.05507100
F	-4.94966100	-2.73216700	-4.26463400
F	-7.16019100	1.03000700	-2.20622200
F	-4.94442000	1.47325200	-0.61609200
F	-2.77225600	-2.36886700	-2.60681700

F	2.77108200	-2.37024300	-2.60698900
F	4.94801100	-2.73427500	-4.26525500
F	7.16067900	-1.06026900	-4.05644900
F	7.15987500	1.02769200	-2.20790400
F	4.94455400	1.47170700	-0.61736100
F	4.07694700	-2.63839600	0.55949000
F	6.26204100	-3.16242500	2.16308300
F	7.08744800	-1.29320000	4.05984800
F	5.73527500	1.12694600	4.30812100
F	3.60676600	1.70387300	2.64553200
H	-0.00027100	-1.27326600	0.01964600

8. $[Fe^{II}py_2]^0$, Complex **B**

E = -5568.56189964 hartrees

Fe	0.00534000	-0.03525400	0.00374000
N	-1.40388300	-0.12037900	-1.24793800
O	-1.26470500	-0.15164200	-2.59836000
B	0.00017000	0.49439600	-3.16005000
O	1.28668100	-0.13517300	-2.59047100
N	1.41968900	-0.11698300	-1.24596800
C	2.63732900	-0.29943800	-0.73743100
C	2.64768700	-0.26990500	0.72841300
N	1.43636900	-0.07928900	1.24022500
O	1.28168500	-0.01886900	2.58320300
O	-1.22982900	-0.04700300	2.56408400
N	-1.41746600	-0.09084400	1.26525600
C	-2.63189600	-0.27681400	0.73099400
C	-2.61509600	-0.29809800	-0.73351700
N	-0.01584900	1.96160700	0.03795200
C	-1.19401400	2.66346400	0.05061100
C	1.15401800	2.67783700	0.03059800
C	-1.23353000	4.06333300	0.06246900
H	-2.11514300	2.08519100	0.05363500
C	1.17813500	4.07767000	0.04225500
H	2.08171000	2.11017000	0.01233300
C	-0.03212100	4.79250500	0.05760200
H	-2.20421700	4.56418200	0.07353100
H	2.14283900	4.59010800	0.03569700
H	-0.03855500	5.88548400	0.06360600
N	-0.00714700	-2.05759000	0.02292500
C	0.00686500	-2.77078100	-1.14777800
C	-0.02879900	-2.74883000	1.20765100
C	0.00418900	-4.17289700	-1.16309900
H	0.01811800	-2.19654100	-2.07369300
C	-0.03172300	-4.14896600	1.25300000
H	-0.05350200	-2.15263500	2.12025800

C	-0.01379200	-4.87985800	0.05104000
H	0.01555700	-4.69102800	-2.12437000
H	-0.05059600	-4.65078600	2.22336300
H	-0.01591400	-5.97299900	0.06173800
F	0.01215600	0.15968200	-4.49829600
F	0.00051300	1.86304700	-2.90048300
C	-3.82195400	-0.43696900	-1.57702300
C	-4.87348900	0.49665700	-1.50727200
C	-3.96001800	-1.47871800	-2.51491800
C	-6.01024900	0.41029800	-2.31921100
C	-5.08095800	-1.58645700	-3.34755500
C	-6.11150700	-0.63882600	-3.24587100
C	-3.83751300	-0.45368800	1.56342600
C	-4.22894000	0.51401200	2.51121100
C	-4.62614800	-1.61871200	1.48875300
C	-5.33958800	0.33461000	3.34534500
C	-5.74849300	-1.82083800	2.30100200
C	-6.10340200	-0.83805600	3.23788300
C	3.84227800	-0.44426200	-1.57962900
C	4.90485000	0.47713000	-1.50518800
C	3.96867900	-1.48072000	-2.52601300
C	6.03961400	0.38433600	-2.31899000
C	5.08661600	-1.59360600	-3.36186500
C	6.12786700	-0.65827300	-3.25441600
C	3.85544500	-0.44143600	1.56206700
C	4.63356800	-1.61387900	1.49609800
C	4.26670700	0.54278300	2.48330200
C	5.76583000	-1.80825400	2.29648500
C	5.39008900	0.37257200	3.30216900
C	6.14271400	-0.80853500	3.20672900
F	-7.20538700	-1.02245400	4.04899000
F	-6.48963500	-2.98490600	2.20370100
F	-4.25937100	-2.63560100	0.60467800
F	-5.70197000	1.31017400	4.25515200
F	-3.52743800	1.70943300	2.59629800
F	-7.22505100	-0.73966200	-4.05445000
F	-5.19041400	-2.62761600	-4.24894300
F	-7.01566500	1.35469900	-2.22808200
F	-4.76713000	1.57942300	-0.63073500
F	-2.97941200	-2.45770300	-2.60010300
F	2.97849600	-2.44951200	-2.61565600
F	5.18356800	-2.62918400	-4.27079200
F	7.23905200	-0.76518700	-4.06512900
F	7.05553700	1.31673500	-2.22166200
F	4.81131000	1.55497000	-0.62074700
F	4.24788900	-2.64092300	0.63400700

F	6.49628300	-2.97894600	2.21174600
F	7.25459100	-0.98520600	4.00436800
F	5.77319300	1.36299200	4.18575900
F	3.56992200	1.74103800	2.55800700
H	0.19842000	0.03616600	2.68565000

9. $[Fe^{II}py]^0$, Complex **B**

E = -5320.28201423 hartrees

Fe	-0.00305000	0.53094800	-0.02510900
N	-1.37233700	0.19319400	-1.28212300
O	-1.24028800	0.16062000	-2.62843400
B	0.00207800	0.86075500	-3.16413200
O	1.27504300	0.20343600	-2.61588300
N	1.39181100	0.21789000	-1.27365100
C	2.57737200	-0.13694400	-0.75676700
C	2.58500600	-0.12478200	0.69088600
N	1.39494000	0.19444000	1.21125600
O	1.25970500	0.21055200	2.55825400
O	-1.24564100	0.27039200	2.52500400
N	-1.40519000	0.22040300	1.22790000
C	-2.58992600	-0.12110800	0.67910600
C	-2.55736200	-0.15623000	-0.76647800
N	-0.00256900	2.55584800	0.14729500
C	-1.18259800	3.24449400	0.20788200
C	1.17528000	3.25050600	0.14003400
C	-1.21724200	4.64411500	0.26242000
H	-2.09498300	2.64684700	0.21562700
C	1.20664800	4.65010600	0.19397800
H	2.08923000	2.65730500	0.09011400
C	-0.00639100	5.36120100	0.25342400
H	-2.18067200	5.15630600	0.30937400
H	2.16857600	5.16721800	0.18550500
H	-0.00797400	6.45372500	0.29202500
F	0.01738300	0.63592600	-4.51894900
F	-0.01542200	2.20778500	-2.78495800
C	-3.70345700	-0.52882100	-1.62081200
C	-4.90927900	0.19671000	-1.59007900
C	-3.62653900	-1.60856400	-2.52381300
C	-5.99376100	-0.12134500	-2.41575800
C	-4.69368200	-1.94477500	-3.36609300
C	-5.88146200	-1.19819000	-3.30916800
C	-3.75902800	-0.45407400	1.51513600
C	-4.28084200	0.47486200	2.43727500
C	-4.37352800	-1.72051300	1.47120700
C	-5.35620500	0.16631300	3.27846800
C	-5.45659700	-2.05468200	2.29382800

C	-5.94649200	-1.10540900	3.20413900
C	3.73089900	-0.50084300	-1.60295300
C	4.93763400	0.22240200	-1.55509200
C	3.66063400	-1.57050600	-2.51907600
C	6.02885700	-0.08793500	-2.37471300
C	4.73377900	-1.89788100	-3.35723000
C	5.92224500	-1.15391300	-3.28184400
C	3.75231700	-0.45802200	1.53311500
C	4.36687100	-1.72392800	1.48351100
C	4.28021400	0.47405400	2.44803500
C	5.45693200	-2.05556700	2.29811000
C	5.36499300	0.16860700	3.27821800
C	5.95508800	-1.10318900	3.20080900
F	-7.01172100	-1.42007200	4.02243700
F	-6.02825500	-3.31114600	2.22985700
F	-3.86975900	-2.69484300	0.61112100
F	-5.85267400	1.10593300	4.16149500
F	-3.74702800	1.75715800	2.48534300
F	-6.94145400	-1.52530600	-4.12856300
F	-4.59631300	-3.01513700	-4.23189300
F	-7.15799000	0.62198800	-2.36750400
F	-5.02111300	1.29948700	-0.74048800
F	-2.48361100	-2.39096300	-2.55380800
F	2.51702000	-2.35109700	-2.56686300
F	4.64205900	-2.95793900	-4.23612000
F	6.98857600	-1.47327400	-4.09601500
F	7.19389200	0.65279500	-2.30782200
F	5.04324400	1.31608500	-0.69216800
F	3.85780700	-2.69723500	0.62699600
F	6.02867900	-3.31110400	2.23161400
F	7.02741100	-1.41524500	4.00966700
F	5.86841000	1.11003100	4.15437100
F	3.73882500	1.75233800	2.50305600
H	0.18978400	0.28669200	2.67873600

10. $[Fe^{II}(gly)^{\bullet}py_2]^{-}$, Complex **B**
E = -5568.65181896 hartrees

Fe	-0.00841800	-0.04707500	0.00961000
N	-1.40108100	-0.14022600	-1.24002900
O	-1.26264200	-0.18207400	-2.60341200
B	0.00538600	0.44134200	-3.16390800
O	1.27332700	-0.17937600	-2.60755700
N	1.40362900	-0.14137400	-1.24167400
C	2.63897600	-0.31570600	-0.72908100
C	2.65542700	-0.26543100	0.72091400
N	1.42681500	-0.06831500	1.24172000

O	1.28011100	-0.08979100	2.60825000
O	-1.24677900	-0.08744200	2.57742600
N	-1.42221700	-0.07856400	1.26510600
C	-2.65188500	-0.26206800	0.72273700
C	-2.63255700	-0.30417400	-0.72916500
N	-0.01094500	1.94261700	0.00392500
C	-1.18535800	2.65069200	0.00218800
C	1.16438800	2.64944800	-0.00697300
C	-1.21608500	4.05120400	-0.00146400
H	-2.10617400	2.07071400	0.00765800
C	1.19641800	4.04978000	-0.01112600
H	2.08438700	2.06852000	-0.01255300
C	-0.00951100	4.77295000	-0.00847500
H	-2.18400800	4.55875800	-0.00090800
H	2.16480600	4.55635800	-0.01960600
H	-0.00887800	5.86681100	-0.01421200
N	-0.01190900	-2.06341600	0.04927300
C	0.02075600	-2.78105400	-1.11767500
C	-0.04720100	-2.74631900	1.23700000
C	0.02317400	-4.18362900	-1.12539700
H	0.04514500	-2.20546900	-2.04297400
C	-0.04519300	-4.14709900	1.28971200
H	-0.08607300	-2.13812100	2.14147500
C	-0.00807300	-4.88448200	0.09233300
H	0.05058100	-4.70699700	-2.08396400
H	-0.07443500	-4.64401600	2.26291900
H	-0.00512900	-5.97835700	0.10877500
F	0.00150300	0.10342900	-4.51721300
F	0.00272200	1.83031800	-2.95119800
C	-3.82993400	-0.42412200	-1.57771400
C	-4.91215600	0.47680100	-1.47291300
C	-3.95390100	-1.42883900	-2.56384900
C	-6.04818200	0.39512900	-2.28541700
C	-5.07116200	-1.52338800	-3.40128200
C	-6.12802900	-0.61088800	-3.25922800
C	-3.84477400	-0.44278100	1.56106300
C	-4.18827100	0.48564800	2.57151300
C	-4.68774100	-1.57082000	1.44935000
C	-5.28528500	0.30095700	3.42064600
C	-5.80241100	-1.76984600	2.27247900
C	-6.10083500	-0.83100000	3.27034900
C	3.83699500	-0.44135900	-1.57410700
C	4.92372400	0.45535400	-1.47229000
C	3.95708300	-1.44753800	-2.55976100
C	6.06057700	0.36514800	-2.28276000
C	5.07441900	-1.54990300	-3.39581200

C	6.13676700	-0.64351100	-3.25390800
C	3.85388700	-0.43051700	1.55449800
C	4.70410100	-1.55529500	1.44340800
C	4.21094800	0.51588800	2.54480000
C	5.83585900	-1.73185200	2.24730500
C	5.32714100	0.35447200	3.37201500
C	6.14908400	-0.77403000	3.22303900
F	-7.20043500	-1.01497400	4.09697500
F	-6.59052400	-2.90615300	2.13642800
F	-4.38091800	-2.57516700	0.52541300
F	-5.60185000	1.24840800	4.38496800
F	-3.46928700	1.66860700	2.69290200
F	-7.24809900	-0.70778000	-4.07169500
F	-5.16701400	-2.53930300	-4.34122300
F	-7.07724300	1.31947400	-2.16078500
F	-4.83717600	1.54489800	-0.57140400
F	-2.97571900	-2.40840800	-2.67806700
F	2.97336500	-2.42201500	-2.67405000
F	5.16577200	-2.56869700	-4.33336700
F	7.25885500	-0.75068300	-4.06265700
F	7.09411900	1.28524300	-2.16005900
F	4.85190200	1.53126700	-0.57905200
F	4.38436000	-2.57908200	0.54599500
F	6.62623400	-2.86725400	2.11776800
F	7.26797900	-0.93515900	4.02825900
F	5.65837100	1.32242200	4.31068100
F	3.48091500	1.69296200	2.66434900
H	0.21554900	-0.01870600	2.70804400

11. $[Fe^{I}py]^{-}$, Complex **B**

E = -5320.40924106 hartrees

Fe	0.00528800	0.56107900	-0.06958700
N	-1.33798500	0.10066600	-1.29018100
O	-1.23446800	0.06363400	-2.65596200
B	0.00100600	0.74559300	-3.18789600
O	1.26328400	0.10784600	-2.65942100
N	1.36054300	0.12774500	-1.29418900
C	2.57090000	-0.18696600	-0.77924700
C	2.58223600	-0.13589500	0.64983700
N	1.36240800	0.17235800	1.15610100
O	1.24102600	0.18039200	2.51276500
O	-1.21518200	0.23479500	2.49801400
N	-1.35248900	0.20369100	1.17795100
C	-2.56929100	-0.12322700	0.65483600
C	-2.54914000	-0.19750500	-0.77240700
N	-0.00926500	2.52342200	0.23385300

C	-1.19136800	3.21564600	0.24571700
C	1.16720100	3.22518900	0.25909000
C	-1.22867900	4.61587300	0.27108800
H	-2.10090000	2.61256000	0.23982600
C	1.19319600	4.62555700	0.28676600
H	2.08160400	2.62936600	0.26077500
C	-0.02075200	5.33830900	0.28865800
H	-2.19546800	5.12537200	0.27672400
H	2.15574000	5.14280300	0.30458300
H	-0.02522200	6.43201600	0.30475400
F	0.00382300	0.53766200	-4.56237800
F	-0.02179200	2.11553100	-2.83553200
C	-3.70377600	-0.53451300	-1.62424800
C	-4.89972800	0.20988200	-1.58590000
C	-3.65938700	-1.60528500	-2.54374100
C	-5.99369800	-0.07681800	-2.41126800
C	-4.73382600	-1.90414100	-3.39072600
C	-5.90764700	-1.13912700	-3.32198900
C	-3.71978200	-0.43514100	1.51743400
C	-4.19549800	0.48829400	2.47396000
C	-4.38407600	-1.67878700	1.47318900
C	-5.25376500	0.19454200	3.34129500
C	-5.45742100	-1.99315600	2.31661500
C	-5.89107100	-1.05267900	3.26119100
C	3.72433100	-0.52480900	-1.63125000
C	4.92659600	0.20903100	-1.58499300
C	3.67207700	-1.58578600	-2.56206400
C	6.01900900	-0.07843500	-2.41219300
C	4.74438400	-1.88445100	-3.41175100
C	5.92461700	-1.13005900	-3.33436800
C	3.73675300	-0.44379900	1.51062300
C	4.40674400	-1.68417800	1.45934100
C	4.21873600	0.48406400	2.45938800
C	5.49127800	-1.99112300	2.29121400
C	5.28948800	0.19827700	3.31371100
C	5.93192700	-1.04608700	3.22810900
F	-6.94955600	-1.35017700	4.10673800
F	-6.07320500	-3.23539700	2.24695200
F	-3.94246800	-2.66765100	0.59265500
F	-5.70388500	1.13701500	4.25552800
F	-3.64748300	1.76472600	2.52823800
F	-6.98196000	-1.43624600	-4.14631300
F	-4.66511100	-2.97243500	-4.27109600
F	-7.14776000	0.69269100	-2.35196400
F	-5.00190400	1.31171200	-0.73097900
F	-2.54806400	-2.43142500	-2.58413400

F	2.55458300	-2.40323700	-2.61045300
F	4.66760700	-2.94320200	-4.30291900
F	6.99704300	-1.42765600	-4.16102500
F	7.17958400	0.68056100	-2.34370700
F	5.03719500	1.30188600	-0.71913500
F	3.96120400	-2.67504700	0.58416500
F	6.11181700	-3.23025100	2.21738800
F	7.00092500	-1.33689300	4.06203500
F	5.74579700	1.14499300	4.21991400
F	3.65862200	1.75495200	2.52113100
H	0.14130400	0.24074100	2.63312800

12. $[Fe^{0}py]^{2-}$, Complex **B**

E = -5320.41480778 hartrees

Fe	0.00705500	0.27296400	-0.00781300
N	-1.33841300	-0.11268000	-1.22304300
O	-1.24427300	-0.16579600	-2.59728500
B	0.00819100	0.41992500	-3.18085200
O	1.26321300	-0.16278700	-2.60054800
N	1.35475900	-0.11232600	-1.22550000
C	2.61063600	-0.28146900	-0.72224800
C	2.62321900	-0.20922100	0.71528900
N	1.37482200	-0.00639000	1.22067600
O	1.23741300	-0.06170200	2.58108700
O	-1.20809200	-0.04147500	2.57271800
N	-1.35799600	0.00670700	1.23957400
C	-2.60491200	-0.19814000	0.72003700
C	-2.59227000	-0.27479700	-0.71852600
N	-0.00965500	2.17700300	-0.02286100
C	-1.19366200	2.88436100	-0.03727800
C	1.16960300	2.89289800	-0.03325900
C	-1.22473000	4.28231600	-0.05384800
H	-2.10747700	2.28752400	-0.03164900
C	1.19114300	4.29079300	-0.04992200
H	2.08761300	2.30236400	-0.02522800
C	-0.01950200	5.01413800	-0.06043700
H	-2.19544300	4.78738800	-0.06438900
H	2.15830600	4.80266600	-0.05768000
H	-0.02331500	6.10852200	-0.07647700
F	0.00668500	0.04628500	-4.53734600
F	0.00669700	1.83233000	-3.04697200
C	-3.77051500	-0.44374200	-1.56786500
C	-4.91684600	0.37966600	-1.44753100
C	-3.84184900	-1.43994100	-2.57697300
C	-6.04334700	0.24553100	-2.26514300
C	-4.94821300	-1.57691600	-3.42167400

C	-6.06193000	-0.73691700	-3.26550800
C	-3.76354500	-0.44318200	1.57976600
C	-4.10436700	0.43854000	2.63841900
C	-4.60048100	-1.57845200	1.44876100
C	-5.17627200	0.20188400	3.50477400
C	-5.69384600	-1.82322700	2.28784100
C	-5.98298100	-0.93335100	3.33129200
C	3.78703400	-0.45557800	-1.57330900
C	4.93343100	0.36854100	-1.46273400
C	3.85249600	-1.45631000	-2.57794800
C	6.05627500	0.22955000	-2.28482700
C	4.95492800	-1.59838000	-3.42698500
C	6.06960100	-0.75806700	-3.28001100
C	3.78706200	-0.43981600	1.57264800
C	4.63144300	-1.57064700	1.44432800
C	4.13346600	0.45604600	2.61778100
C	5.73491500	-1.79785500	2.27479500
C	5.21667200	0.23787900	3.47431600
C	6.02973500	-0.89366500	3.30464200
F	-7.06480100	-1.16707700	4.18016200
F	-6.46821300	-2.97329000	2.13178500
F	-4.30701500	-2.55616300	0.49135800
F	-5.49508100	1.11497800	4.50960300
F	-3.42532100	1.64342700	2.78216200
F	-7.17773500	-0.88244600	-4.08957900
F	-4.99381500	-2.59188800	-4.37509200
F	-7.12983700	1.11111900	-2.12989100
F	-4.91713000	1.44369100	-0.53342700
F	-2.83501400	-2.38993300	-2.68480300
F	2.84303800	-2.40420700	-2.67749700
F	4.99511500	-2.61728600	-4.37621400
F	7.18163500	-0.90881500	-4.10800200
F	7.14437500	1.09432600	-2.15828300
F	4.93857700	1.43689300	-0.55367600
F	4.33571300	-2.55995300	0.50029000
F	6.51411300	-2.94508600	2.12500800
F	7.12047400	-1.11165300	4.14581800
F	5.54079000	1.16584500	4.46336900
F	3.44175400	1.65424500	2.75791800
H	0.11270000	-0.04083700	2.68618300

13. $[Fe^{I}py\ldots H]^{0}$, Complex **B**

E = -5320.87506508 hartrees

Fe	-0.01220200	0.44712700	0.05471000
N	-1.35684400	0.08031500	-1.18884700
O	-1.26858800	0.11671500	-2.53691400

B	0.01581900	0.70377900	-3.09500400
O	1.20456300	-0.04571600	-2.53341300
N	1.32320300	0.01555100	-1.18506600
C	2.56128300	-0.23965200	-0.69870000
C	2.61104500	-0.15729300	0.72370000
N	1.40576000	0.12960000	1.25107500
O	1.37897600	0.21331600	2.63981000
O	-1.29581600	-0.15387400	2.66185200
N	-1.37514800	-0.06476800	1.21836400
C	-2.61570200	-0.28461500	0.70364800
C	-2.59478200	-0.23364000	-0.70993000
N	0.00083900	2.44598500	0.20883000
C	-1.18295600	3.12957700	0.27565500
C	1.17426600	3.14467600	0.13119200
C	-1.22439500	4.52981400	0.26737300
H	-2.09121500	2.52734600	0.33625200
C	1.19606700	4.54538700	0.11756200
H	2.09049000	2.55474200	0.07862200
C	-0.01907900	5.25212900	0.18404900
H	-2.18937200	5.03873300	0.31967300
H	2.15353700	5.06641900	0.05047800
H	-0.02707600	6.34522100	0.16896600
F	-0.00285500	0.46784800	-4.45058700
F	0.10155500	2.06032200	-2.74325600
C	-3.74295200	-0.48196400	-1.60347300
C	-4.88482800	0.33987500	-1.58927200
C	-3.72684900	-1.53729900	-2.53831700
C	-5.96448000	0.13757400	-2.45761000
C	-4.78703000	-1.75690800	-3.42633400
C	-5.91101500	-0.91658100	-3.38236100
C	-3.81347000	-0.53116800	1.53112900
C	-4.27726200	0.43781500	2.44620400
C	-4.56199700	-1.72186300	1.43486000
C	-5.42025900	0.23891000	3.22861800
C	-5.71496400	-1.94414700	2.20002900
C	-6.14326200	-0.95872600	3.10269500
C	3.70531600	-0.54464800	-1.57845100
C	4.84984700	0.27439000	-1.61138400
C	3.68872100	-1.65367600	-2.44910400
C	5.92968100	0.01924000	-2.46475100
C	4.74991200	-1.92710200	-3.32100800
C	5.87570600	-1.08829900	-3.32497500
C	3.81592200	-0.38799700	1.54704000
C	4.49132100	-1.62427300	1.53961500
C	4.33605200	0.61499600	2.38875800
C	5.62678800	-1.86009200	2.32564200

C	5.46420000	0.40567200	3.19050500
C	6.11253800	-0.83914200	3.15682700
F	-7.27255000	-1.16561800	3.86679200
F	-6.41512300	-3.12960600	2.08745700
F	-4.13116900	-2.73407300	0.58096200
F	-5.85274800	1.21541900	4.10500100
F	-3.60947000	1.65299900	2.54583600
F	-6.96759100	-1.13111300	-4.24394600
F	-4.74809500	-2.80458700	-4.32498200
F	-7.06688100	0.97219300	-2.41915900
F	-4.93819500	1.42229600	-0.70596600
F	-2.64825400	-2.40722300	-2.56171600
F	2.61001000	-2.52307500	-2.42299900
F	4.71033900	-3.02650600	-4.15585000
F	6.93275000	-1.35518400	-4.17128000
F	7.03263000	0.85383700	-2.47635600
F	4.90216200	1.40896900	-0.79671300
F	4.00302400	-2.66623000	0.75482000
F	6.25573700	-3.09048000	2.30230900
F	7.22831700	-1.05736200	3.93879700
F	5.95321500	1.41618800	3.99665700
F	3.73838500	1.87003300	2.40162800
H	0.39875000	0.23298800	2.83683500
H	-1.33237500	-1.11855500	2.85141100

14. $[Fe^{III}Hpy]^{0}$, Complex **B**

E = -5320.87251639 hartrees

Fe	0.00101800	0.26380500	-0.02070800
N	-1.38071600	0.04562200	-1.26563000
O	-1.25078800	0.00348600	-2.60686600
B	-0.00066900	0.68075700	-3.16209500
O	1.27559700	0.03063500	-2.60848600
N	1.40111300	0.05732300	-1.27148400
C	2.61288200	-0.19534800	-0.75923400
C	2.62491500	-0.18313700	0.68778200
N	1.41694800	0.04604400	1.20944600
O	1.27447100	0.03342500	2.54957500
O	-1.22938500	0.07141600	2.52618200
N	-1.39679200	0.05074500	1.23378600
C	-2.61327000	-0.18620300	0.69078900
C	-2.59199200	-0.20669700	-0.74904700
N	-0.01833500	2.31179600	0.13177700
C	-1.19906400	3.00027500	0.15615600
C	1.15483900	3.01373300	0.14408200
C	-1.24064000	4.40018300	0.19337900
H	-2.11268900	2.40491200	0.14756400

C	1.18162800	4.41401300	0.18163200
H	2.07491300	2.42854700	0.12338400
C	-0.03348500	5.12277900	0.20453100
H	-2.20743500	4.90783100	0.21111600
H	2.14278700	4.93256600	0.18916100
H	-0.03958000	6.21565900	0.23045000
F	0.00495800	0.42350100	-4.51066800
F	-0.00823000	2.03439900	-2.81397800
C	-3.76593900	-0.47439000	-1.60501600
C	-4.90326200	0.35362100	-1.57281400
C	-3.78272900	-1.55505800	-2.50987600
C	-6.01158500	0.13248500	-2.39854600
C	-4.87530300	-1.79585900	-3.35240300
C	-5.99361000	-0.94904800	-3.29338400
C	-3.79841800	-0.43933200	1.53341600
C	-4.24778800	0.51612500	2.46607800
C	-4.50145400	-1.65865600	1.48287800
C	-5.33779700	0.27770300	3.31134700
C	-5.60077600	-1.92210400	2.30984900
C	-6.01705800	-0.94833600	3.23080200
C	3.78917900	-0.46370000	-1.60995400
C	4.93252300	0.35587900	-1.56570200
C	3.80289800	-1.53585900	-2.52564400
C	6.04303900	0.13502900	-2.38835600
C	4.89703900	-1.77532400	-3.36659800
C	6.02113200	-0.93716300	-3.29440400
C	3.81350500	-0.44398700	1.52739800
C	4.50455700	-1.66947300	1.47237800
C	4.28462900	0.51565800	2.44419400
C	5.61486900	-1.93577800	2.28379300
C	5.38804400	0.27525800	3.27138100
C	6.05525100	-0.95743000	3.18874000
F	-7.09746900	-1.19331000	4.05284600
F	-6.26106400	-3.13382100	2.23855000
F	-4.07510300	-2.65752600	0.61000000
F	-5.75998100	1.24230300	4.20585100
F	-3.62163900	1.75542900	2.52398600
F	-7.07845800	-1.18148400	-4.11246500
F	-4.87072600	-2.86800200	-4.22125900
F	-7.10672000	0.97410000	-2.34885300
F	-4.91793100	1.45976500	-0.71982700
F	-2.70968200	-2.43010300	-2.54479600
F	2.72477400	-2.40393800	-2.57283000
F	4.88880600	-2.83880600	-4.24581100
F	7.10780800	-1.16916800	-4.11098600
F	7.14387900	0.96821900	-2.32533300

F	4.95051200	1.45433300	-0.70235600
F	4.05608200	-2.66804400	0.61169600
F	6.26340000	-3.15294000	2.21122700
F	7.14655700	-1.20510300	3.99428000
F	5.83237200	1.24246000	4.15121100
F	3.66208900	1.75612300	2.50816900
H	0.19895400	0.08983900	2.66966400
H	-0.01195400	-1.25044400	-0.01321300

15. $[Fe^{0}py\ldots H]^{-}$, Complex **B**

E = -5320.99155268 hartrees

Fe	-0.00502700	0.23715400	0.08313000
N	-1.34962100	-0.08885200	-1.16768500
O	-1.25819200	-0.07282500	-2.53245800
B	0.01024500	0.50156900	-3.10414400
O	1.23153400	-0.15526200	-2.51916500
N	1.34063200	-0.08617900	-1.15790600
C	2.59960400	-0.26284600	-0.67787600
C	2.64394600	-0.18910100	0.75169600
N	1.41359000	-0.00078100	1.27581200
O	1.37661100	0.02968800	2.68159000
O	-1.30865800	-0.35160200	2.69205500
N	-1.38836300	-0.15808100	1.23656800
C	-2.64657900	-0.32991100	0.73071100
C	-2.61005400	-0.30242000	-0.69368100
N	-0.01927100	2.14952600	0.09705300
C	-1.21309900	2.83323800	0.12276800
C	1.14732500	2.87637200	0.04728200
C	-1.26646100	4.23102300	0.10450500
H	-2.11837600	2.22561800	0.15805900
C	1.14830700	4.27532400	0.03057100
H	2.07425200	2.30252400	0.01727200
C	-0.07248000	4.97663000	0.05799400
H	-2.24286600	4.72248100	0.12271700
H	2.10527400	4.80220300	-0.01107100
H	-0.09321200	6.06982700	0.03899500
F	0.00529000	0.16977700	-4.45828100
F	0.05525300	1.89615700	-2.89697700
C	-3.77164600	-0.44231200	-1.58790100
C	-4.86645900	0.44318900	-1.53693000
C	-3.83345000	-1.45762800	-2.56774200
C	-5.96192000	0.34228200	-2.40318500
C	-4.90732200	-1.57000900	-3.45900700
C	-5.97963600	-0.66933000	-3.37333100
C	-3.84554300	-0.50570200	1.55804400

C	-4.17725000	0.41551300	2.58308300
C	-4.74634900	-1.58362900	1.38826700
C	-5.31197800	0.27248900	3.38738900
C	-5.89932600	-1.73794500	2.16781700
C	-6.18293900	-0.80885400	3.17924000
C	3.75542400	-0.48963600	-1.55841400
C	4.88345100	0.35680400	-1.55015200
C	3.78648300	-1.55985400	-2.48139900
C	5.97620400	0.17077400	-2.40511800
C	4.85718800	-1.75672000	-3.36153100
C	5.96061300	-0.89125500	-3.32023600
C	3.85256500	-0.35808200	1.57622200
C	4.65306400	-1.51912500	1.50832200
C	4.27155300	0.63003500	2.49506000
C	5.79918400	-1.69406400	2.29426400
C	5.40299400	0.47399600	3.30369300
C	6.17439800	-0.69341100	3.20169500
F	-7.31403300	-0.95667900	3.96829800
F	-6.73880100	-2.82746900	1.97890500
F	-4.46444500	-2.58058100	0.45171800
F	-5.61136500	1.21353300	4.36305400
F	-3.39667500	1.55272900	2.76162500
F	-7.05683100	-0.78343600	-4.23950000
F	-4.94469600	-2.58874400	-4.39894100
F	-7.01336400	1.24658300	-2.32642500
F	-4.85675400	1.50457800	-0.62449600
F	-2.83473300	-2.41719600	-2.62580400
F	2.75888800	-2.49061800	-2.48933700
F	4.86204400	-2.82749600	-4.24296300
F	7.03521600	-1.08932400	-4.17482200
F	7.05817700	1.04150400	-2.37391100
F	4.90840800	1.46679600	-0.69751300
F	4.27972600	-2.56875300	0.66821300
F	6.54483700	-2.86180400	2.20869800
F	7.30255300	-0.85493800	3.99191100
F	5.79097700	1.47747500	4.18048400
F	3.58011200	1.83285200	2.57305500
H	0.39278700	0.04657800	2.85530200
H	-1.28218900	-1.32901900	2.78646600

16. $[Fe^{II}Hpy]^{-}$, Complex **B**

E = 5320.99877613 hartrees

Fe	0.01207200	0.16116400	-0.00700400
N	-1.37592400	-0.04456000	-1.24502500
O	-1.25807900	-0.08915900	-2.59874500
B	0.00407500	0.52564800	-3.16899700

O	1.27695300	-0.07718500	-2.59388700
N	1.39317000	-0.03939100	-1.24290200
C	2.62373400	-0.22398700	-0.74026700
C	2.63571000	-0.19049400	0.71475000
N	1.41569400	0.00445500	1.22532200
O	1.26619500	-0.01283800	2.57218800
O	-1.22307900	0.01280900	2.56213800
N	-1.39266600	0.00453500	1.25623400
C	-2.61263800	-0.19197000	0.72368000
C	-2.59551100	-0.23010300	-0.73293300
N	-0.01992400	2.16620600	0.02836900
C	-1.20025600	2.86502500	0.02832000
C	1.15072300	2.88193200	0.03582400
C	-1.24222700	4.26488700	0.04229100
H	-2.11439400	2.27068200	0.01757600
C	1.17365400	4.28191300	0.04945100
H	2.07305900	2.29987900	0.02907200
C	-0.03959300	4.99574000	0.05248400
H	-2.21289700	4.76767100	0.04167400
H	2.13719300	4.79829000	0.05372300
H	-0.04733600	6.08946300	0.05988900
F	0.01071500	0.17871600	-4.51547400
F	0.00200200	1.91573300	-2.96194700
C	-3.78318700	-0.44129800	-1.58071100
C	-4.91014100	0.40156300	-1.50439400
C	-3.84509900	-1.48682500	-2.52835300
C	-6.03604500	0.23380700	-2.31890100
C	-4.95197900	-1.66660600	-3.36750200
C	-6.05446000	-0.80598000	-3.25950700
C	-3.79688000	-0.42935700	1.56719400
C	-4.19118500	0.49402400	2.56010000
C	-4.57254600	-1.60328900	1.46787800
C	-5.28024800	0.26313100	3.40926600
C	-5.67773800	-1.85142500	2.29156700
C	-6.03007500	-0.91435700	3.27304800
C	3.80811200	-0.43366700	-1.58880700
C	4.94228800	0.40002000	-1.50403600
C	3.86424300	-1.47023800	-2.54795400
C	6.06698900	0.23303700	-2.32001900
C	4.96938000	-1.64754700	-3.38973500
C	6.07817500	-0.79606400	-3.27256100
C	3.81983800	-0.43375800	1.56009200
C	4.57981800	-1.61779700	1.46410000
C	4.23712300	0.49946000	2.53309600
C	5.69304300	-1.86682700	2.27692300
C	5.33691900	0.26959400	3.36854100

C	6.07066500	-0.91874900	3.23832200
F	-7.11860800	-1.14692800	4.09994900
F	-6.40491600	-3.02710600	2.16703300
F	-4.21407700	-2.59193100	0.54998600
F	-5.64686100	1.20261200	4.36223100
F	-3.52666800	1.70828500	2.67327300
F	-7.16061600	-0.98469100	-4.07555300
F	-4.98781400	-2.71190100	-4.27681700
F	-7.11708300	1.09898900	-2.22146900
F	-4.90132500	1.48537100	-0.61997700
F	-2.81269800	-2.40709500	-2.60651200
F	2.82827500	-2.38607600	-2.63266600
F	4.99887800	-2.68444900	-4.30885400
F	7.18328500	-0.97382300	-4.09032800
F	7.15403500	1.08975400	-2.21310000
F	4.94073900	1.47585400	-0.60913400
F	4.19943000	-2.61087600	0.56207900
F	6.40452000	-3.05183800	2.15968200
F	7.16697700	-1.15237400	4.05323500
F	5.72657300	1.21755300	4.30269300
F	3.57813200	1.71660900	2.64455000
H	0.17107200	0.02381700	2.67665000
H	-0.01846300	-1.36254700	0.03496200

17. [Fe^{II}Hpy…H] , Complex **B**
E = -5321.45835734 hartrees

Fe	-0.01335100	0.20313200	0.08640400
N	-1.38842100	-0.00029300	-1.15631200
O	-1.27303300	-0.03049100	-2.49334500
B	-0.02549300	0.62034200	-3.08765600
O	1.23754100	-0.01061400	-2.52112600
N	1.36733600	0.01022300	-1.18309100
C	2.60159300	-0.19427000	-0.71147700
C	2.65156400	-0.18867900	0.74219000
N	1.46096000	0.00734800	1.28917600
O	1.41691300	-0.03620600	2.66981500
O	-1.32325700	0.05737700	2.69732500
N	-1.45221900	0.03395400	1.27312500
C	-2.66333800	-0.19392900	0.76145700
C	-2.62918100	-0.23048100	-0.68178000
N	0.03904400	2.22397200	0.14442900
C	-1.13130000	2.93746600	0.13691700
C	1.21998400	2.91775800	0.14517100
C	-1.15303400	4.33776100	0.13571000
H	-2.05548700	2.35901000	0.12412800
C	1.26402100	4.31812700	0.14451800

H	2.13585500	2.32664800	0.14225100
C	0.06162700	5.04794400	0.13886000
H	-2.11458300	4.85640800	0.12515100
H	2.23405100	4.82067700	0.14269000
H	0.07058400	6.14096200	0.13243500
F	-0.04082400	0.29969000	-4.42625000
F	-0.03850400	1.98970000	-2.81761500
C	-3.78606000	-0.48847400	-1.55812600
C	-4.92706000	0.33692100	-1.54332800
C	-3.78882200	-1.55973800	-2.47704100
C	-6.01761000	0.12764000	-2.39523600
C	-4.85933300	-1.78429300	-3.35166600
C	-5.97928100	-0.93880500	-3.30702800
C	-3.87747300	-0.42776200	1.57575700
C	-4.40011900	0.56910400	2.42907900
C	-4.59936500	-1.63809200	1.49510700
C	-5.57602500	0.37770800	3.16552100
C	-5.78215300	-1.85206900	2.21486200
C	-6.27012100	-0.83814800	3.05459900
C	3.76431100	-0.42046500	-1.59089000
C	4.88882000	0.42608400	-1.55985000
C	3.79191200	-1.48257000	-2.51914400
C	5.98948000	0.24415900	-2.40488100
C	4.87411500	-1.68103600	-3.38581100
C	5.97817300	-0.81609400	-3.32461200
C	3.87448500	-0.43611100	1.53781800
C	4.58459400	-1.64819800	1.44020100
C	4.37151200	0.52350200	2.44112500
C	5.73714300	-1.90103300	2.19521400
C	5.51746800	0.29590700	3.21270300
C	6.20298700	-0.92266000	3.08698500
F	-7.42733300	-1.03810400	3.77499400
F	-6.45424300	-3.05387500	2.12129000
F	-4.11292200	-2.66998400	0.69976500
F	-6.06380800	1.37728300	3.98282800
F	-3.75703000	1.79635200	2.51570500
F	-7.04638600	-1.15992000	-4.15359800
F	-4.83652700	-2.84626100	-4.23384800
F	-7.11539600	0.96817100	-2.35556800
F	-4.96430000	1.43356600	-0.67555700
F	-2.72164000	-2.44292400	-2.49619000
F	2.74029700	-2.38340500	-2.55620300
F	4.87728200	-2.73540200	-4.27755700
F	7.05561500	-1.01047700	-4.16477000
F	7.07033500	1.10538700	-2.35146600
F	4.89620800	1.51692400	-0.68515400

F	4.11357000	-2.64970000	0.59532500
F	6.40215000	-3.10677600	2.08220800
F	7.33523800	-1.15761000	3.83913700
F	5.98418800	1.26307100	4.08197500
F	3.73097300	1.75117100	2.55214200
H	0.43999700	0.02835500	2.85957000
H	-1.88872100	-0.66607600	3.05524500
H	0.02399500	-1.31918800	0.12006700