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Supplementary information

Insights on the effect of distal histidine and water hydrogen bonding on NO ligation to the Ferrous and Ferric Heme: a DFT study

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This supplementary file contains Figures and Tables:

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Figure S1:

The optimized structures of complexes of ferrous with NO ligand investigated with/without HIS64 (MI) distal group at the OPTX-PBE/DZVP-GGA/GEN-A2* level of theory.

Figure S2:

The optimized structures of complexes of ferric with NO ligand investigated with/without HIS64 (MI) distal group at the OPTX-PBE/DZVP-GGA/GEN-A2* level of theory.

Table S1:

Binding energy in presence of distal group for ferrous complexes at B3LYP/def2-TZVP level of theory

Table S2:

Binding energy in presence of distal group for ferric complexes at B3LYP/def2-TZVP level of theory

Table S3:

The QTAIM analysis of the topological and energetic features of the electron density distribution ρ(r) calculated at the band critical points (BCP of Fe-N, N…H_{MI}, O…H_{MI} and O…H_W) for ferrous-heme. All values in the table are in atomic units

Table S4:

The QTAIM analysis of the topological and energetic features of the electron density distribution ρ(r) calculated at the band critical points (BCP of Fe-N) for ferric-heme. All values in the table are in atomic units

Table S5:

xyz coordinates of the optimized Ferrous-Heme systems.

Table S6:

xyz coordinates of the optimized Ferrous-Heme systems.

Figure S1:

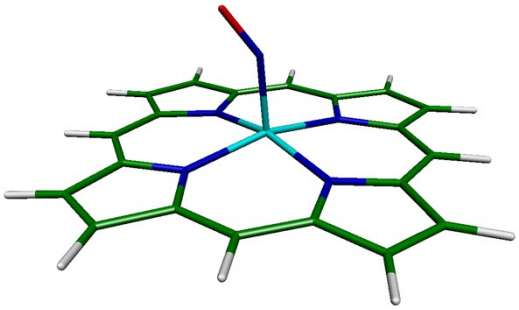
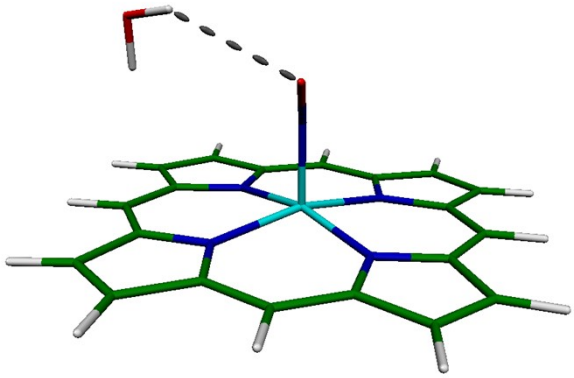
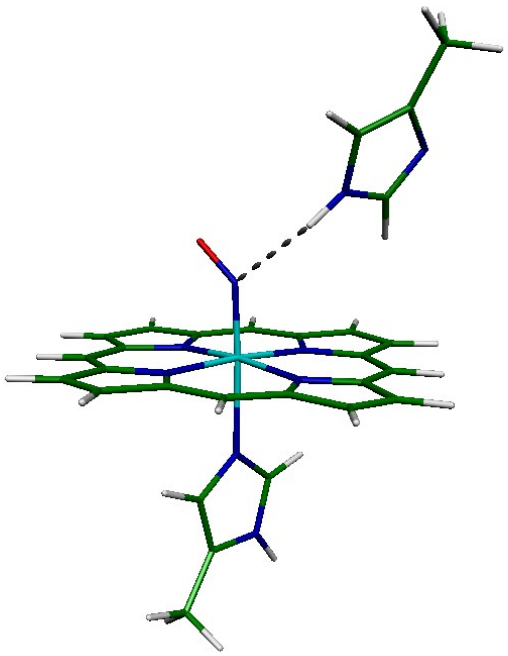
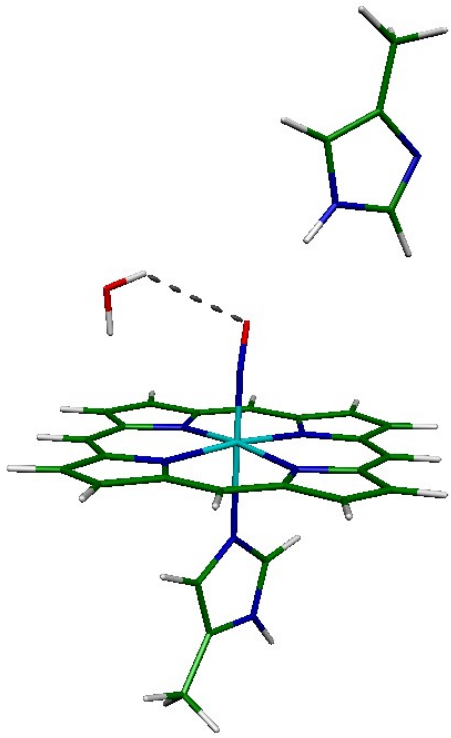
$[Fe^{II}P\text{-}NO]$	$[Fe^{II}P\text{-}NO]\ldots H_2O$
	
$[MI\text{-}Fe^{II}\ P\text{-}NO\ldots MI]$	**$[MI\text{-}Fe^{II}\ P\text{-}NO\ldots MI]\ldots H_2O$**
	

Figure S2:

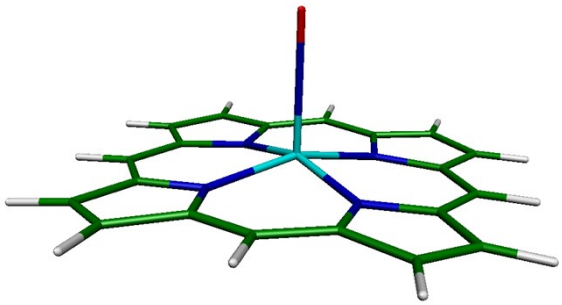
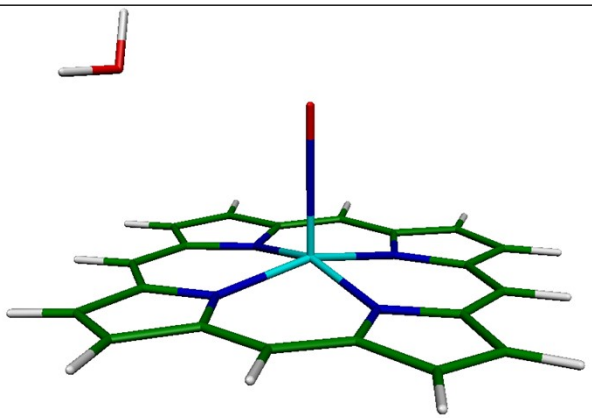
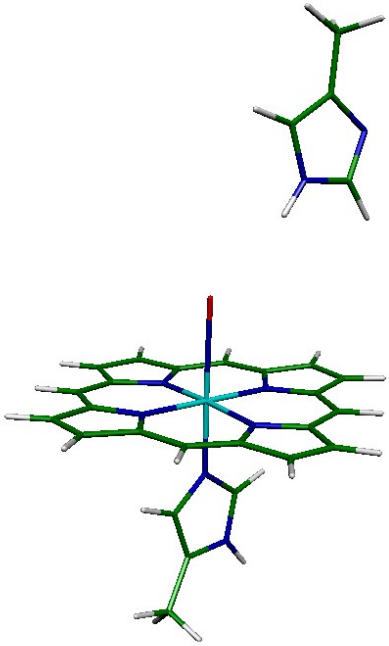
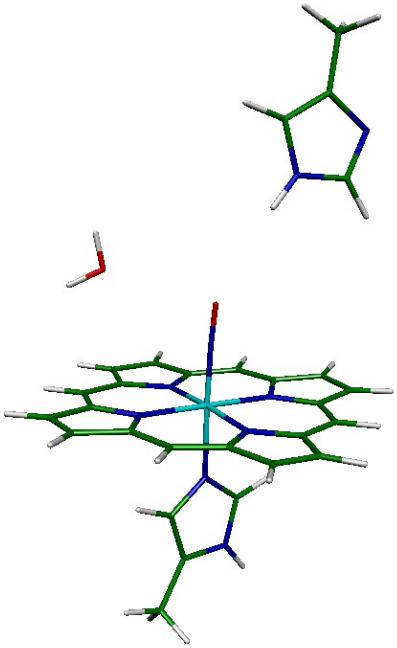
$[Fe^{III}P\text{-}NO]^+$	$[Fe^{III}P\text{-}NO]^+\ldots H_2O$
	
$[MI\text{-}Fe^{III}\ P\text{-}NO\ldots MI]^+$	**$[MI\text{-}Fe^{III}\ P\text{-}NO\ldots MI]^+\ldots H_2O$**
	

Table S1:

$\Delta E_{binding} = E_{complex}$ (S=1/2, LS) - ($E_{[MI\text{-}Fe^{II}P]}$ (S=2, HS) + E_{NO} (S=1/2))

$\Delta E_{binding} = E_{complex}$ (S=1/2, LS) - ($E_{[MI\text{-}Fe^{II}P\ldots MI]}$ (S=2, HS) + E_{NO} (S=1/2))

Complex	ΔGD3BJ	BSSE	ΔE (kcal mol^{-1}) (gas)	ΔEc (kcal mol^{-1}) (gas)	ΔE (kcal mol^{-1}) (solvent)	ΔEc (kcal mol^{-1}) (solvent)
Ferrous-Heme						
[Fe^{II}P-NO]	-5.737	1.008	-11.836	-16.565	-10.897	-15.796
[Fe^{II}P-NO…MI]	-7.386	1.082	-10.237	-16.541	-8.473	-14.777
[MI-Fe^{II}P-NO]	-5.163	1.284	-14.007	-17.887	-13.007	-16.887
[MI-Fe^{II}P-NO…MI]	-5.739	1.218	-14.566	-19.087	-12.177	-16.697
Ferrous-Heme (Microhydration effect)						
[Fe^{II}P-NO]…H_2O	-6.067	-0.776	-10.378	-17.221	-9.199	-14.092
[Fe^{II}P-NO…MI]…H_2O	-8.570	1.292	-12.661	-19.939	-9.717	-16.994
[MI-Fe^{II}P-NO]…H_2O	-6.097	1.354	-15.081	-19.823	-12.262	-17.004
[MI-Fe^{II}P-NO…MI]…H_2O	-5.832	1.483	-15.236	-19.586	-12.227	-16.576

Table S2:

$\Delta E_{binding} = E_{complex}$ (S=0, LS) - ($E_{[MI\text{-}Fe^{III}P]^+}$ (S=5/2, HS) + E_{NO} (S=1/2))

$\Delta E_{binding} = E_{complex}$ (S=0, LS) - ($E_{[MI\text{-}Fe^{III}P\ldots MI]^+}$ (S=5/2, HS) + E_{NO} (S=1/2))

Complex	ΔGD3BJ	BSSE	ΔE (kcal mol^{-1}) (gas)	ΔEc (kcal mol^{-1}) (gas)	ΔE (kcal mol^{-1}) (solvent)	ΔEc (kcal mol^{-1}) (solvent)
Ferric-Heme						
[Fe^{III}P-NO]$^+$	-5.570	1.211	-6.810	-11.169	0.162	-4.197
[Fe^{III}P-NO…MI]$^+$	-3.980	1.346	-5.381	-8.015	3.096	0.462
[MI-Fe^{III}P-NO]$^+$	-7.398	1.486	-6.424	-12.336	-4.141	-10.103
[MI-Fe^{III}P-NO…MI]$^+$	-6.010	1.606	-8.884	-13.288	-2.749	-7.152
Ferric-Heme (Microhydration effect)						
[Fe^{III}P-NO]$^+$…H_2O	-6.108	1.294	-3.302	-8.115	4.131	-0.682
[Fe^{III}P-NO…MI]$^+$…H_2O	-5.877	1.327	-0.373	-4.923	7.103	2.553
[MI-Fe^{III}P-NO]$^+$…H_2O	-7.632	1.601	-7.050	-13.081	-2.824	-8.855
[MI-Fe^{III}P-NO…MI]$^+$…H_2O	-4.685	1.640	-4.649	-7.694	0.260	-2.786

***Table S3**:*

Complex		ρ_{BCP}	$\nabla\rho^2_{BCP}$	V_{BCP}	G_{BCP}	H_{BCP}	H_{BCP}/ρ_{BCP}	$\lvert V_{BCP}\rvert/G_{BCP}$	G_{BCP}/ρ_{BCP}
a) Ferrous-Heme									
[Fe^{II}P-NO]	Fe-N	0.188	0.810	-0.376	0.289	-0.087	-0.462	1.300	1.537
[Fe^{II}P-NO…MI]	Fe-N	0.189	0.799	-0.376	0.288	-0.088	-0.465	1.306	1.522
[MI-Fe^{II}P-NO]	Fe-N	0.169	0.788	-0.339	0.268	-0.071	-0.418	1.264	1.581
[MI-Fe^{II}P-NO…MI]	Fe-N	0.173	0.824	-0.344	0.275	-0.069	-0.398	1.251	1.587
	N…H_{MI}	0.006	0.021	-0.003	0.004	0.001	0.187	0.728	0.689
b) Ferrous-Heme (Microhydration effect)									
[Fe^{II}P-NO] …H_2O	Fe-N	0.192	0.788	-0.387	0.292	-0.095	-0.494	1.325	1.520
	N…H_w	0.003	0.011	-0.002	0.002	0.001	0.206	0.704	0.698
[Fe^{II}P-NO…MI] …H_2O	Fe-N	0.194	0.784	-0.384	0.290	-0.094	-0.485	1.324	1.494
	O…H_W	0.004	0.014	-0.002	0.003	0.001	0.222	0.687	0.709
	O…H_{MI}	0.006	0.023	-0.003	0.004	0.001	0.244	0.677	0.755
[MI-Fe^{II}P-NO]…H_2O	Fe-N	0.176	0.830	-0.351	0.279	-0.072	-0.407	1.257	1.584
	O…H_w	0.005	0.017	-0.002	0.003	0.001	0.228	0.682	0.716
[MI-Fe^{II}P-NO…MI] …H_2O	Fe-N	0.176	0.820	-0.349	0.277	-0.072	-0.408	1.260	1.572
	O…H_W	0.004	0.017	-0.002	0.003	0.001	0.229	0.681	0.719

***Table S4**:*

Complex		ρ_{BCP}	$\nabla\rho^2_{BCP}$	V_{BCP}	G_{BCP}	H_{BCP}	H_{BCP}/ρ_{BCP}	$\lvert V_{BCP}\rvert/G_{BCP}$	G_{BCP}/ρ_{BCP}
a) Ferric-Heme									
[Fe^{III}P-NO]$^+$	Fe-N	0.220	1.385	-0.568	0.457	-0.111	-0.505	1.243	2.079
[Fe^{III}P-NO…MI]$^+$	Fe-N	0.217	1.342	-0.550	0.443	-0.107	-0.495	1.242	2.045
[MI-Fe^{III}P-NO]$^+$	Fe-N	0.197	1.406	-0.518	0.435	-0.083	-0.423	1.192	2.207
[MI-Fe^{III}P-NO…MI]$^+$	Fe-N	0.202	1.441	-0.531	0.446	-0.086	-0.424	1.192	2.210
b) Ferric-Heme (Microhydration effect)									
[Fe^{III}P-NO]$^+$ …H_2O	Fe-N	0.218	1.394	-0.563	0.456	-0.107	-0.494	1.236	2.094
[Fe^{III}P-NO…MI]$^+$ …H_2O	Fe-N	0.218	1.276	-0.540	0.429	-0.111	-0.507	1.257	1.968
[MI-Fe^{III}P-NO]$^+$…H_2O	Fe-N	0.202	1.445	-0.532	0.446	-0.085	-0.423	1.191	2.215
[MI-Fe^{III}P-NO…MI]$^+$ …H_2O	Fe-N	0.200	1.426	-0.525	0.441	-0.084	-0.421	1.191	2.201

Table S5:

Ferrous-Heme							
[MI-Fe^{II}-P-NO], Ms=2				**[MI-Fe^{II}-P-NO]…H_2O, Ms=2**			
C	9.483977	29.187638	2.539124	C	8.197362	28.538742	2.147696
H	8.576827	29.050742	3.169765	H	7.363992	28.134443	2.765888
H	9.522139	28.356550	1.806929	H	8.366354	27.845217	1.300287
C	10.728662	29.192235	3.367708	C	9.452362	28.674625	2.950419
N	10.967347	30.104213	4.383070	N	9.565882	29.503813	4.054453
H	10.335945	30.848605	4.665451	H	8.828387	30.098962	4.422143
C	11.851339	28.391775	3.356462	C	10.693012	28.081647	2.837743
H	12.078249	27.537369	2.706002	H	11.038035	27.350891	2.095327
C	12.181219	29.833919	4.931150	C	10.826570	29.388649	4.552557
H	12.625231	30.397229	5.758798	H	11.199748	29.933454	5.426893
N	12.750390	28.795815	4.329145	N	11.540444	28.528801	3.836249
FE	14.746883	27.913188	4.853245	FE	13.740100	27.961370	4.221018
C	15.996375	31.112605	5.123776	C	14.416966	31.326284	4.515945
H	16.422258	32.123330	5.209824	H	14.670963	32.393165	4.605596
C	13.790681	28.021994	8.164421	C	13.034307	27.823073	7.602170
H	13.509199	28.043889	9.228144	H	12.842619	27.768724	8.684243
C	13.333880	24.793970	4.559969	C	12.886517	24.636718	3.926232
H	12.912223	23.782582	4.461069	H	12.655499	23.564850	3.833424
C	15.532091	27.891356	1.510598	C	14.258238	28.140798	0.832627
H	15.809461	27.865249	0.446753	H	14.450121	28.193522	-0.249033
N	14.868894	29.304755	6.357598	N	13.724968	29.313958	5.760058
C	15.458110	30.543932	6.284967	C	14.092772	30.638169	5.693482
C	15.417144	31.190764	7.576822	C	14.056598	31.233705	7.009560
C	14.794108	30.318201	8.432618	C	13.664656	30.246167	7.877381
C	14.459471	29.144255	7.658775	C	13.463918	29.053452	7.085852
N	13.749900	26.651246	6.113672	N	13.057624	26.522077	5.503566
C	13.466496	26.869146	7.439659	C	12.851353	26.651601	6.855700
C	12.763059	25.732240	7.993963	C	12.401423	25.396151	7.418376
C	12.634022	24.819317	6.981121	C	12.360688	24.497173	6.386257
C	13.257834	25.406285	5.815573	C	12.780009	25.212557	5.200016
N	14.485739	26.608725	3.341579	N	13.613976	26.649235	2.691083
C	13.924240	25.354598	3.421353	C	13.293734	25.312216	2.768582
C	13.998955	24.691993	2.140130	C	13.397951	24.696619	1.465734
C	14.618152	25.562267	1.281457	C	13.781035	25.682286	0.593657
C	14.917172	26.752683	2.042131	C	13.910483	26.894658	1.369122
N	15.593834	29.242969	3.563351	N	14.216038	29.437642	2.930924
C	15.843514	29.051378	2.228522	C	14.399666	29.321157	1.573157
C	16.471627	30.224615	1.662004	C	14.757062	30.600285	1.001707
C	16.600127	31.129293	2.681684	C	14.802450	31.493931	2.039071
C	16.051848	30.501982	3.864982	C	14.474598	30.754345	3.238237

O	17.037190	26.399164	4.845625	O	16.411725	27.543743	3.813808
H	9.369294	30.140303	1.974262	H	7.873017	29.520244	1.733090
H	12.420674	25.643532	9.036424	H	12.160518	25.227199	8.480049
H	12.165075	23.824291	7.018299	H	12.079179	23.433409	6.419820
H	13.613008	23.683653	1.927868	H	13.191940	23.636698	1.249609
H	14.847266	25.417006	0.215066	H	13.954939	25.604387	-0.491095
H	16.783943	30.333879	0.612608	H	14.950782	30.784486	-0.066395
H	17.037532	32.138297	2.643883	H	15.042368	32.568317	2.004427
H	15.820512	32.191228	7.800077	H	14.306659	32.282574	7.235901
H	14.579384	30.451682	9.503890	H	13.522845	30.311308	8.968070
N	16.258269	27.211913	5.229134	O	16.427902	24.268794	5.156057
				H	16.829488	25.084879	4.813498
				H	15.475615	24.459128	5.109916
				N	15.394925	27.585848	4.435312

[MI-Fe^{II}-P-NO…MI], Ms=2				[MI-Fe^{II}-P-NO…MI]…H_2O, Ms=2			
C	22.907000	29.056000	6.205000	C	22.907000	29.056000	6.205000
H	23.291812	30.084863	6.026582	H	23.445987	30.006459	6.006145
H	23.485789	28.353634	5.566044	H	23.462530	28.225283	5.715678
C	21.441000	28.978393	5.911044	C	21.497982	29.136627	5.727523
N	20.519294	29.729003	6.625812	N	20.691457	30.201754	6.089189
C	20.796447	28.204250	4.961116	C	20.797922	28.244969	4.932984
H	21.176348	27.487551	4.223635	H	21.086830	27.293889	4.468065
C	19.339333	29.403221	6.108619	C	19.521903	29.944323	5.524789
H	18.364862	29.803863	6.417463	H	18.648000	30.582000	5.610000
N	19.456325	28.485180	5.109108	N	19.528604	28.775659	4.827066
H	18.688634	28.097283	4.570218	H	18.749020	28.391536	4.305614
C	9.738639	29.249592	2.276280	C	8.185009	28.364909	2.152878
H	8.796579	29.011461	2.821192	H	7.337960	27.994453	2.772519
H	9.878898	28.493230	1.479845	H	8.384775	27.621558	1.357066
C	10.915728	29.236182	3.201347	C	9.417486	28.561466	2.979134
N	11.041484	30.080712	4.291268	N	9.487330	29.417190	4.066349
H	10.367189	30.786465	4.574841	H	8.727303	29.997202	4.410560
C	12.063122	28.471261	3.225921	C	10.677999	28.009243	2.895029
H	12.365486	27.675872	2.535184	H	11.054127	27.279872	2.167629
C	12.217614	29.807296	4.917799	C	10.745603	29.356447	4.583351
H	12.574031	30.327580	5.811681	H	11.084787	29.935232	5.448033
N	12.866150	28.829484	4.295276	N	11.497137	28.502194	3.897280
FE	14.836915	27.941258	4.926003	FE	13.714864	28.016519	4.230966
C	16.003608	31.187049	5.199572	C	14.311587	31.406087	4.422288
H	16.393506	32.214704	5.287312	H	14.546243	32.480584	4.493617
C	13.802157	28.059772	8.198176	C	13.037044	27.938841	7.592732
H	13.509457	28.065424	9.261147	H	12.852678	27.899714	8.678478
C	13.419889	24.840642	4.570100	C	12.874578	24.691906	3.970410
H	12.981014	23.835224	4.467007	H	12.644177	23.616157	3.905895
C	15.806109	27.893168	1.630370	C	14.260498	28.129319	0.825829
H	16.148450	27.858678	0.582640	H	14.479829	28.159897	-0.253957
N	14.894825	29.343726	6.404551	N	13.659982	29.396745	5.704159
C	15.447068	30.603389	6.341761	C	13.988819	30.731942	5.605562
C	15.373687	31.250695	7.630813	C	13.928190	31.360768	6.903255
C	14.768530	30.362769	8.481568	C	13.570800	30.385339	7.798694
C	14.472511	29.182729	7.704114	C	13.413836	29.167421	7.040730
N	13.779561	26.725652	6.118919	N	13.068167	26.611815	5.511685
C	13.489723	26.921056	7.450173	C	12.892575	26.750543	6.870218
C	12.768848	25.786943	7.980191	C	12.491347	25.493123	7.458121
C	12.647215	24.886309	6.956783	C	12.441739	24.581351	6.438466
C	13.297275	25.475069	5.809344	C	12.814377	25.287281	5.233747
N	14.647874	26.635018	3.411511	N	13.566869	26.681025	2.695844
C	14.072702	25.384679	3.461028	C	13.237054	25.349316	2.789299
C	14.224883	24.708018	2.195231	C	13.341748	24.711067	1.497547
C	14.908874	25.565052	1.372847	C	13.748336	25.678533	0.616330

C	15.166182	26.759764	2.141540	C	13.886978	26.898973	1.375870
N	15.710528	29.279246	3.664403	N	14.148905	29.481982	2.887516
C	16.053573	29.065586	2.350752	C	14.387456	29.323407	1.542232
C	16.693939	30.237110	1.797500	C	14.761278	30.585803	0.943551
C	16.737569	31.167696	2.800034	C	14.768375	31.509678	1.953820
C	16.128226	30.554986	3.958860	C	14.400606	30.805512	3.161269
O	16.722349	26.103703	5.682405	O	16.059325	27.491818	5.531036
H	9.615223	30.245613	1.795468	H	7.867450	29.316335	1.669054
H	23.107364	28.810743	7.269509	H	22.934000	28.879000	7.306000
H	12.409414	25.699031	9.017567	N	15.351938	27.659024	4.581331
H	12.167412	23.895532	6.969293	H	12.269753	25.338997	8.525818
H	13.850748	23.697082	1.971398	H	12.171398	23.514547	6.485863
H	15.215389	25.411338	0.325681	H	13.136037	23.647994	1.299326
H	17.057822	30.329170	0.761849	H	13.943106	25.581307	-0.464362
H	17.152368	32.187692	2.768600	H	14.997937	30.734908	-0.122491
H	15.750776	32.261910	7.852255	H	15.013480	32.582112	1.897522
H	14.537922	30.489507	9.551620	H	14.141821	32.423573	7.100876
N	16.298338	27.182910	5.408423	H	13.429417	30.475725	8.887606
				O	16.607179	24.446018	3.922263
				H	16.910238	25.066059	4.605850
				H	15.709274	24.760379	3.720130

Ferric-Heme

[MI-Fe^{III}-P-NO]$^{+}$, Ms=1				**[MI-Fe^{III}-P-NO]$^{+}$…H$_2$O, Ms=1**			
C	-0.347385	3.018983	-0.117736	C	8.362258	28.424513	2.170188
C	0.403206	4.251708	-0.142342	H	7.523510	28.034003	2.787392
C	1.713147	3.914751	-0.356938	H	8.544933	27.704678	1.347747
C	1.769562	2.474086	-0.430252	C	9.601939	28.598667	2.985554
N	0.501094	1.941828	-0.290113	N	9.689728	29.449545	4.077660
H	-0.023305	5.256104	-0.023076	H	8.935125	30.028634	4.434285
H	2.578229	4.586388	-0.440583	C	10.850638	28.030369	2.882786
C	2.956774	1.749515	-0.539229	H	11.206519	27.301954	2.152823
H	3.901164	2.308414	-0.635512	C	10.939841	29.386716	4.593931
C	3.017851	0.359599	-0.440518	H	11.279861	29.954260	5.457130
C	2.468248	-1.761220	-0.152831	N	11.674335	28.527095	3.885277
C	3.910288	-1.703742	-0.198679	FE	13.622913	28.031810	4.249648
H	5.256551	0.038548	-0.487309	C	14.387304	31.391591	4.486102
H	4.582597	-2.566571	-0.103059	H	14.664978	32.454904	4.563607
N	1.938237	-0.492531	-0.297012	C	12.968902	27.943237	7.634573
C	4.249934	-0.391209	-0.396114	H	12.799484	27.901269	8.722662
C	1.737886	-2.946980	-0.043783	C	12.800723	24.695011	4.004847
H	2.292931	-3.889665	0.086967	H	12.554173	23.622411	3.931272
C	0.346571	-3.010421	-0.151347	C	14.320523	28.114775	0.876714
C	-1.774827	-2.461919	-0.437895	H	14.571439	28.136617	-0.196826
C	-1.715964	-3.903579	-0.393820	N	13.655746	29.384782	5.741026
H	0.025010	-5.249961	-0.101600	C	14.049841	30.710048	5.655773

H	-2.580069	-4.575348	-0.484972
N	-0.505835	-1.931456	-0.294638
C	-0.403382	-4.243467	-0.197004
C	-2.960481	-1.734097	-0.538336
H	-3.907212	-2.288817	-0.635301
C	-3.018271	-0.344363	-0.429566
C	-2.467253	1.771139	-0.117513
C	-3.909362	1.713276	-0.143404
H	-5.257628	-0.025800	-0.442231
H	-4.580657	2.573571	-0.024294
N	-1.937469	0.506208	-0.288295
C	-4.250481	0.404298	-0.357851
C	-1.736329	2.954032	0.010404
H	-2.289458	3.893655	0.165713
Fe	-0.000319	0.004916	-0.228312
N	-0.001594	0.002972	-2.246007
C	0.539549	-0.921548	-3.040410
C	-0.569015	0.966246	-3.070454
H	1.064179	-1.814331	-2.702820
C	-0.366884	0.616567	-4.385179
H	-1.082571	1.843651	-2.672363
H	0.648011	-1.115684	-5.139476
C	-0.767030	1.291954	-5.657732
H	0.122658	1.550439	-6.272181
H	-1.431785	0.640735	-6.265995
H	-1.314688	2.229093	-5.432679
N	0.336262	-0.580087	-4.334420
N	0.004375	-0.005605	1.391132
O	0.012702	-0.025093	2.540961

C	14.048432	31.313912	6.965760
C	13.655145	30.344239	7.852112
C	13.413880	29.146456	7.083918
N	12.958747	26.633821	5.530299
C	12.745318	26.785256	6.888863
C	12.294797	25.538401	7.463408
C	12.246681	24.625626	6.444127
C	12.671890	25.312983	5.247988
N	13.585697	26.687179	2.762932
C	13.236821	25.352220	2.854823
C	13.365444	24.715145	1.567127
C	13.800032	25.673377	0.689098
C	13.931867	26.898420	1.439310
N	14.165875	29.462041	2.947722
C	14.408482	29.307371	1.595991
C	14.803814	30.567505	1.011547
C	14.809426	31.490145	2.023086
C	14.421933	30.792566	3.226599
O	16.255880	27.399229	4.800350
H	8.038008	29.386858	1.716245
N	15.164831	27.658188	4.566079
H	12.049540	25.385019	8.523145
H	11.950933	23.569608	6.497211
H	13.151270	23.658211	1.360256
H	14.019825	25.559147	-0.381073
H	15.049088	30.724250	-0.047382
H	15.061219	32.557844	1.967918
H	14.325612	32.354466	7.183151
H	13.544133	30.433193	8.941454
O	16.814510	24.508622	3.935521
H	17.699878	24.211281	4.192781
H	16.452396	23.765011	3.432329

[MI-Fe^{III}-P-NO…MI]$^{+}$, Ms=1

C	22.907000	29.056000	6.205000
H	23.442538	30.010422	6.012183
H	23.466161	28.235563	5.706371
C	21.507079	29.149304	5.698733
N	20.656751	30.142877	6.149137
C	20.866444	28.360606	4.758174
H	21.207027	27.494113	4.185814
C	19.527144	29.958945	5.491022
H	18.648000	30.582000	5.610000
N	19.593030	28.892441	4.635453
H	18.863912	28.562383	4.011500
C	7.892931	27.378532	2.880902

[MI-Fe^{III}-P-NO…MI]$^{+}$…H$_2$O, Ms=1

C	22.907000	29.056000	6.205000
H	23.450204	30.006570	6.013419
H	23.463741	28.232942	5.707303
C	21.510620	29.157876	5.691196
N	20.651467	30.135187	6.161052
C	20.885685	28.397024	4.719491
H	21.239421	27.552831	4.122077
C	19.531064	29.967182	5.483213
H	18.648000	30.582000	5.610000
N	19.610247	28.926896	4.598557
H	18.894599	28.623230	3.946325
C	7.722333	27.442889	2.369027
H	6.909240	26.959305	2.952925

H	8.113117	26.607263	2.116527	H	7.960786	26.789510	1.505677
C	9.103226	27.617679	3.724872	C	8.946497	27.654422	3.198492
N	9.150537	28.528532	4.771253	N	8.982059	28.423392	4.352501
H	8.374747	29.100557	5.090391	H	8.189488	28.905928	4.765270
C	10.369799	27.084908	3.666090	C	10.237257	27.208235	3.034291
H	10.757047	26.333303	2.976685	H	10.636290	26.570847	2.243844
C	10.398327	28.541412	5.295564	C	10.245671	28.439403	4.839678
H	10.712449	29.165400	6.129055	H	10.554344	28.972381	5.736299
N	11.168615	27.669365	4.641541	N	11.037090	27.705721	4.054643
FE	13.168147	27.386082	4.922701	FE	13.051816	27.445647	4.266363
C	13.610261	30.806382	4.817223	C	13.371893	30.868027	4.605143
H	13.787870	31.893954	4.787486	H	13.508298	31.956102	4.716250
C	12.749781	27.543525	8.345181	C	12.671517	27.143055	7.680891
H	12.658393	27.584368	9.442671	H	12.591986	27.038838	8.775267
C	12.691269	23.972568	5.024220	C	12.649140	24.041992	3.921489
H	12.566403	22.878485	5.061698	H	12.528712	22.950774	3.813545
C	13.621571	27.226098	1.507191	C	13.479996	27.748189	0.860058
H	13.802304	27.170849	0.421150	H	13.649525	27.841151	-0.225576
N	13.166125	28.861478	6.289197	N	13.016196	28.733351	5.812528
C	13.405929	30.206229	6.060635	C	13.209320	30.104069	5.761705
C	13.408044	30.928336	7.309197	C	13.207830	30.655426	7.095194
C	13.172540	30.012338	8.301436	C	13.018431	29.608239	7.959934
C	13.024201	28.728653	7.660913	C	12.900900	28.415945	7.156029
N	12.733464	26.056873	6.362146	N	12.674729	25.925594	5.523038
C	12.600784	26.306930	7.716182	C	12.555396	25.993429	6.899539
C	12.327578	25.079278	8.426212	C	12.328107	24.675249	7.445889
C	12.304947	24.077755	7.493930	C	12.316536	23.804534	6.390146
C	12.567612	24.692163	6.213247	C	12.543940	24.589542	5.199417
N	13.159944	25.913944	3.558184	N	13.076390	26.166154	2.723248
C	12.973623	24.562592	3.791678	C	12.908525	24.794671	2.775978
C	13.108548	23.823057	2.560277	C	13.032263	24.228170	1.455565
C	13.376947	24.735445	1.573813	C	13.278113	25.267395	0.596643
C	13.405032	26.034570	2.200484	C	13.298541	26.470611	1.391427
N	13.475973	28.735603	3.464998	N	13.300078	28.986595	2.994749
C	13.637608	28.482045	2.114984	C	13.464606	28.915883	1.624440
C	13.875230	29.714588	1.400533	C	13.657178	30.237846	1.075103
C	13.868158	30.720291	2.329692	C	13.617194	31.114382	2.126444
C	13.627420	30.102458	3.612647	C	13.403011	30.327896	3.318857
O	15.890975	27.053622	5.303268	O	15.789131	27.245550	4.616190
H	7.587927	28.307438	2.351150	H	7.334629	28.405810	1.969727
H	22.934000	28.879000	7.306000	H	22.934000	28.879000	7.306000
H	12.174279	24.998476	9.510865	N	14.653811	27.295600	4.458069
H	12.129462	23.006190	7.656563	H	12.194136	24.449324	8.512583
H	13.015080	22.733055	2.463909	H	12.169276	22.716744	6.413515
H	13.546857	24.543122	0.506059	H	12.943141	23.160769	1.212070
H	14.032742	29.796823	0.316508	H	13.436346	25.222543	-0.489536

H	14.020694	31.795057	2.163204	H	13.808929	30.466680	0.011358
H	13.580632	32.008021	7.416542	H	13.731923	32.206628	2.100588
H	13.111200	30.190966	9.383590	H	13.347066	31.716471	7.344588
N	14.758205	27.184918	5.143602	H	12.970414	29.641262	9.057115
				O	16.263501	24.279445	3.982502
				H	17.159470	23.929966	4.111980
				H	15.783907	23.542310	3.568400