Supporting Information

Iron L-edge X-ray Absorption Spectroscopy of Oxy-Picket Fence Porphyrin: Experimental Insight into Fe–O_2 Bonding

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SI Table S1. First Shell Bond Lengths of Oxy-Heme Complexes.

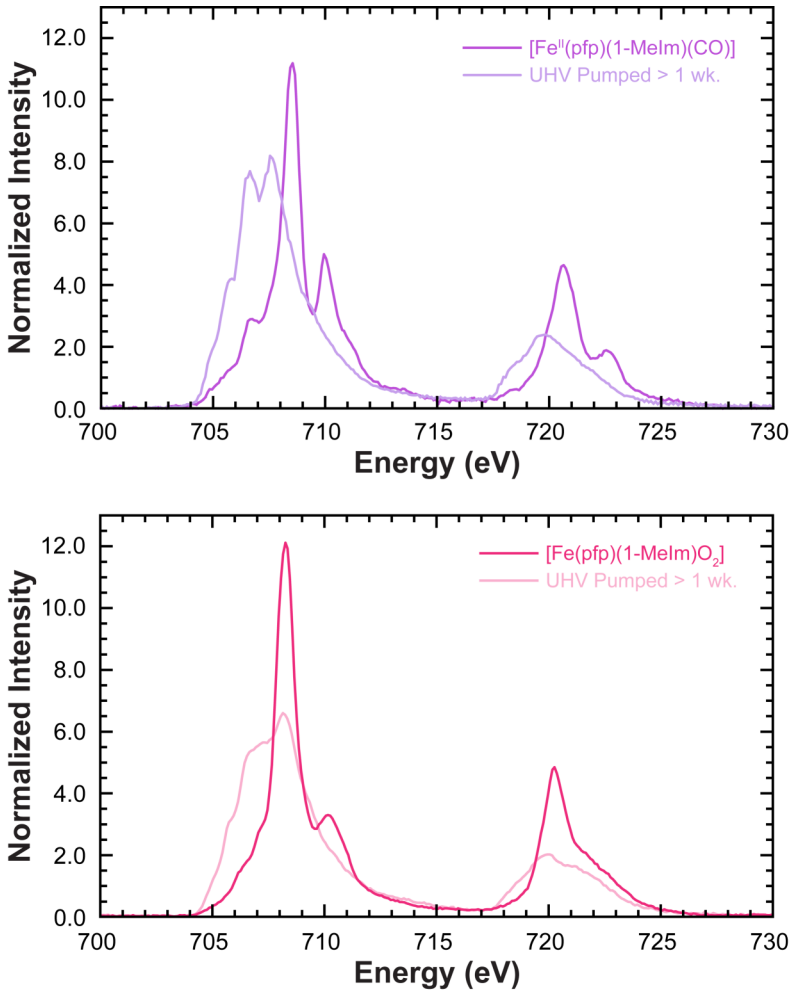
	Fe–O_2	Fe-N–Transaxial	Fe–N Equatorial	Fe Out-of-Plane	∠ Fe–O–O	O–O	Ref.
Oxy-pfp Crystal	1.75	2.07	1.98	0.03	129.33	1.16	1,2
Fe^{II}–O_2	1.75	2.07	2.00	0.05	120.97	1.30	
Fe^{III}–OO^-	1.79	2.07	2.00	0.03	119.82	1.30	
Hemoglobin–O_2	1.78-1.82	2.06	2.02	0.03	125.87	1.41	3
Myoglobin–O_2	1.81	2.06	2.01	0.02	122.53	1.24	4

First shell bond lengths (in Å) of geometry optimized using Gaussian 09[5] with BP86[6,7] (Fe^{II}–O_2) and UBP86 (Fe^{III}–OO^-) with 6-311G* on iron and 6-31G* on other light atoms (C, N, O, H). Values compared to crystal structure geometries where available.

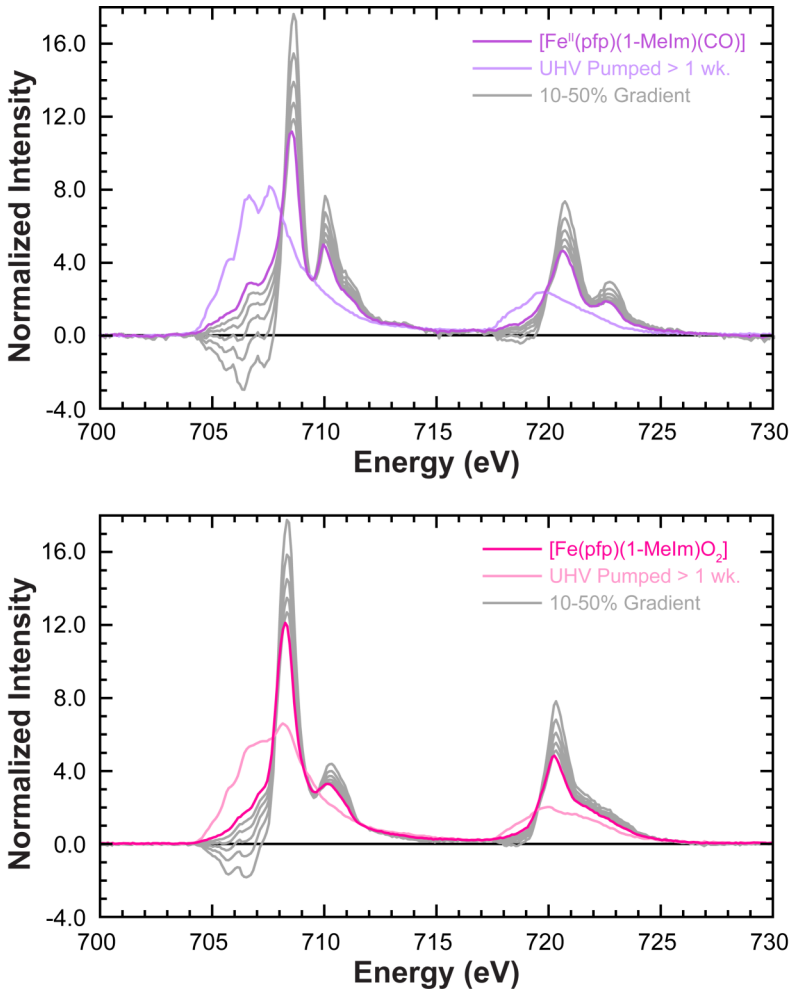
SI Table S2. DFT Parameters for [Fe(pfp)(1-MeIm)O_2].

	Fe–O_2	Fe–O_2^- (S)	Fe–O_2^- (T)
Fragment		Mulliken Fragment Charges	
Fe	1.22	1.23	1.25
O_2	–0.34	–0.35	–0.41
pfp	–1.01	–1.02	–0.99
1-MeIm	0.14	0.14	0.15
Fragment		Mulliken Spin Densities	
Fe	0.00	0.72	1.02
O_2	0.00	–0.69	–0.96
pfp	0.00	0.02	0.01
1-MeIm	0.00	0.00	0.00
$\langle S^2 \rangle$	0.00	0.45	2.02
Vibration		Frequencies (cm^{-1})	
Fe–O	670	554	532
O–O	1203	1188	1205
		Energy Difference (kcal/mol)	
Δ kcal/mol	0.0	–0.9 (–2.4)	4.2

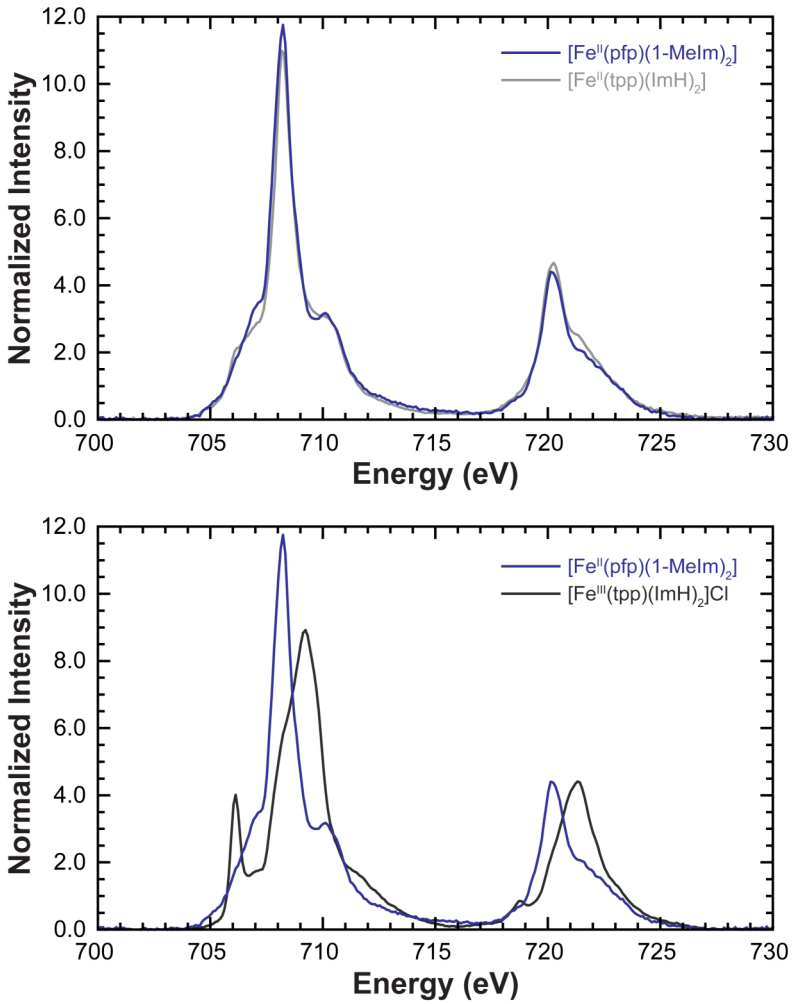
Optimized using UBP86 with 6-311G* on iron and 6-31G* on other light atoms.[5-7] Vertical triplet (T) state energy calculated in order to apply Yamaguchi's spin-projected correction[8,9] of the spin contaminated singlet (S) state, $E_S = (E_C - aE_{S+1}) / (1 - a)$ where $a = [\langle S^2 \rangle_C - s(s+1)] / 2(s+1)$, E_C is the spin-contaminated energy for the singlet state, E_{S+1} is the energy of the triplet state $\langle S^2 \rangle_C$ is the calculated spin expectation value of the spin-contaminated singlet state, and $s = 0$ for the ground state. Corrected singlet energy given in parenthesis.



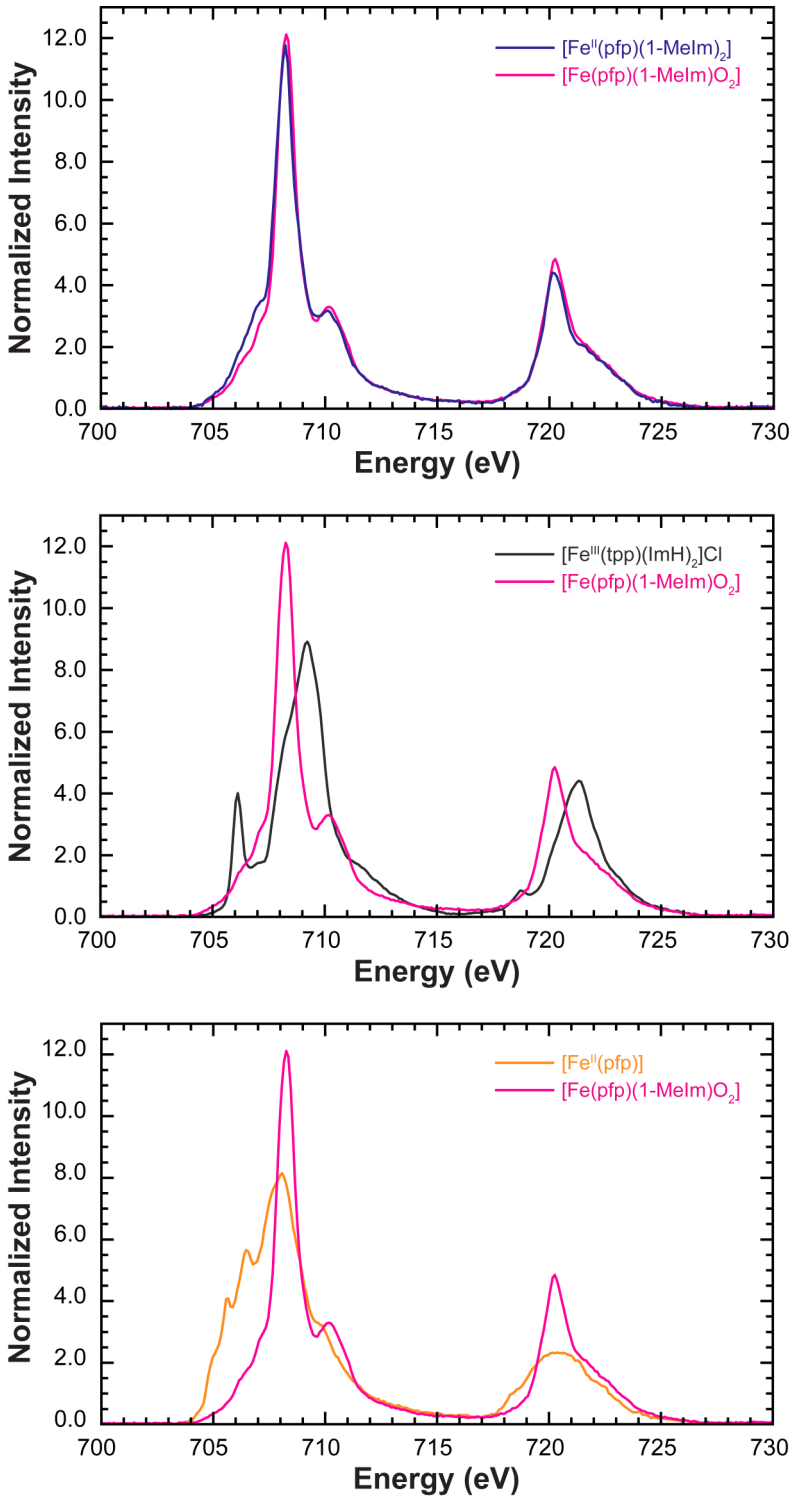
SI Figure S1. Top: Normalized L-edge data for [Fe^{II}(pfp)(1-MeIm)(CO)] vs. the same sample pumped for one week under UHV conditions. Bottom: Normalized L-edge data for [Fe(pfp)(1-MeIm)O_2] vs. the same sample pumped for one week under UHV conditions.



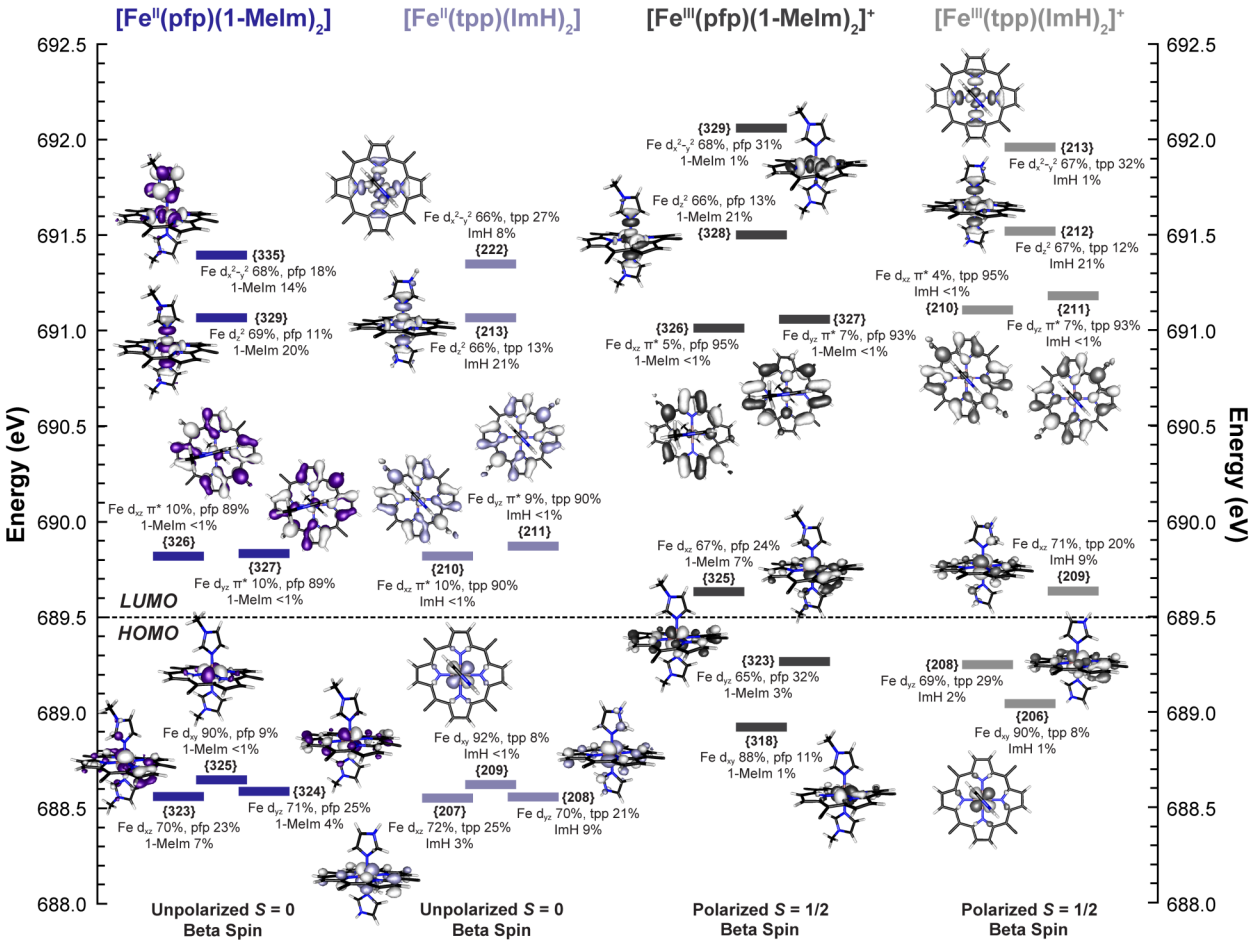
SI Figure S2. Top: Pumped subtraction and renormalization (grey) from 10–50% pumped contribution for [Fe^{II}(pfp)(1-MeIm)(CO)]. Subtraction allowed for < 20% pumped contribution in [Fe^{II}(pfp)(1-MeIm)(CO)]. Bottom: Pumped subtraction and renormalization for [Fe(pfp)(1-MeIm)O_2]. Subtraction allowed for < 15% pumped contribution in the renormalized data of [Fe(pfp)(1-MeIm)O_2].



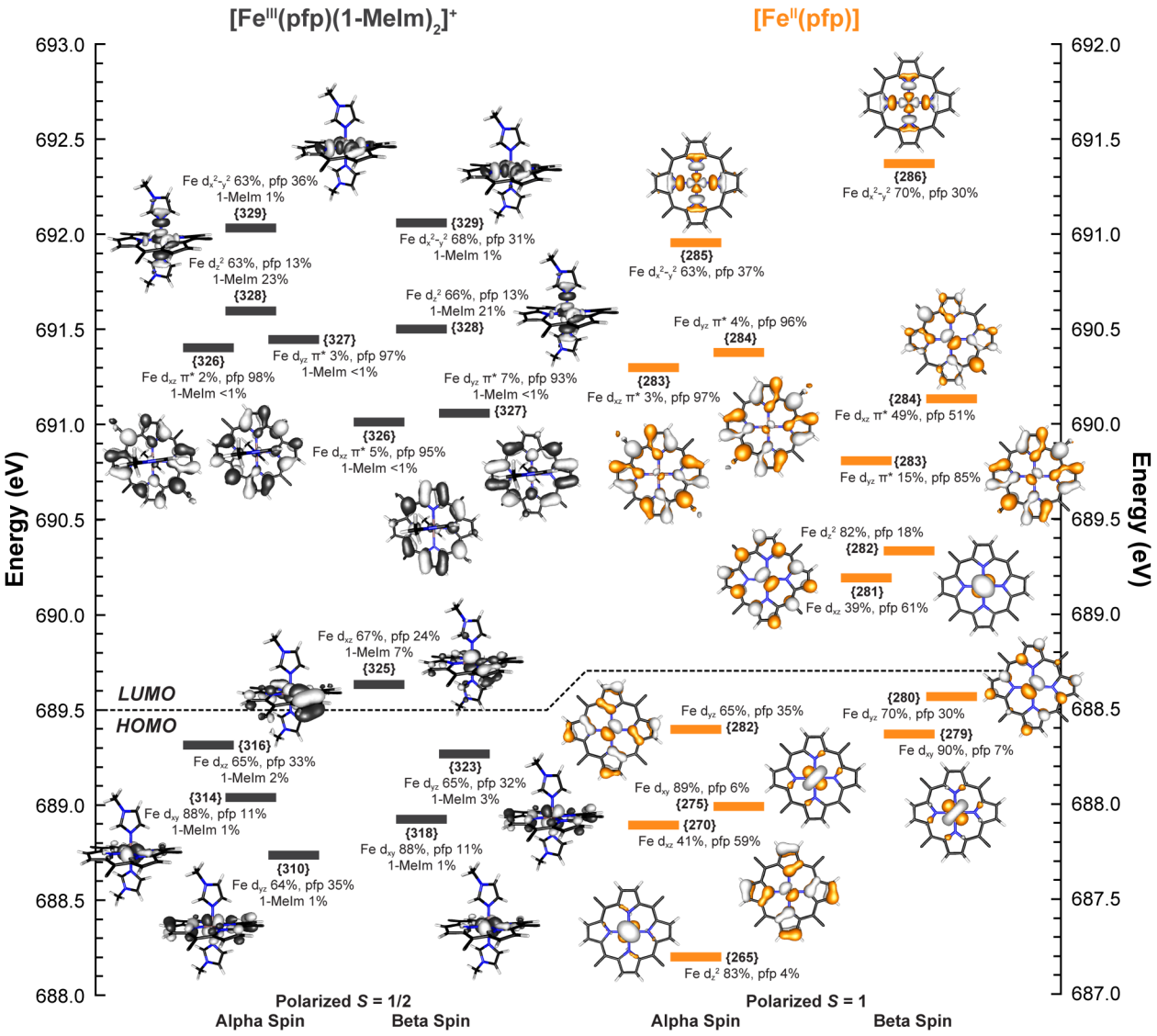
SI Figure S3. Top: Comparison of L-edge data for low-spin (S = 0) ferrous [Fe^{II}(pfp)(1-MeIm)$_2$] vs. [Fe^{II}(tpp)(ImH)$_2$]. The two samples are very similar with respect to spectral shape and normalized intensity indicating that the two sets of ligands are very similar with respect to their bonding interactions with iron. Bottom: Comparison of L-edge data for [Fe^{II}(pfp)(1-MeIm)$_2$] vs. low-spin (S = 1/2) ferric [Fe^{III}(tpp)(ImH)$_2$]Cl.



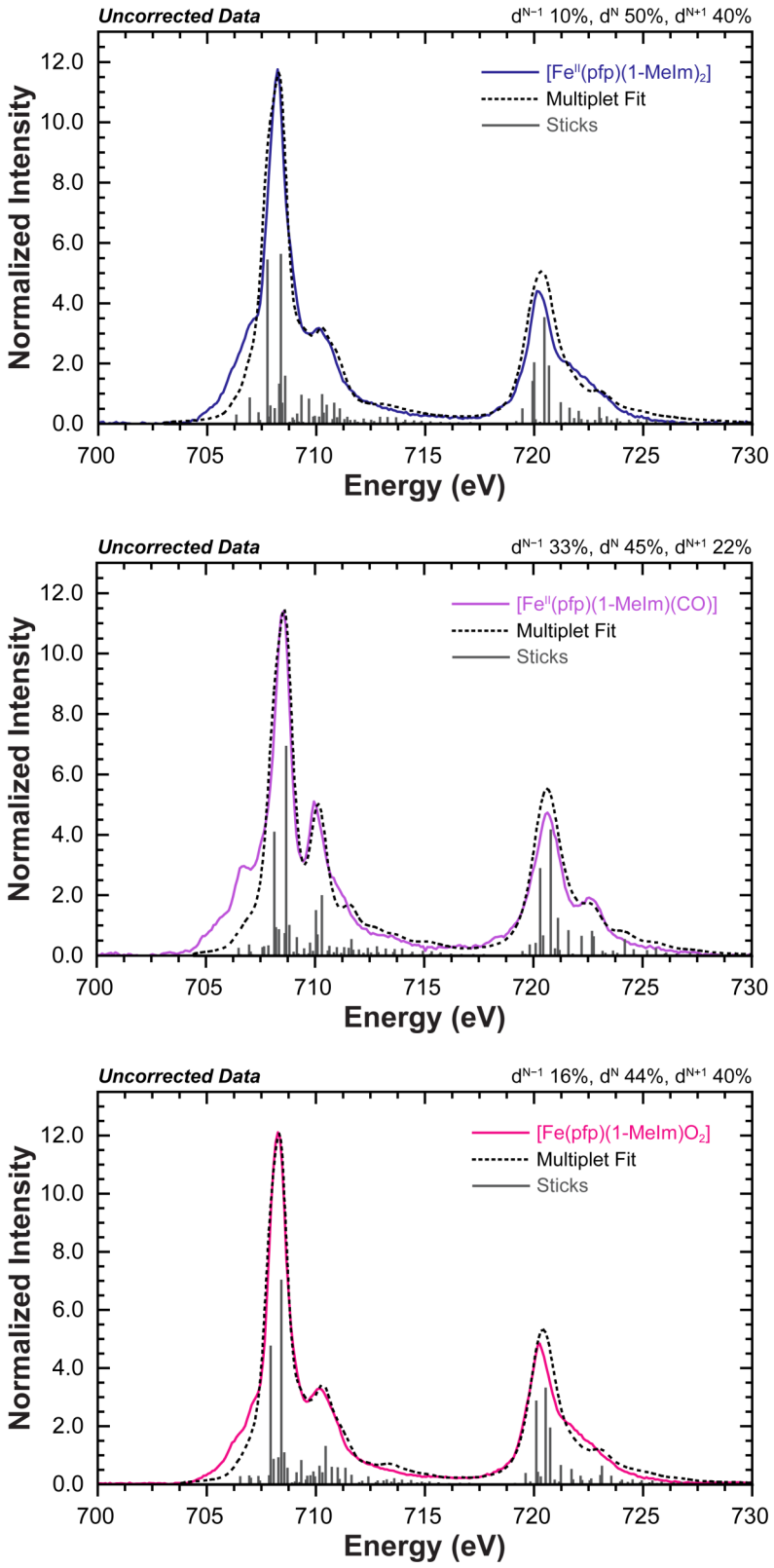
SI Figure S4. Uncorrected L-edge spectra of low-spin ferrous (S = 0) [Fe^{II}(pfp)(1-MeIm)$_2$], low-spin ferric (S = 1/2) [Fe^{III}(tpp)(ImH)$_2$]Cl, and intermediate-spin ferrous (S = 1) [Fe^{II}(pfp)]. All spectra plotted vs. [Fe(pfp)(1-MeIm)O$_2$].



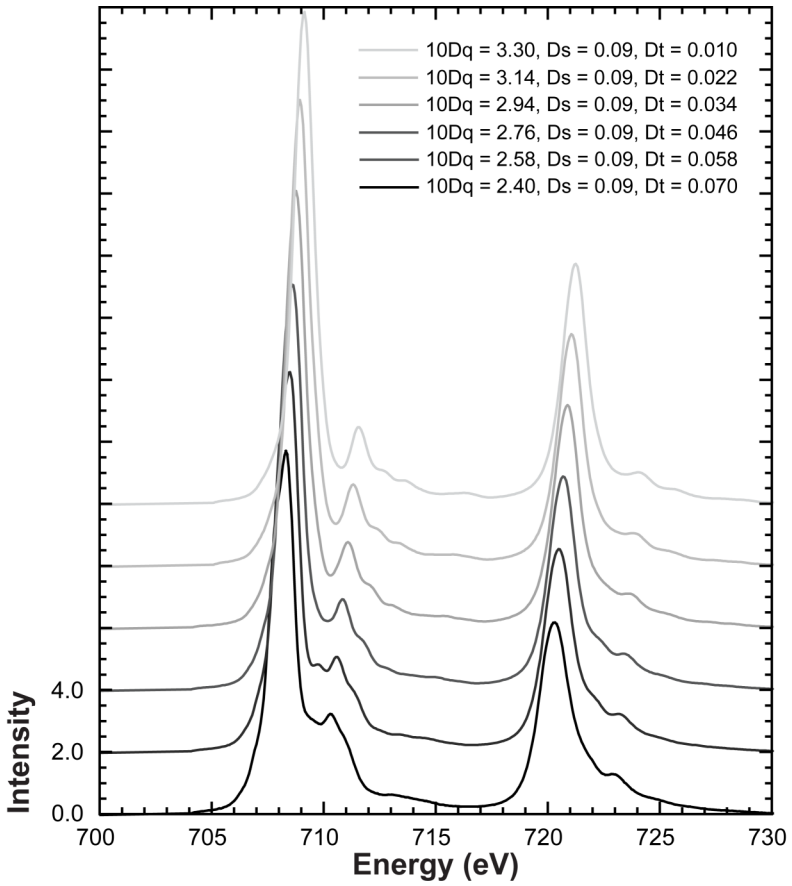
SI Figure S5. Comparison of the molecular orbitals for low-spin (S = 0) ferrous [Fe^{II}(pfp)(1-MeIm)$_2$] (blue) vs. [Fe^{II}(tpp)(ImH)$_2$] (blue-grey) and low-spin (S = 1/2) ferric [Fe^{III}(pfp)(1-MeIm)$_2$]$^+$ (black) vs. [Fe^{III}(tpp)(ImH)$_2$]$^+$ (silver). Orbitals are numbered according to the Gaussian output with the predominant fragment components in each molecular orbital listed above or below. Energy axes are shifted up with the lowest energy Fe 2p orbital set to zero. Geometry optimization and single point calculations were done using UBP86 with 6-311G* on iron, and 6-31G* on all other atoms (C, N, O, H). Orbitals plotted with an isodensity value of ± 0.03. The pickets and phenyl rings have been removed for clarity but were included in all calculations.



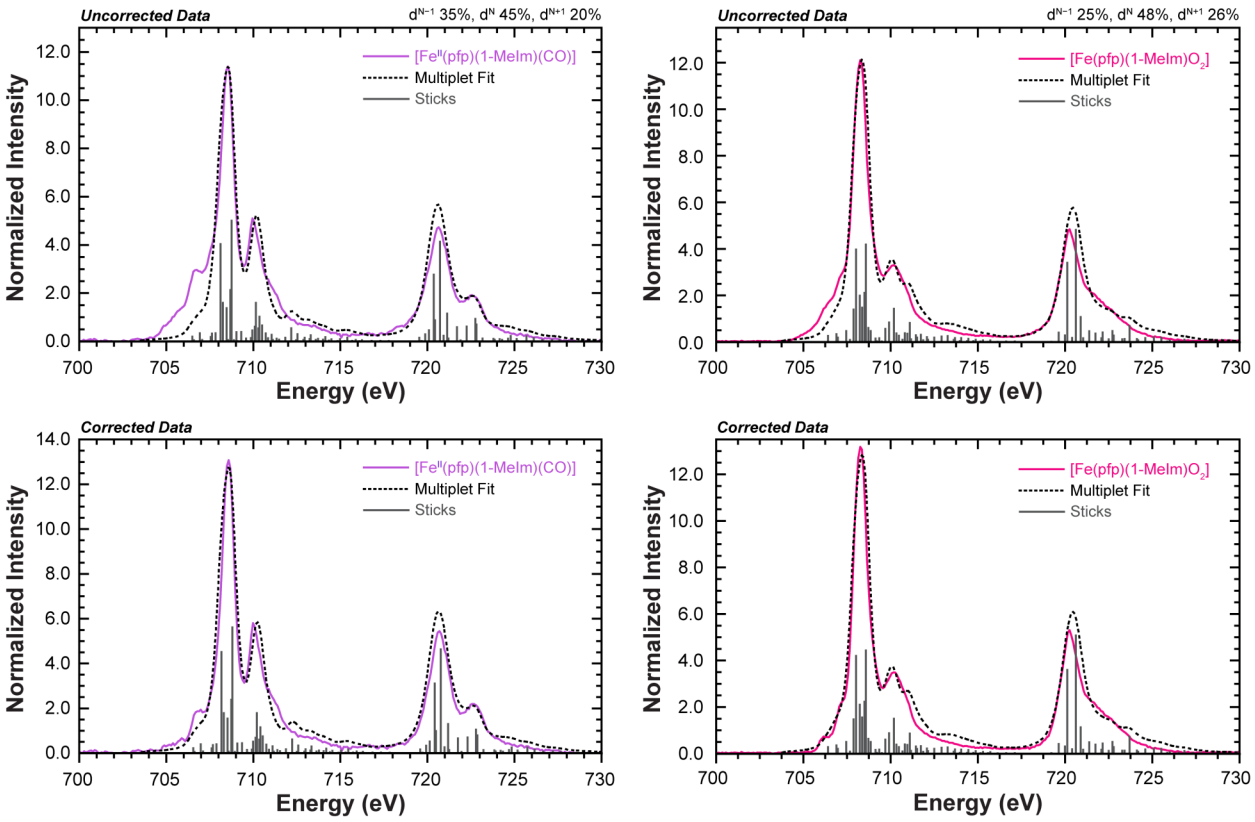
SI Figure S6. Comparison of the molecular orbitals for low-spin ferric (S = 1/2) $[Fe^{III}(pfp)(1\text{-MeIm})_2]^+$ (black) plotted on the left energy axis and intermediate spin (S = 1) $[Fe^{II}(pfp)]$ (orange) on the right axis. Orbitals are numbered according to the Gaussian output with the predominant fragment components in each molecular orbital listed above or below. Energy axes are shifted up with the lowest energy Fe 2p orbital set to zero. Geometry optimization and single point calculations were done using UBP86 with 6-311G* on iron, and 6-31G* on all other atoms. Orbitals are plotted with an isodensity value of ± 0.03. The pickets have been removed for clarity but were included in all calculations.



SI Figure S7. Final VBCI fits (----) given in Figures 4, 6, and 11 for $[Fe^{II}(pfp)(1\text{-MeIm})]_2$, $[Fe^{II}(pfp)(1\text{-MeIm})(CO)]$ and $[Fe(pfp)(1\text{-MeIm})O_2]$ vs. the uncorrected data.



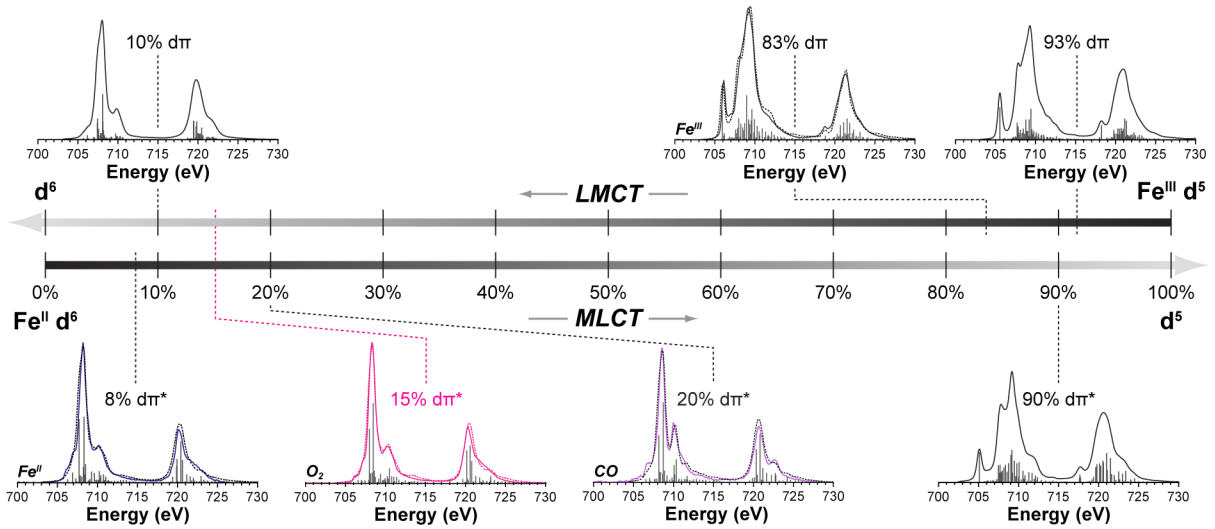
SI Figure S8. Systematic multiplet progression showing the effects of increased ligand field on the spectrum starting from the low-spin d^6 fit to $[Fe^{II}(pfp)(1\text{-MeIm})_2]$. Reference Figure 10 in text.



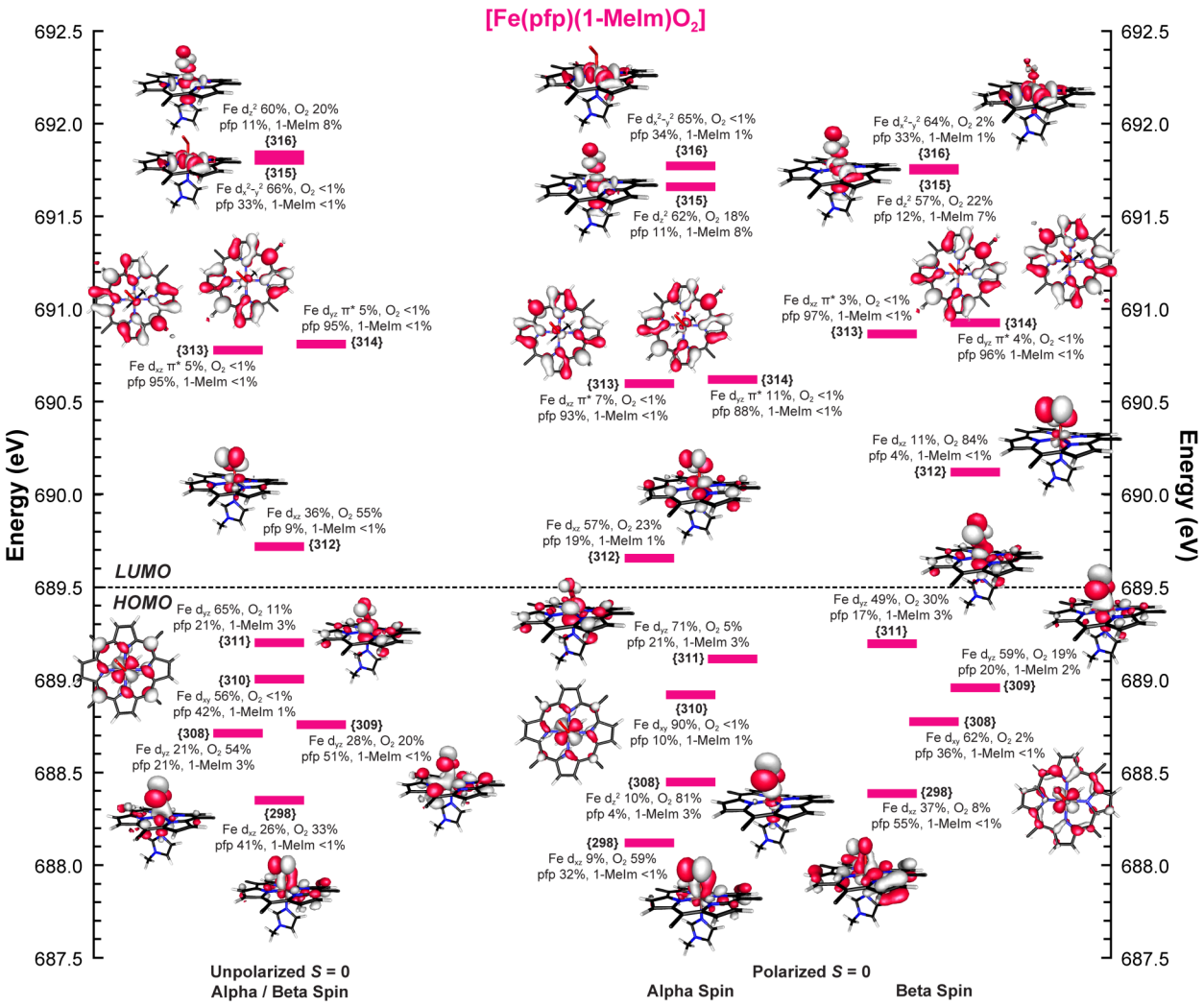
	Crystal Field	Configuration Energies			Mixing Parameters (T)				
Compound	10Dq, Ds, Dt	Δ	Δ_{BB}	Q – U	x^2-y^2 (b_{1g})	z^2 (a_{1g})	xy (b_{2g})	xz/yz (e_g)	xz/yz π*
[Fe^{II}(pfp)(1-MeIm)(CO)]	2.50, 0.15, 0.02	−0.60	−2.90	1.2	2.15	2.35	0.50	2.80	1.80
[Fe(pfp)(1-MeIm)O_2]	2.40, 0.09, 0.05	−0.60	−1.95	1.2	2.15	2.00	0.50	1.70	1.30

	% Total Metal Character			% Metal Character per Orbital (DOC)				
Compound	TI	Intensity	Total	x^2-y^2 (b_{1g})	z^2 (a_{1g})	xy (b_{2g})	xz/yz (e_g)	xz/yz π*
[Fe^{II}(pfp)(1-MeIm)(CO)]	41 (2)	326	328	64	60	—	—	20
[Fe(pfp)(1-MeIm)O_2]	39 (2)	310	306	62	61	—	—	15

SI Figure S9. Alternative VBCI multiplet fits (----) for [Fe^{II}(pfp)(1-MeIm)(CO)] and [Fe(pfp)(1-MeIm)O_2] with Δ fixed to a value of –0.60 eV, Q – U = 1.2. Top plots show the fit compared to the normalized uncorrected data, lower traces show the fit compared to the corrected L-edge spectrum at 20% and 15% pumped for [Fe^{II}(pfp)(1-MeIm)(CO)] and [Fe(pfp)(1-MeIm)O_2] respectively (SI Figure S2).



SI Figure S10. Schematic representation of the relative amounts of dπ hole character and the multiplet simulations for the heme complexes presented in this study. The top section shows the effect of increasing LMCT on a d^5 multiplet wavefunction, right to left, with increased charge donation into the iron dπ hole. The bottom section illustrates the effect of increasing MLCT on a d^6 multiplet wavefunction, left to right, with increasing backbonding through charge donation into the unoccupied ligand π* orbital and the formation of a dπ hole on the metal. Multiplet simulations labeled ferrous, ferric, CO, and O_2 represent the final fits of $[Fe^{II}(pfp)(1\text{-MeIm})_2]$ and $[Fe^{III}(tpp)(ImH)_2]Cl$, $[Fe^{II}(pfp)(1\text{-MeIm})(CO)]$, and $[Fe^{II}(pfp)(1\text{-MeIm})O_2]$, whose DOC values were projected and given in Tables 4 and 5. All others were adapted from limiting cases in Figure 10.



SI Figure S11. Comparison of the unpolarized (spin-restricted) and polarized molecular orbitals of [Fe(pfp)(1-MeIm)O_2]. Orbitals are numbered according to the Gaussian output with the predominant fragment components in each molecular orbital listed above or below. Energy axes are shifted up with the lowest energy Fe 2p orbital set to zero. Geometry optimization and single point calculations were done using UBP86 with 6-311G* on iron, and 6-31G* on all other atoms (C, N, O, H). Orbitals plotted with an isodensity value of ± 0.03. The pickets have been removed for clarity but were included in all calculations.

Optimized Molecular Coordinates

[Fe^{II}(pfp)(1-MeIm)$_2$]

N	0.00000	0.00000	1.99298	C	-2.45185	-2.44631	0.19649	H	-1.32707	-5.07337	0.45046
N	0.13257	-0.68618	4.11135	C	-2.43154	2.42368	-0.37719	H	-5.09032	-1.36528	-0.09341
N	-0.01155	-0.02728	-1.97057	C	3.51204	3.52096	-0.11914	H	-5.06723	1.33097	-0.46840
N	-0.53027	-0.57375	-4.06481	C	3.95099	4.33898	0.96214	H	5.27264	5.92536	1.59114
C	0.24380	-1.04393	2.79516	C	4.95277	5.31395	0.74711	H	6.28780	6.23657	-0.67234
C	-0.19575	0.66021	4.14672	C	5.51302	5.47536	-0.52627	H	5.53129	4.80429	-2.59790
C	-0.27519	1.06958	2.83093	C	5.09392	4.67759	-1.60168	H	3.76147	3.07952	-2.21372
C	0.33868	-1.56281	5.26122	C	4.10073	3.71229	-1.38588	H	3.99684	2.58729	5.03788
C	-0.76909	-0.81560	-2.74136	C	3.59367	4.80231	3.42149	H	2.56707	2.18185	4.04223
C	0.43531	0.42161	-4.13670	C	2.71507	4.32717	4.61613	H	2.37410	2.50903	5.78062
C	0.74513	0.75101	-2.83446	C	2.92833	2.81430	4.87313	H	0.59500	4.31609	5.16468
C	-1.15716	-1.25907	-5.19033	C	1.22435	4.61561	4.30594	H	0.86416	4.06838	3.41605
H	0.48167	-2.05282	2.46618	C	3.14130	5.12199	5.86665	H	1.05958	5.69282	4.12591
H	-0.34412	1.19110	5.08424	C	3.46970	-3.51615	-0.37374	H	4.19890	4.93379	6.11640
H	-0.51386	2.04761	2.42278	C	4.43614	-3.89321	0.60575	H	2.51705	4.82496	6.72914
H	-0.54513	-1.54055	5.92013	C	5.33057	-4.95518	0.34091	H	3.02988	6.20650	5.70571
H	1.23000	-1.25253	5.83210	C	5.27867	-5.62796	-0.88655	H	6.04660	-5.23530	1.11415
H	0.48566	-2.59234	4.90188	C	4.34213	-5.26308	-1.86550	H	5.98254	-6.44698	-1.07326
H	-1.48701	-1.54987	-2.38332	C	3.44819	-4.21731	-1.59720	H	4.30348	-5.78726	-2.82662
H	0.80255	0.79647	-5.08974	C	5.27104	-3.37268	2.93108	H	2.70380	-3.92168	-2.34462
H	1.44702	1.49029	-2.45718	C	5.13013	-2.33859	4.08822	H	4.64655	-2.47199	6.22263
H	-0.41750	-1.86764	-5.73859	C	4.65753	-3.12927	5.33350	H	5.33533	-3.97666	5.52772
H	-1.60740	-0.52642	-5.88087	C	4.15927	-1.17455	3.80497	H	3.63785	-3.53340	5.19013
H	-1.95073	-1.91907	-4.80898	C	6.54840	-1.77207	4.34972	H	4.45887	-0.58289	2.92014
Fe	0.00000	0.00000	0.00000	C	-3.50087	-3.52483	0.20776	H	4.14903	-0.48312	4.66740
N	0.00000	2.00053	-0.03541	C	-4.38552	-3.73468	1.30751	H	3.11825	-1.52056	3.65672
N	1.99803	0.00983	-0.01833	C	-5.32483	-4.79038	1.26717	H	6.90195	-1.16829	3.49429
N	-0.00339	-1.99281	0.03978	C	-5.39864	-5.62333	0.14375	H	7.26314	-2.59520	4.51034
N	-1.99740	-0.00255	-0.01360	C	-4.54445	-5.42589	-0.95167	H	6.54032	-1.12429	5.24533
N	3.35786	4.13298	2.22827	C	-3.60788	-4.38427	-0.90575	H	-5.97529	-4.93814	2.12977
N	4.46462	-3.17236	1.82357	C	-4.98928	-2.88685	3.60679	H	-6.13519	-6.43467	0.13106
N	-4.28958	-2.85718	2.41257	C	-4.71399	-1.71739	4.59806	H	-4.60282	-6.07519	-1.83200
N	-3.89988	4.21095	1.40835	C	-4.09863	-2.35035	5.87112	H	-2.92585	-4.22264	-1.74810
O	4.42310	5.71121	3.54139	C	-6.09123	-1.10125	4.94840	H	-3.98684	-1.58687	6.66317
O	6.07028	-4.31225	3.03920	C	-3.78203	-0.61523	4.05543	H	-3.10171	-2.78248	5.66282
O	-5.79420	-3.77733	3.91097	C	-3.45273	3.42833	-0.84880	H	-4.74811	-3.15773	6.24759
O	-5.36014	5.77545	2.28585	C	-4.17134	4.29584	0.02223	H	-5.97827	-0.34309	5.74487
C	-1.09704	2.84071	-0.22204	C	-5.11765	5.20256	-0.50884	H	-6.78155	-1.88618	5.29666
C	1.09709	2.86079	0.01154	C	-5.34732	5.24638	-1.88982	H	-6.54450	-0.60892	4.06879
C	2.84820	1.11247	-0.00740	C	-4.64812	4.39822	-2.76171	H	-4.18175	-0.14516	3.13754
C	2.84460	-1.08866	-0.13969	C	-3.71071	3.50015	-2.23259	H	-2.76276	-0.98827	3.84079
C	1.10196	-2.84132	-0.00946	C	-4.47482	4.92495	2.44683	H	-3.67559	0.18411	4.81116
C	-1.09905	-2.84388	0.19253	C	-3.95962	4.60950	3.88157	H	-5.65643	5.85392	0.17962
C	-2.85196	-1.10090	0.06273	C	-5.17501	4.07645	4.68124	H	-6.08468	5.95571	-2.28260
C	-2.83695	1.08325	-0.23956	C	-3.49221	5.95444	4.49128	H	-4.82782	4.43397	-3.84176
C	-0.68548	4.22925	-0.25443	C	-2.80699	3.58858	3.94491	H	-3.15216	2.82923	-2.89455
C	0.67372	4.24338	-0.09491	H	2.64881	3.39587	2.23578	H	-6.01354	4.78905	4.61759
C	4.23365	0.69726	-0.10990	H	3.85091	-2.35566	1.83736	H	-4.90349	3.94115	5.74441
C	4.23005	-0.66646	-0.21831	H	-3.64329	-2.07853	2.27035	H	-5.51923	3.10229	4.28808
C	0.69648	-4.22142	0.15756	H	-3.18314	3.52291	1.64691	H	-4.29419	6.70593	4.41327
C	-0.66561	-4.22194	0.29602	H	-1.36051	5.07384	-0.39340	H	-2.60166	6.34496	3.96551
C	-4.23408	-0.69053	-0.10046	H	1.34559	5.10153	-0.08591	H	-3.22957	5.82002	5.55668
C	-4.22273	0.66371	-0.29673	H	5.08628	1.37516	-0.12348	H	-2.49944	3.44511	4.99705
C	2.44848	2.46303	0.02924	H	5.08050	-1.33646	-0.34487	H	-1.91564	3.94040	3.39194
C	2.44420	-2.43788	-0.15158	H	1.37803	-5.07108	0.17840	H	-3.09978	2.59424	3.55841

[Fe^{III}(pfp)(1-MeIm)$_2$]$^+$

N	0.00000	0.00000	2.00139
N	-0.71715	-0.04583	4.10552
N	0.02730	0.04242	-1.96865
N	-0.42546	0.60838	-4.06414
C	-1.07803	-0.10471	2.79399
C	0.66004	0.10693	4.15446
C	1.09359	0.13164	2.84664
C	-1.61824	-0.11549	5.25834
C	-0.71343	0.83655	-2.75632
C	0.54621	-0.38470	-4.11478
C	0.82042	-0.72531	-2.80970
C	-1.03082	1.28532	-5.21385
H	-2.10388	-0.22606	2.45681
H	1.19693	0.18621	5.09701
H	2.10375	0.22882	2.46048
H	-1.57485	0.82606	5.82978
H	-1.33200	-0.95666	5.90971
H	-2.64530	-0.27268	4.89892
H	-1.43942	1.57051	-2.41491
H	0.94622	-0.74863	-5.05868
H	1.51857	-1.46060	-2.41906
H	-1.55309	0.55441	-5.85222
H	-0.25346	1.79848	-5.80264
H	-1.75560	2.02842	-4.85065
Fe	0.00000	0.00000	0.00000
C	1.08315	-2.84205	0.08537
N	-0.00274	-1.97236	-0.05417
O	-6.23261	-5.05826	1.74589
C	0.65880	-4.20634	-0.11502
N	-1.99718	0.03106	-0.03199
O	-3.77179	5.80535	4.01076
C	-0.68058	-4.17026	-0.41194
N	0.00000	1.99506	0.03333
O	6.10593	4.70932	2.59961
C	-1.08877	-2.78677	-0.36501
N	1.99965	-0.02728	0.02688
O	3.45346	-5.85524	4.06078
C	-2.42080	-2.36914	-0.55017
N	-4.49856	-3.69555	1.04998
C	-2.83424	-1.04493	-0.30911
N	-2.84978	4.28716	2.52701
C	-4.22041	-0.63159	-0.26325
N	4.37335	3.52821	1.62543
C	-4.23166	0.69778	0.06795
N	2.67709	-4.28701	2.54641
C	-2.84999	1.12360	0.15153
C	-2.44756	2.47021	0.25747
C	-1.09159	2.85378	0.14788
C	-0.66024	4.22782	0.04071
C	0.69781	4.20593	-0.15700
C	1.10348	2.82001	-0.15440
C	2.44599	2.40769	-0.28049
C	2.84443	1.06558	-0.13270
C	4.22863	0.64807	-0.05000
C	4.22616	-0.69745	0.20560
C	2.84200	-1.12269	0.20490
C	2.43064	-2.47019	0.26965
C	-3.40063	-3.36933	-1.10244
C	-3.29136	-3.68918	-2.47258
C	-4.15107	-4.61221	-3.08174
C	-5.13916	-5.23665	-2.30544
C	-5.27021	-4.94899	-0.94120
C	-4.40564	-4.01487	-0.32461
C	-5.38382	-4.19806	1.99846
C	-5.26675	-3.61954	3.43762
C	-4.91618	-4.80640	4.37001
C	-6.66587	-3.06631	3.80824
C	-4.21515	-2.50197	3.60323
C	-3.50939	3.53395	0.29517
C	-4.34964	3.68044	-0.83142
C	-5.37494	4.63283	-0.87170
C	-5.57573	5.46142	0.24268
C	-4.75852	5.35185	1.37395
C	-3.71231	4.40064	1.41210
C	-2.87946	5.00259	3.72091
C	-1.70932	4.74560	4.71383
C	-0.62777	3.77322	4.20156
C	-1.06359	6.12478	5.00216
C	-2.34394	4.19474	6.01541
C	3.47258	3.44738	-0.64109
C	3.49167	3.91170	-1.97337
C	4.40968	4.87966	-2.40056
C	5.32690	5.40129	-1.47549
C	5.33131	4.96830	-0.14386
C	4.40793	3.98851	0.29036
C	5.20423	3.87378	2.69264
C	4.92434	3.09713	4.01226
C	3.43375	3.20647	4.41807
C	5.32006	1.61081	3.81541
C	5.79806	3.71750	5.12203
C	3.48062	-3.54039	0.36086
C	4.38600	-3.69022	-0.71309
C	5.40269	-4.65269	-0.69158
C	5.52672	-5.48518	0.43122
C	4.64294	-5.37100	1.51107
C	3.60558	-4.41001	1.48717
C	2.60897	-5.01781	3.72872
C	1.38915	-4.73185	4.65287
C	1.95800	-4.17134	5.98059
C	0.35167	-3.75051	4.06875
C	0.70918	-6.09819	4.92035
H	1.31698	-5.07356	-0.07020
H	-1.34461	-5.00337	-0.63952
H	-3.82643	-2.99828	1.37077
H	-2.06447	3.64874	2.39925
H	-5.07045	-1.28789	-0.44891
H	3.65875	2.82409	1.81406
H	-5.09234	1.34967	0.20787
H	1.92885	-3.61260	2.38574
H	-1.32205	5.09252	0.08272
H	1.37484	5.04850	-0.29215
H	5.08479	1.31285	-0.15989
H	5.07954	-1.35783	0.34976
H	-2.51085	-3.19241	-3.05979
H	-4.04767	-4.84105	-4.14741
H	-5.82013	-5.96389	-2.76056
H	-6.02768	-5.43773	-0.32818
H	-4.93939	-4.48150	5.42612
H	-5.64501	-5.62194	4.23692
H	-3.90837	-5.20659	4.15433
H	-6.68340	-2.75350	4.86777
H	-6.93211	-2.19146	3.18708
H	-7.43281	-3.84194	3.65501
H	-4.23392	-2.14464	4.64936
H	-3.18674	-2.86074	3.40162
H	-4.43336	-1.63135	2.95420
H	-4.18171	3.02360	-1.69250
H	-6.00720	4.72429	-1.76077
H	-6.37619	6.20902	0.23741
H	-4.91072	5.98811	2.24602
H	0.16593	3.66715	4.96275
H	-1.02918	2.75882	4.01055
H	-0.13997	4.13905	3.27878
H	-0.30308	6.02991	5.79808
H	-0.56823	6.53212	4.10205
H	-1.83071	6.84497	5.32802
H	-1.57648	4.09780	6.80485
H	-3.13319	4.87538	6.37373
H	-2.80307	3.20092	5.85238
H	2.76866	3.48873	-2.67992
H	4.40761	5.21982	-3.44119
H	6.05253	6.16035	-1.78709
H	6.03635	5.37409	0.58190
H	3.28541	2.72862	5.40426
H	3.11816	4.26122	4.50458
H	2.74873	2.70438	3.70832
H	5.16645	1.05133	4.75651
H	4.72789	1.11420	3.02383
H	6.38554	1.51958	3.54037
H	5.64952	3.16589	6.06766
H	6.86585	3.67893	4.85451
H	5.53871	4.77631	5.29026
H	4.27398	-3.03301	-1.58279
H	6.08667	-4.74957	-1.54084
H	6.31922	-6.24010	0.47299
H	4.73458	-6.01148	2.38854
H	1.14944	-4.05802	6.72584
H	2.71754	-4.85736	6.38947
H	2.43305	-3.18364	5.83235
H	-0.49211	-3.64817	4.77600
H	0.77061	-2.73706	3.91520
H	-0.07052	-4.11303	3.11259
H	-0.09127	-5.98375	5.67361
H	0.25706	-6.50950	3.99938
H	1.44758	-6.82486	5.29427

[Fe^{II}(pfp)(1-MeIm)(CO)]

Fe	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.73416
O	0.00226	-0.00008	2.90952
O	4.01960	-5.48256	3.95515
O	-5.65472	-4.34221	3.36281
O	-3.96865	5.48908	3.98072
O	5.62924	4.34682	3.39575
N	2.00993	-0.01236	-0.05349
N	-0.00040	-2.00889	-0.04734
N	-2.01043	0.01346	-0.05454
N	0.00000	2.01002	-0.04223
N	3.04909	-4.04874	2.42160
N	-4.14209	-3.25476	1.99236
N	-3.01719	4.05349	2.43664
N	4.14318	3.24171	2.01048
C	2.85094	1.08875	-0.13824
C	4.23942	0.67000	-0.13065
C	4.24148	-0.69198	-0.00885
C	2.85356	-1.11261	0.02230
C	2.44843	-2.46094	0.07734
C	1.09720	-2.85745	0.03009
C	0.67122	-4.24359	-0.00107
C	-0.69298	-4.23573	-0.09493
C	-1.10495	-2.84548	-0.12373
C	-2.44966	-2.43623	-0.19561
C	-2.85090	-1.08782	-0.14422
C	-4.23930	-0.66934	-0.13673
C	-4.24236	0.69230	-0.00889
C	-2.85487	1.11368	0.02482
C	-2.44962	2.46219	0.08488
C	-1.09766	2.85907	0.03852
C	-0.67079	4.24475	0.01272
C	0.69397	4.23644	-0.07892
C	1.10542	2.84658	-0.11354
C	2.45025	2.43706	-0.18536
C	3.51492	-3.52202	0.09176
C	4.25982	-3.75949	-1.08118
C	5.27902	-4.72100	-1.12384
C	5.56535	-5.46172	0.03306
C	4.84531	-5.25365	1.21636
C	3.81284	-4.28832	1.25776
C	3.15739	-4.64144	3.67140
C	2.12619	-4.18239	4.74287
C	2.93491	-3.47326	5.85908
C	1.47895	-5.46838	5.31423
C	1.02228	-3.24026	4.22001
C	-3.50201	-3.50187	-0.33988
C	-3.66621	-4.13962	-1.58519
C	-4.61326	-5.15770	-1.76771
C	-5.41069	-5.55082	-0.68190
C	-5.27337	-4.93897	0.57105
C	-4.32205	-3.90960	0.75404
C	-4.79598	-3.46680	3.19689
C	-4.38024	-2.53625	4.37453
C	-3.40942	-1.39988	3.99049
C	-5.68647	-1.92753	4.94208
C	-3.72819	-3.44615	5.44641
C	-3.51541	3.52361	0.11330
C	-4.27879	3.76135	-1.04782
C	-5.29816	4.72303	-1.07693
C	-5.56574	5.46615	0.08298
C	-4.82757	5.25872	1.25507
C	-3.79590	4.29195	1.28282
C	-3.10869	4.64920	3.68681
C	-2.05638	4.20049	4.74223
C	-0.97760	3.23438	4.21123
C	-1.38071	5.49183	5.26750
C	-2.84420	3.52680	5.89433
C	3.50228	3.50415	-0.32063
C	3.66879	4.14892	-1.56205
C	4.61178	5.17214	-1.73614
C	5.40211	5.56458	-0.64496
C	5.26333	4.94527	0.60409
C	4.31787	3.90876	0.77792
C	4.78991	3.45493	3.21871
C	4.39241	2.50400	4.38569
C	3.71001	3.38651	5.46189
C	3.45404	1.34501	3.98805
C	5.71154	1.92579	4.95546
H	5.09140	1.34517	-0.20638
H	5.09531	-1.36620	0.03939
H	2.30031	-3.36462	2.30195
H	-3.45177	-2.50268	1.97367
H	1.34394	-5.10040	0.02856
H	-2.26870	3.37075	2.30760
H	-1.37310	-5.08493	-0.14561
H	3.46800	2.47621	1.98307
H	-5.09129	-1.34427	-0.21432
H	-5.09708	1.36513	0.04345
H	-1.34241	5.10231	0.04685
H	1.37466	5.08553	-0.12396
H	4.02454	-3.16729	-1.97281
H	5.84092	-4.88683	-2.04925
H	6.36090	-6.21533	0.02220
H	5.06300	-5.81757	2.12395
H	2.27094	-3.21520	6.70428
H	3.73859	-4.13200	6.22771
H	3.39548	-2.53908	5.48828
H	0.83079	-5.21799	6.17363
H	0.85724	-5.97570	4.55391
H	2.25817	-6.17274	5.64685
H	0.31718	-3.00952	5.03880
H	1.41758	-2.26914	3.86838
H	0.43359	-3.70216	3.40515
H	-3.02956	-3.82000	-2.41785
H	-4.72378	-5.63752	-2.74612
H	-6.15353	-6.34724	-0.80409
H	-5.88170	-5.24049	1.42458
H	-3.21174	-0.76878	4.87564
H	-2.42583	-1.77377	3.64889
H	-3.83126	-0.73987	3.20959
H	-5.47072	-1.35745	5.86404
H	-6.15562	-1.23813	4.21643
H	-6.40958	-2.72537	5.17574
H	-3.50633	-2.86207	6.35832
H	-4.40822	-4.27241	5.71214
H	-2.78062	-3.88205	5.08003
H	-4.05862	3.16700	-1.94210
H	-5.87464	4.88746	-1.99363
H	-6.36045	6.22067	0.08323
H	-5.03036	5.82408	2.16520
H	-0.25610	3.00817	5.01690
H	-1.39443	2.26328	3.88570
H	-0.40167	3.67407	3.37513
H	-0.70806	5.25230	6.11099
H	-0.77913	5.97880	4.47829
H	-2.14336	6.20920	5.61084
H	-2.16298	3.28383	6.73019
H	-3.63290	4.20245	6.26441
H	-3.32176	2.58812	5.55825
H	3.03750	3.83010	-2.39909
H	4.72472	5.65658	-2.71201
H	6.14106	6.36565	-0.76006
H	5.86639	5.24612	1.46157
H	3.50018	2.78831	6.36742
H	4.36504	4.22930	5.73845
H	2.75226	3.79875	5.09433
H	3.26965	0.70250	4.86786
H	2.46194	1.69481	3.64519
H	3.89643	0.70220	3.20414
H	5.50733	1.34616	5.87402
H	6.20034	1.25185	4.22825
H	6.41352	2.74054	5.19509
N	0.00093	0.00149	-2.05645
N	-0.46317	0.55509	-4.16012
C	-0.69241	0.82857	-2.84238
C	0.42889	-0.50877	-4.21186
C	0.70574	-0.83896	-2.90219
C	-1.04748	1.25482	-5.30104
H	-1.35398	1.62152	-2.49960
H	0.77492	-0.92082	-5.15753
H	1.35488	-1.61839	-2.51031
H	-1.63381	0.55685	-5.92206
H	-0.25664	1.71441	-5.91747
H	-1.71441	2.04724	-4.92970

[Fe^{II}(pfp)]

Fe	0.00223	-0.00282	-1.58583
N	1.97310	-0.20566	-1.58079
N	0.21330	1.96712	-1.58219
N	-1.96873	0.20001	-1.58289
N	-0.20879	-1.97273	-1.58154
C	0.79713	-2.93983	-1.59505
O	-4.86913	-4.96570	2.15240
C	-1.39479	-2.71401	-1.59012
O	-4.99725	4.86076	2.09865
C	-2.94148	-0.80448	-1.58903
O	4.86211	4.97533	2.15031
C	-2.70400	1.38630	-1.60617
O	4.99488	-4.86147	2.11190
C	-0.79264	2.93413	-1.59845
C	1.39933	2.70841	-1.59014
C	2.94590	0.79877	-1.58625
C	2.70841	-1.39198	-1.60163
C	0.23714	-4.27128	-1.59580
N	-3.66615	-3.63504	0.69325
C	-1.12376	-4.13197	-1.60073
N	-3.65351	3.65482	0.65387
C	-4.27140	-0.24300	-1.60074
N	3.66290	3.63977	0.69249
C	-4.12323	1.11677	-1.62194
N	3.65335	-3.65762	0.66336
C	-0.23270	4.26560	-1.60012
C	1.12824	4.12635	-1.60298
C	4.27581	0.23722	-1.59516
C	4.12764	-1.12254	-1.61525
C	-2.69468	-2.18561	-1.59644
C	-2.17371	2.68577	-1.61832
C	2.69924	2.17996	-1.59472
C	2.17818	-2.69147	-1.61303
C	-3.86748	-3.12480	-1.67317
C	-4.34595	-3.82977	-0.53020
C	-5.46358	-4.68624	-0.65184
C	-6.09322	-4.84128	-1.89395
C	-5.63104	-4.15571	-3.02795
C	-4.52397	-3.30360	-2.90661
C	-3.92541	-4.19599	1.93417
C	-2.94835	-3.80863	3.08322
C	-1.80171	-2.86248	2.66868
C	-2.35644	-5.13484	3.62297
C	-3.80356	-3.13880	4.18773
C	-3.11139	3.85898	-1.70547
C	-3.83103	4.33657	-0.57111
C	-4.68362	5.45608	-0.70215
C	-4.82117	6.08822	-1.94509
C	-4.12132	5.62687	-3.07064
C	-3.27242	4.51838	-2.93993
C	-4.22838	3.91457	1.88827
C	-3.85870	2.93402	3.04022
C	-3.20061	3.78474	4.15517
C	-2.91053	1.78563	2.63514
C	-5.19347	2.34500	3.56152
C	3.87246	3.11859	-1.67098
C	4.34751	3.82801	-0.52929
C	5.46653	4.68274	-0.65052
C	6.10058	4.83224	-1.89107
C	5.64157	4.14266	-3.02391
C	4.53339	3.29195	-2.90290
C	3.91735	4.20708	1.93152
C	2.93205	3.83044	3.07716
C	2.33799	5.16199	3.60105
C	3.77859	3.16939	4.19356
C	1.78741	2.88180	2.66283
C	3.11607	-3.86473	-1.69691
C	3.83339	-4.34084	-0.56046
C	4.68650	-5.46031	-0.68847
C	4.82686	-6.09378	-1.93041
C	4.12927	-5.63390	-3.05797
C	3.27982	-4.52547	-2.93027
C	4.22652	-3.91544	1.89896
C	3.85620	-2.93253	3.04872
C	5.19063	-2.34066	3.56770
C	3.19985	-3.78128	4.16622
C	2.90634	-1.78628	2.64165
H	-2.85677	-3.01607	0.62829
H	-3.03770	2.84252	0.59488
H	2.85227	3.02249	0.62715
H	3.03749	-2.84549	0.60235
H	0.82563	-5.18780	-1.60182
H	-1.88735	-4.90876	-1.61831
H	-5.18990	-0.82780	-1.60508
H	-4.89750	1.88300	-1.65270
H	-0.82118	5.18210	-1.60823
H	1.89171	4.90325	-1.62077
H	5.19430	0.82204	-1.59824
H	4.90186	-1.88891	-1.64376
H	-5.81621	-5.21008	0.23727
H	-6.95834	-5.50964	-1.96943
H	-6.12441	-4.28101	-3.99762
H	-4.14717	-2.75870	-3.77938
H	-2.17456	-1.88392	2.31039
H	-1.15438	-3.30702	1.88901
H	-1.15765	-2.65736	3.54297
H	-1.74303	-4.94084	4.52160
H	-1.71377	-5.62465	2.86862
H	-3.16735	-5.83205	3.88897
H	-4.21341	-2.17041	3.84652
H	-3.18831	-2.95319	5.08702
H	-4.64787	-3.79140	4.46352
H	-5.21806	5.80846	0.18074
H	-5.48691	6.95468	-2.02787
H	-4.23279	6.12218	-4.04101
H	-2.71630	4.14235	-3.80589
H	-3.02920	3.16695	5.05555
H	-3.85405	4.63064	4.42391
H	-2.22635	4.19188	3.82776
H	-3.34726	1.14052	1.84922
H	-2.71716	1.13975	3.51078
H	-1.92705	2.15690	2.28885
H	-5.67595	1.70628	2.79911
H	-5.89140	3.15731	3.82134
H	-5.01286	1.72831	4.46069
H	5.81667	5.20972	0.23771
H	6.96664	5.49942	-1.96623
H	6.13829	4.26368	-3.99241
H	4.15915	2.74385	-3.77476
H	1.71707	4.97648	4.49630
H	1.70224	5.64647	2.83744
H	3.14779	5.86022	3.86776
H	3.15711	2.99412	5.09065
H	4.62260	3.82277	4.46837
H	4.18823	2.19673	3.86450
H	2.16217	1.90046	2.31422
H	1.14497	3.32064	1.87590
H	1.13798	2.68352	3.53472
H	5.21920	-5.81152	0.19593
H	5.49301	-6.96015	-2.01079
H	4.24290	-6.13029	-4.02754
H	2.72549	-4.15050	-3.79783
H	5.88958	-3.15160	3.82907
H	5.00985	-1.72188	4.46540
H	5.67187	-1.70329	2.80340
H	3.85398	-4.62634	4.43598
H	2.22539	-4.18953	3.84079
H	3.02918	-3.16177	5.06556
H	2.71231	-1.13912	3.51619
H	1.92331	-2.15966	2.29636
H	3.34195	-1.14197	1.85446

[Fe(pfp)(1-MeIm)O_2] - Unpolarized

O	0.00000	0.00000	1.74705
O	-0.77201	0.80079	2.41472
Fe	0.00000	0.00000	0.00000
O	4.47975	4.14475	4.68075
N	0.00000	1.98165	-0.07719
N	2.01296	-0.00590	0.02040
C	-1.08964	2.81831	-0.28642
C	-0.67855	4.20496	-0.25146
C	0.66238	4.21244	0.02851
C	1.08311	2.82925	0.11432
C	2.42282	2.43226	0.29699
C	2.84182	1.09030	0.21314
C	4.23267	0.68105	0.21424
C	4.24731	-0.66856	-0.01295
C	2.86437	-1.09021	-0.12219
C	-2.42515	2.40463	-0.43963
N	3.43700	3.11081	2.89505
C	3.71184	3.27752	4.24532
C	2.97684	2.31422	5.22217
C	2.19284	1.17113	4.54425
C	2.00795	3.19177	6.05581
C	4.05928	1.71642	6.15462
N	-3.54970	4.17573	1.55925
C	-3.88919	4.93205	2.67335
O	-4.71413	5.85427	2.64390
C	-3.17072	4.56618	4.00412
C	-2.45356	5.85269	4.48572
C	-2.15146	3.41491	3.89519
C	-4.28138	4.18840	5.01660
C	3.46306	3.50072	0.49565
C	3.96442	4.20240	-0.61775
C	4.92304	5.21589	-0.47578
C	5.38842	5.53631	0.80885
C	4.91198	4.85832	1.93833
C	3.94824	3.83318	1.79473
C	-3.47804	3.43012	-0.75667
C	-3.95267	3.52219	-2.07996
C	-4.93630	4.45313	-2.44244
C	-5.45912	5.30819	-1.46026
C	-5.01526	5.23834	-0.13335
C	-4.02371	4.29902	0.23401
H	2.77562	2.37148	2.64972
H	-2.85274	3.44079	1.69729
H	1.77346	0.50667	5.32114
H	1.33228	1.52174	3.94455
H	2.84251	0.54646	3.90285
H	2.55567	4.02143	6.53290
H	1.21047	3.62018	5.42158
H	1.52806	2.58321	6.84401
H	4.74021	1.04552	5.59933
H	4.66210	2.52069	6.60587
H	3.58235	1.12914	6.96013
H	-3.16507	6.69318	4.53194
H	-2.02337	5.69320	5.49120
H	-1.63049	6.13248	3.80289
H	-2.61694	2.46140	3.58581
H	-1.32841	3.64498	3.19352
H	-1.69011	3.23572	4.88303
H	-4.79967	3.25932	4.71638
H	-3.84244	4.02621	6.01801
H	-5.02962	4.99523	5.08242
H	1.32388	5.06964	0.14932
H	-1.34399	5.05445	-0.40316
H	5.07718	1.35622	0.35107
H	5.10588	-1.33491	-0.08910
H	5.26171	5.10408	2.94150
H	6.13516	6.32725	0.94215
H	5.29861	5.74728	-1.35682
H	3.58365	3.93900	-1.61134
H	-5.41844	5.89370	0.63919
H	-6.22897	6.04270	-1.72277
H	-5.28785	4.50828	-3.47836
H	-3.52900	2.84437	-2.82959
N	0.02979	-2.01131	-0.02549
N	-1.97696	-0.02053	-0.10188
C	2.47007	-2.43226	-0.28175
C	-2.82416	1.06485	-0.29067
C	1.12742	-2.84458	-0.18972
C	-1.06060	-2.86014	0.09817
C	-2.81475	-1.11660	0.05615
C	3.53763	-3.45860	-0.54684
C	-4.20711	0.64176	-0.25381
C	0.71565	-4.23509	-0.17942
C	-0.63657	-4.24515	0.03131
C	-2.40762	-2.45970	0.18431
C	-4.20190	-0.70756	-0.02133
C	4.07786	-3.55565	-1.84412
C	4.03773	-4.32230	0.47198
H	-5.06168	1.30635	-0.37494
H	1.38788	-5.08324	-0.30770
H	-1.30467	-5.10225	0.10923
C	-3.47010	-3.51900	0.30117
H	-5.05213	-1.38228	0.07522
C	5.08436	-4.48230	-2.15147
H	3.68700	-2.88595	-2.61839
N	3.48648	-4.20120	1.76638
C	5.05436	-5.25485	0.16280
C	-3.89344	-4.20787	-0.85236
C	-4.07068	-3.83973	1.55381
C	5.56533	-5.32752	-1.13973
H	5.48626	-4.54182	-3.16867
C	3.79009	-4.91944	2.91363
H	2.74704	-3.50105	1.84490
H	5.42431	-5.90149	0.95924
C	-4.89045	-5.19219	-0.79384
H	-3.42513	-3.95349	-1.81004
N	-3.61464	-3.15299	2.70066
C	-5.08023	-4.82847	1.61153
H	6.35295	-6.05704	-1.35981
O	4.65936	-5.79904	2.95757
C	2.97274	-4.55729	4.18781
C	-5.47932	-5.49203	0.44416
H	-5.20416	-5.71313	-1.70478
C	-4.06263	-3.25914	4.01021
H	-2.85848	-2.48835	2.52615
H	-5.53043	-5.05374	2.57873
C	2.33819	-5.87584	4.69610
C	1.86723	-3.50294	3.97010
C	3.99247	-4.03978	5.23385
H	-6.26253	-6.25569	0.51053
O	-4.98528	-4.00863	4.35465
C	-3.35064	-2.35638	5.05857
H	3.11233	-6.65172	4.81077
H	1.84877	-5.71128	5.67333
H	1.57443	-6.25151	3.99066
H	2.27239	-2.52083	3.66142
H	1.11957	-3.83134	3.22372
H	1.32470	-3.33600	4.91797
H	4.45030	-3.08664	4.91152
H	3.48973	-3.86725	6.20285
H	4.79840	-4.77793	5.37880
C	-2.11228	-1.60145	4.53525
C	-2.93463	-3.27971	6.23045
C	-4.41255	-1.34219	5.55683
H	-1.65384	-1.02853	5.36110
H	-1.33588	-2.29038	4.15328
H	-2.34691	-0.86453	3.74520
H	-3.80013	-3.86166	6.58558
H	-2.14633	-3.98970	5.91943
H	-2.53992	-2.67495	7.06705
H	-4.72133	-0.65429	4.74866
H	-5.30837	-1.87223	5.92096
H	-3.99941	-0.73493	6.38288
N	0.08521	-0.03866	-2.07074
N	0.67612	0.43195	-4.16307
C	0.88861	0.69899	-2.84059
C	-0.32253	-0.53054	-4.23438
C	-0.67655	-0.81153	-2.93147
C	1.36036	1.05946	-5.29066
H	-1.41825	-1.51162	-2.55420
H	-0.67835	-0.91765	-5.18696
H	1.62125	1.41986	-2.48361
H	0.64882	1.64131	-5.90067
H	1.83987	0.29311	-5.92220
H	2.13621	1.73721	-4.90420

[Fe(pfp)(1-MeIm)O_2] - Polarized

Fe	0.00000	0.00000	0.00000
O	0.00000	0.00000	1.78937
O	-0.77530	0.81879	2.43568
O	4.48573	4.16691	4.67576
N	0.00000	1.98462	-0.07499
N	2.00851	-0.00713	0.04145
N	0.08646	-0.04402	-2.06438
N	0.68591	0.41313	-4.15694
C	0.89627	0.68578	-2.83531
H	1.63156	1.40452	-2.47952
C	-0.31757	-0.54435	-4.22639
H	-0.67272	-0.93433	-5.17804
C	-0.67711	-0.81723	-2.92328
H	-1.42390	-1.51112	-2.54462
C	1.37671	1.03135	-5.28573
H	0.66999	1.61400	-5.90052
H	1.85375	0.25922	-5.91208
H	2.15516	1.70678	-4.90046
C	-1.08736	2.82165	-0.29313
C	-0.67434	4.20831	-0.26578
C	0.66547	4.21544	0.01850
C	1.08353	2.83173	0.11386
C	2.42176	2.43338	0.30235
C	2.83804	1.08970	0.23039
C	4.22763	0.67840	0.24432
C	4.24232	-0.67367	0.02987
C	2.86045	-1.09441	-0.08466
C	-2.42322	2.40950	-0.44746
N	3.43828	3.12505	2.89736
C	3.71491	3.29921	4.24643
C	2.97777	2.34451	5.23004
C	2.19184	1.19824	4.56000
C	2.01007	3.23020	6.05649
C	4.05854	1.75148	6.16740
N	-3.54854	4.20242	1.53288
C	-3.89126	4.96789	2.63972
O	-4.71904	5.88722	2.60126
C	-3.17326	4.61590	3.97449
C	-2.46658	5.91060	4.44942
C	-2.14535	3.47141	3.87524
C	-4.28360	4.23664	4.98685
C	3.46403	3.50088	0.49547
C	3.96635	4.19530	-0.62208
C	4.92711	5.20761	-0.48644
C	5.39385	5.53425	0.79612
C	4.91648	4.86369	1.92962
C	3.95045	3.83977	1.79246
C	-3.47361	3.43417	-0.77561
C	-3.94551	3.51464	-2.10066
C	-4.92740	4.44318	-2.47382
C	-5.45153	5.30769	-1.50065
C	-5.01038	5.24966	-0.17227
C	-4.02032	4.31300	0.20574
H	2.77501	2.38577	2.65691
H	-2.84963	3.47082	1.67828
H	1.77100	0.53984	5.34124
H	1.33219	1.54680	3.95799
H	2.84013	0.56814	3.92263
H	2.55907	4.06207	6.52824
H	1.21424	3.65581	5.41827
H	1.52789	2.62839	6.84845
H	4.73825	1.07502	5.61738
H	4.66293	2.55777	6.61293
H	3.58009	1.17116	6.97705
H	-3.18422	6.74622	4.48803
H	-2.03795	5.76093	5.45709
H	-1.64366	6.19172	3.76694
H	-2.60338	2.51197	3.57316
H	-1.32366	3.70277	3.17237
H	-1.68342	3.30330	4.86475
H	-4.79497	3.30234	4.69108
H	-3.84579	4.08343	5.99017
H	-5.03737	5.03885	5.04622
H	1.32817	5.07225	0.13548
H	-1.33792	5.05781	-0.42543
H	5.07227	1.35354	0.38064
H	5.10063	-1.34165	-0.03365
H	5.26725	5.11445	2.93117
H	6.14234	6.32434	0.92462
H	5.30330	5.73321	-1.37068
H	3.58448	3.92707	-1.61397
H	-5.41472	5.91230	0.59343
H	-6.22021	6.04040	-1.77148
H	-5.27670	4.48911	-3.51095
H	-3.52112	2.82939	-2.84309
N	0.02433	-2.00792	-0.00097
N	-1.98034	-0.01459	-0.09515
C	2.46559	-2.43722	-0.23456
C	-2.82488	1.07106	-0.29199
C	1.12158	-2.84597	-0.14934
C	-1.06884	-2.85371	0.12316
C	-2.82065	-1.10810	0.06533
C	3.53336	-3.46807	-0.48020
C	-4.20905	0.65104	-0.25663
C	0.70680	-4.23475	-0.13012
C	-0.64718	-4.23964	0.07111
C	-2.41591	-2.45113	0.20002
C	-4.20703	-0.69704	-0.01760
C	4.08517	-3.57903	-1.77147
C	4.02209	-4.32274	0.55168
H	-5.06196	1.31670	-0.38346
H	1.37792	-5.08562	-0.24536
H	-1.31754	-5.09469	0.15212
C	-3.47997	-3.50892	0.31634
H	-5.05880	-1.36978	0.07929
C	5.09229	-4.51089	-2.06045
H	3.70294	-2.91611	-2.55583
N	3.45934	-4.18750	1.83968
C	5.03927	-5.26061	0.26097
C	-3.89360	-4.20666	-0.83540
C	-4.09117	-3.82019	1.56627
C	5.56195	-5.34722	-1.03607
H	5.50334	-4.58135	-3.07328
C	3.75069	-4.89508	2.99674
H	2.72112	-3.48466	1.90471
H	5.40040	-5.90026	1.06705
C	-4.89095	-5.19067	-0.77783
H	-3.41720	-3.95958	-1.79100
N	-3.64559	-3.12409	2.71156
C	-5.10082	-4.80889	1.62304
H	6.34981	-6.08067	-1.24175
O	4.61721	-5.77640	3.05716
C	2.92320	-4.51772	4.25990
C	-5.49003	-5.48138	0.45744
H	-5.19695	-5.71853	-1.68742
C	-4.10296	-3.22238	4.01849
H	-2.89043	-2.45808	2.53777
H	-5.55872	-5.02722	2.58822
C	2.28387	-5.82991	4.77856
C	1.81997	-3.46557	4.02094
C	3.93482	-3.98847	5.30798
H	-6.27354	-6.24479	0.52307
O	-5.02472	-3.97350	4.36181
C	-3.40260	-2.30902	5.06542
H	3.05650	-6.60494	4.90811
H	1.78717	-5.65367	5.75005
H	1.52519	-6.21321	4.07174
H	2.22756	-2.48698	3.70449
H	1.07847	-3.80229	3.27216
H	1.26963	-3.28771	4.96230
H	4.39595	-3.03954	4.97805
H	3.42431	-3.80405	6.27070
H	4.73899	-4.72536	5.46838
C	-2.17041	-1.54404	4.54243
C	-2.98147	-3.22394	6.24210
C	-4.47558	-1.30311	5.55660
H	-1.72137	-0.96058	5.36600
H	-1.38469	-2.22610	4.16740
H	-2.41123	-0.81549	3.74660
H	-3.84283	-3.81194	6.59740
H	-2.18615	-3.92826	5.93614
H	-2.59435	-2.61240	7.07734
H	-4.78767	-0.62062	4.74507
H	-5.36791	-1.84019	5.91889
H	-4.07111	-0.68947	6.38221

[Fe^{II}(tpp)(ImH)$_2$]

N	0.00000	0.00000	1.97433
N	-0.51903	0.49469	4.07020
C	-0.78374	0.75073	2.75449
C	0.48019	-0.46584	4.13368
C	0.79120	-0.76211	2.82415
H	-0.98296	0.93456	4.86134
H	-1.52860	1.46132	2.40485
H	0.86637	-0.84028	5.07859
H	1.52118	-1.46412	2.43005
N	-0.00001	0.00003	-1.97434
N	0.51917	-0.49448	-4.07022
C	0.78397	-0.75043	-2.75452
C	-0.79143	0.76192	-2.82415
C	-0.48030	0.46578	-4.13368
H	1.52907	-1.46079	-2.40488
H	-1.52163	1.46368	-2.43005
H	0.98324	-0.93420	-4.86135
H	-0.86657	0.84014	-5.07859
Fe	0.00000	0.00000	0.00000
N	0.00000	2.00218	0.00342
N	-2.00375	0.01458	0.00741
C	1.10837	2.84356	-0.02592
C	-1.09680	2.86219	-0.01700
C	-2.85597	1.11841	0.01388
C	-2.85403	-1.08776	0.02208
C	0.70005	4.23145	-0.09481
C	-0.66691	4.24408	-0.09124
C	-4.24219	0.69831	0.04435
C	-4.24007	-0.66885	0.02987
C	-2.44925	2.46755	0.00205
C	2.45291	2.43491	-0.02376
C	-3.50305	3.53458	0.00377
C	-4.39391	3.68095	-1.08385
C	-5.37907	4.68065	-1.08132
C	-5.49377	5.55791	0.00952
C	-4.61476	5.42710	1.09711
C	-3.63114	4.42600	1.09308
C	3.51441	3.49488	-0.01878
C	3.70297	4.31831	1.11375
C	4.69518	5.31105	1.12577
C	5.51920	5.49947	0.00394
C	5.34249	4.68873	-1.12936
C	4.34928	3.69665	-1.14043
H	1.38143	5.07900	-0.15852
H	-1.33371	5.10311	-0.15414
H	-5.09891	1.37043	0.07151
H	-5.09580	-1.34279	0.02831
H	-4.30357	3.00199	-1.93916
H	-6.05569	4.77770	-1.93832
H	-6.26251	6.33898	0.01159
H	-4.69695	6.10450	1.95513
H	-2.94739	4.32631	1.94377
H	3.06425	4.16636	1.99099
H	4.82795	5.93605	2.01665
H	6.29464	6.27400	0.01271
H	5.97717	4.83190	-2.01169
H	4.20690	3.06915	-2.02730
N	0.00001	-2.00218	-0.00357
N	2.00374	-0.01457	-0.00723
C	-2.45288	-2.43488	0.02412
C	2.85404	1.08777	-0.02128
C	-1.10837	-2.84357	0.02556
C	1.09679	-2.86220	0.01627
C	2.85596	-1.11840	-0.01341
C	-3.51442	-3.49486	0.01938
C	4.24008	0.66885	-0.02828
C	-0.70007	-4.23149	0.09355
C	0.66690	-4.24414	0.08974
C	2.44925	-2.46754	-0.00228
C	4.24221	-0.69831	-0.04293
C	-3.70414	-4.31739	-1.11360
C	-4.34814	-3.69747	1.14172
H	5.09582	1.34278	-0.02609
H	-1.38147	-5.07906	0.15687
H	1.33372	-5.10320	0.15205
C	3.50303	-3.53459	-0.00412
H	5.09894	-1.37040	-0.06969
C	-4.69636	-5.31012	-1.12537
H	-3.06629	-4.16477	-1.99137
C	-5.34138	-4.68952	1.13089
H	-4.20487	-3.07064	2.02893
C	4.39317	-3.68180	1.08399
C	3.63183	-4.42521	-1.09399
C	-5.51925	-5.49940	-0.00285
H	-4.83005	-5.93443	-2.01659
H	-5.97519	-4.83337	2.01375
C	5.37830	-4.68149	1.08138
H	4.30227	-3.00345	1.93973
C	4.61543	-5.42633	-1.09811
H	2.94866	-4.32487	-1.94507
H	-6.29469	-6.27392	-0.01142
C	5.49372	-5.55795	-0.01003
H	6.05436	-4.77918	1.93876
H	4.69817	-6.10311	-1.95657
H	6.26243	-6.33904	-0.01217

[Fe^{III}(tpp)(ImH)$_2$]$^+$

N	0.00000	0.00000	1.98156
N	-0.53556	0.48747	4.06447
C	-0.80468	0.73786	2.75702
C	0.48365	-0.45254	4.13505
C	0.80726	-0.74666	2.83028
H	-1.00966	0.91884	4.85661
H	-1.56352	1.43260	2.40618
H	0.87364	-0.81674	5.08217
H	1.55278	-1.43546	2.44363
N	0.00010	0.00016	-1.98157
N	0.53628	-0.48652	-4.06451
C	0.80561	-0.73675	-2.75708
C	-0.80792	0.74605	-2.83026
C	-0.48394	0.45240	-4.13504
H	1.56520	-1.43070	-2.40628
H	-1.55418	1.43402	-2.44357
H	1.01088	-0.91728	-4.85667
H	-0.87427	0.81629	-5.08214
Fe	0.00000	0.00000	0.00000
N	0.00000	2.00294	-0.00713
N	-2.00768	0.03632	0.00215
C	1.11945	2.82832	-0.04790
C	-1.09334	2.87037	-0.05047
C	-2.85595	1.14534	-0.00336
C	-2.85451	-1.06719	0.01825
C	0.72072	4.21357	-0.14177
C	-0.64850	4.23965	-0.14519
C	-4.23737	0.72583	0.02403
C	-4.23638	-0.64291	0.01589
C	-2.45011	2.49343	-0.03011
C	2.46387	2.41732	-0.03482
C	-3.49669	3.56675	-0.04609
C	-4.37884	3.70232	-1.14182
C	-5.35527	4.71006	-1.15521
C	-5.46866	5.59824	-0.07321
C	-4.59816	5.47462	1.02196
C	-3.61979	4.46883	1.03462
C	3.52992	3.47262	-0.03835
C	3.71806	4.30172	1.08979
C	4.71612	5.28834	1.09296
C	5.53841	5.46375	-0.03212
C	5.35842	4.64700	-1.16052
C	4.36282	3.65766	-1.16407
H	1.41022	5.05315	-0.21543
H	-1.30687	5.10327	-0.22355
H	-5.09230	1.39974	0.04132
H	-5.09205	-1.31628	0.01340
H	-4.28923	3.01628	-1.99172
H	-6.02575	4.80404	-2.01640
H	-6.23150	6.38400	-0.08390
H	-4.68221	6.16111	1.87154
H	-2.94418	4.37438	1.89254
H	3.08212	4.15978	1.97082
H	4.85390	5.91859	1.97842
H	6.31665	6.23446	-0.02973
H	5.99209	4.78259	-2.04383
H	4.21753	3.02701	-2.04833
N	0.00001	-2.00288	0.00678
N	2.00774	-0.03630	-0.00175
C	-2.46381	-2.41728	0.03528
C	2.85457	1.06723	-0.01636
C	-1.11943	-2.82833	0.04659
C	1.09335	-2.87040	0.04870
C	2.85599	-1.14531	0.00480
C	-3.52993	-3.47255	0.03914
C	4.23644	0.64294	-0.01148
C	-0.72071	-4.21376	0.13793
C	0.64850	-4.23985	0.14107
C	2.45010	-2.49342	0.02981
C	4.23745	-0.72580	-0.01999
C	-3.72094	-4.29914	-1.09034
C	-4.36008	-3.65990	1.16649
H	5.09211	1.31629	-0.00727
H	-1.41025	-5.05341	0.21027
H	1.30689	-5.10359	0.21787
C	3.49670	-3.56676	0.04571
H	5.09241	-1.39970	-0.03594
C	-4.71909	-5.28568	-1.09317
H	-3.08713	-4.15536	-1.97261
C	-5.35580	-4.64912	1.16325
H	-4.21258	-3.03112	2.05173
C	4.37688	-3.70420	1.14277
C	3.62179	-4.46689	-1.03638
C	-5.53864	-5.46344	0.03355
H	-4.85908	-5.91402	-1.97963
H	-5.98736	-4.78651	2.04780
C	5.35336	-4.71190	1.15613
H	4.28573	-3.01964	1.99370
C	4.60018	-5.47266	-1.02373
H	2.94772	-4.37096	-1.89535
H	-6.31696	-6.23407	0.03140
C	5.46873	-5.59817	0.07277
H	6.02232	-4.80734	2.01834
H	4.68578	-6.15766	-1.87436
H	6.23159	-6.38391	0.08345

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