

The dramatic effect of N-methylimidazole on trans axial ligand binding to ferric heme: experiment and theory

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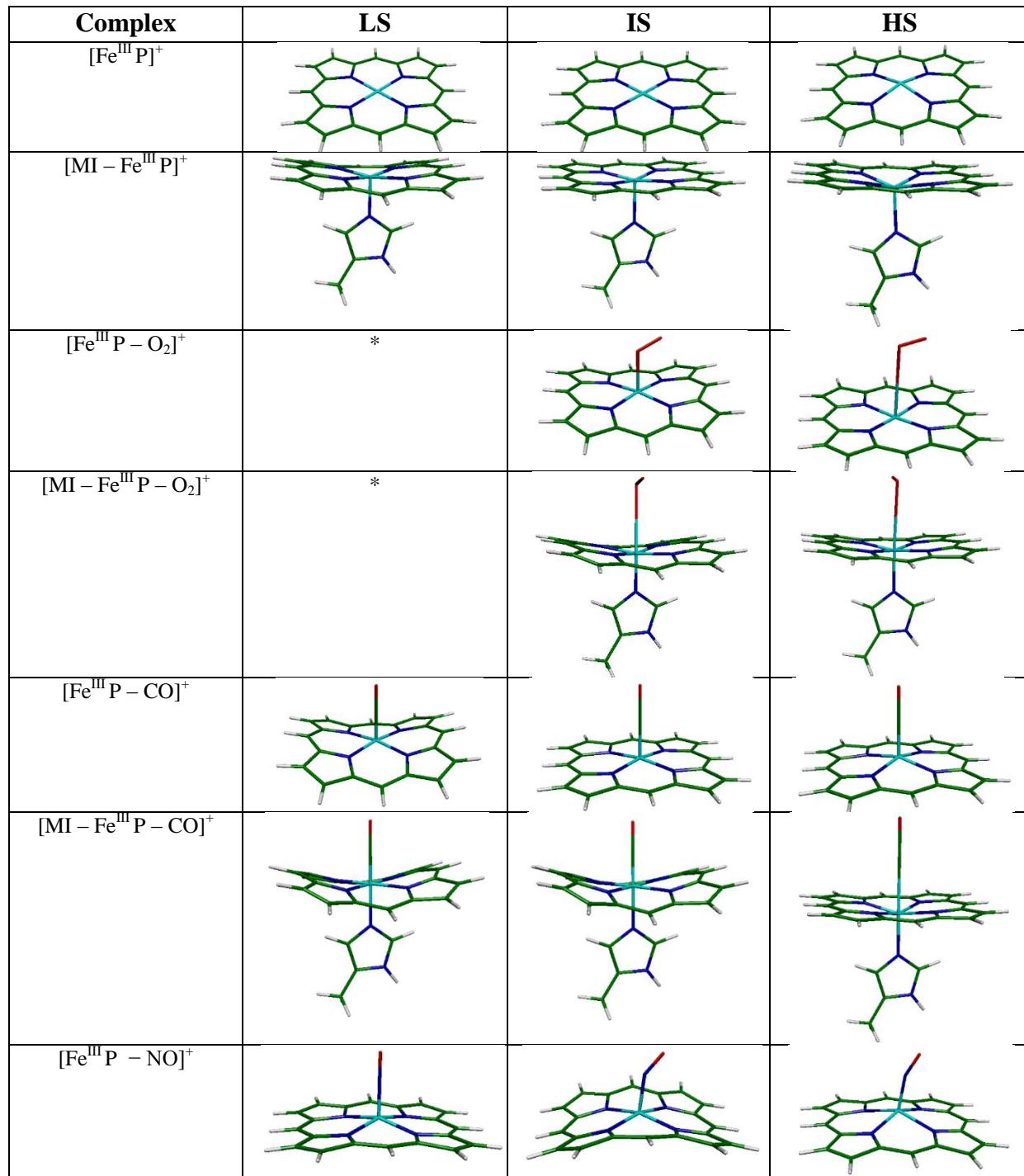
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Electronic Supplementary Information:

This supplementary material section contains 1 Figure and 5 Tables.

It is noteworthy that the star sign (*) presented in each cell in following tables indicates that the relevant geometry optimization ceased to converge due to the spin contamination or technical problems, thus we were unable to present their corresponding information.

Figure S1. The spin state optimized structures of the ferric porphyrin complexes investigated in this study with/without MI(Methylimidazole) at the OPTX-PBE/DZVP-GGA level of theory.



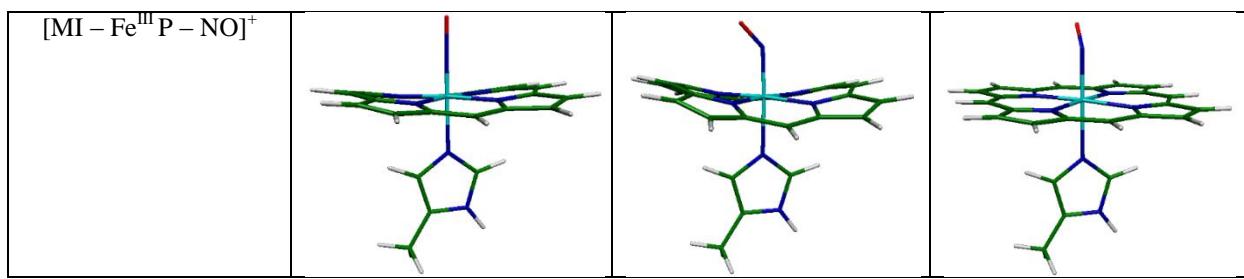


Table S1 Optimized geometry parameters (in Å and degree, respectively for bond lengths and bond angles), for spin states. A description of the coordinates is reported in figure 3 of the article. Np indicates the pyrrolic nitrogens. N_{MI} indicates the Nitrogen of Methylimidazole bounds to Fe. The displacement of the Fe from the porphyrin plane is defined as doming describe in Figure 3C of the article. ^{a)}Average value of the four Fe-Np bond lengths ^bExperimental data for the structure of ferric Heme-nitrosyl complex in solution taken from Ref. 1 . The values in bold correspond to the lowest spin state

Complex	S	Fe-XO	X-O	Doming	∠FeXO	Fe-N _P ^a	Fe - N _{MI}
[Fe ^{III} P] ⁺	1/2	-	-	0.00	-	1.970	-
	3/2	-	-	0.00	-	1.957	-
	5/2	-	-	0.293	-	2.044	-
[MI-Fe ^{III} P] ⁺	1/2	-	-	-0.178	-	1.967	1.897
	3/2	-	-	-0.185	-	1.984	2.138
	5/2	-	-	-0.428	-	2.070	2.096
[Fe ^{III} P-O ₂] ⁺	1/2				*		
	3/2	2.120	1.233	0.136	119.6	1.958	-
	5/2	3.614	1.218	-0.052	108.6	1.957	-
[MI-Fe ^{III} P-O ₂] ⁺	3/2	3.315	1.218	-0.160	99.60	1.961	1.890
	5/2	3.534	1.218	-0.180	88.21	1.981	2.146
	7/2				*		
[Fe ^{III} P-CO] ⁺	1/2	1.693	1.164	0.166	180.0	1.955	-
	3/2	2.315	1.144	0.172	179.9	1.972	-
	5/2	2.225	1.143	0.332	180.0	2.049	-
[MI-Fe ^{III} P-CO] ⁺	1/2	1.753	1.159	0.020	179.8	1.963	2.030
	3/2	1.784	1.156	0.001	176.2	1.963	2.014
	5/2	3.493	1.149	-0.317	179.3	2.057	2.093
[Fe ^{III} P-NO] ⁺	0	1.599	1.158	0.333	180.0	1.987	-
	1	1.723	1.165	0.265	144.8	1.975	-
	2	1.736	1.167	0.519	156.8	2.104	-
[MI-Fe ^{III} P-NO] ⁺	0	1.619	1.150	0.064	179.3	2.002	2.018
	1	1.770	1.172	0.068	139.0	1.978	2.119
	2	1.896	1.168	0.052	137.3	2.078	2.226

Table S2. Relative energies for different spin states of ferric-porphyrin complexes (in kcal mol^{-1}). The experimental information has been adopted from literature.

Complex	Spin State (Theor.)	B3LYP		Spin State (Exp.)
		TZP	def2-TZVP	
$[\text{Fe}^{\text{III}} \text{P}]^+$	1/2	6.81	7.09	$3/2^2$
	3/2	0.00	0.00	
	5/2	12.07	12.42	
$[\text{MI-Fe}^{\text{III}} \text{P}]^+$	1/2	10.65	10.93	$5/2^3$
	3/2	0.00	0.00	
	5/2	5.52	5.18	
$[\text{Fe}^{\text{III}} \text{P-O}_2]^+$	1/2	*	*	-
	3/2	23.17	24.66	
	5/2	0.00	0.00	
$[\text{MI-Fe}^{\text{III}} \text{P-O}_2]^+$	3/2	10.86	11.27	-
	5/2	0.00	0.00	
	7/2	*	*	
$[\text{Fe}^{\text{III}} \text{P-CO}]^+$	1/2	13.20	13.93	$3/2^4$
	3/2	0.00	0.00	
	5/2	10.74	10.34	
$[\text{MI-Fe}^{\text{III}} \text{P-CO}]^+$	1/2	0.83	2.01	-
	3/2	42.40	43.57	
	5/2	0.00	0.00	
$[\text{Fe}^{\text{III}} \text{P-NO}]^+$	0	0.00	*	0^5
	1	7.82	*	
	2	2.04	*	
$[\text{MI-Fe}^{\text{III}} \text{P-NO}]^+$	0	0.00	0.00	0^5
	1	13.33	13.20	
	2	40.44	17.02	

Table S3 Computed spin density of $[Fe^{III}P-O_2]^+$ and $[MI-Fe^{III}P-O_2]^+$: Spin-up and spin-down densities are shown as white and blue, respectively.

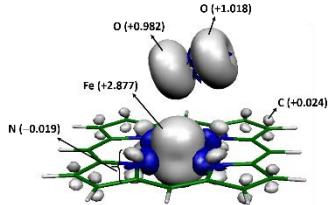
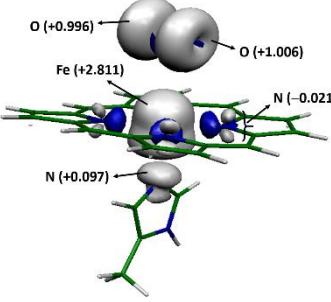
Molecule	Spin	Spin-density plot (isosurfaces=0.0025)
$[Fe^{III}P-O_2]^+$	5/2	
$[MI-Fe^{III}P-O_2]^+$	5/2	

Table S4: Comparison of binding energies of $[FeP-CO]^+$ and $[FeP-OC]^+$ (in kcal mol⁻¹): Relative energies for the different spin states of ferric-porphyrin ligated to CO and OC (in kcal mol⁻¹).

Complex	B3LYP/TZP (kcal/mol)		B3LYP/def2TZVP (kcal/mol)	
	Relative	Binding	Relative	Binding
$[FeP-CO]^+$				
2	13.20		13.93	
4	0.00	-8.42	0.00	-6.57
6	10.74		10.34	
$[FeP-OC]^+$				
2	14.59		13.45	
4	7.18	-1.24	5.98	-0.58
6	20.10		18.84	

References

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4. S. Dillinger, J. Lang and G. Niedner-Schatteburg, J. Phys. Chem. A. **121** (38), 7191-7196 (2017).
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Table S5. The ground state xyz coordinates of the spin state optimized geometry of the ferric porphyrin complexes investigated in this study at the OPBE/DZVP-GGA level of theory.

[Fe^{III}P]⁺ S=1/2

C	-0.351495	3.010124	-0.312146
C	0.398666	4.251776	-0.311978
C	1.718661	3.911929	-0.312183
C	1.767335	2.465479	-0.312383
N	0.509989	1.903467	-0.312147
H	-0.041079	5.259562	-0.311519
H	2.590994	4.580327	-0.311587
C	2.978816	1.744299	-0.312194
H	3.925635	2.308733	-0.312833
C	3.025653	0.366402	-0.311542
C	2.457176	-1.746872	-0.311014
C	3.903256	-1.709551	-0.312548
H	5.271222	0.036609	-0.314281
H	4.563900	-2.588285	-0.313978
N	1.908906	-0.484980	-0.310441
C	4.259322	-0.392397	-0.312723
C	1.727882	-2.955472	-0.311590
H	2.292699	-3.902133	-0.312844
C	0.351475	-3.010110	-0.311162
C	-1.767350	-2.465472	-0.310956
C	-1.718674	-3.911928	-0.312571
H	0.041087	-5.259552	-0.314396
H	-2.591004	-4.580328	-0.314451
N	-0.510012	-1.903457	-0.310470
C	-0.398677	-4.251771	-0.312730
C	-2.978822	-1.744279	-0.311314
H	-3.925653	-2.308696	-0.311483
C	-3.025653	-0.366381	-0.311895
C	-2.457191	1.746902	-0.312446
C	-3.903267	1.709567	-0.312366
H	-5.271240	-0.036585	-0.311744
H	-4.563908	2.588301	-0.312140
N	-1.908911	0.485016	-0.312292
C	-4.259330	0.392413	-0.312148
C	-1.727903	2.955502	-0.311951
H	-2.292707	3.902167	-0.311528
Fe	-0.000015	0.000007	-0.311109

[Fe^{III}P]⁺ S=3/2

C	-0.360123	3.008769	-0.312985
C	0.385295	4.230606	-0.311883
C	1.715525	3.886153	-0.312158
C	1.774400	2.456069	-0.313346
N	0.490255	1.894915	-0.313822
H	-0.050738	5.239736	-0.310667
H	2.586337	4.557105	-0.310924
C	2.967697	1.747225	-0.311959
H	3.917055	2.306139	-0.312034
C	3.008500	0.359827	-0.310865
C	2.456240	-1.774876	-0.310977
C	3.886246	-1.715784	-0.312957
H	5.239631	0.050405	-0.313934
H	4.557425	-2.586448	-0.315079
N	1.894770	-0.490708	-0.309630
C	4.230423	-0.385484	-0.312412
C	1.747457	-2.968134	-0.312019
H	2.306249	-3.917563	-0.314420
C	0.360115	-3.008745	-0.310497
C	-1.774409	-2.456054	-0.310143
C	-1.715535	-3.886126	-0.312549
H	0.050734	-5.239694	-0.315110
H	-2.586361	-4.557059	-0.314920
N	-0.490267	-1.894887	-0.308966
C	-0.385305	-4.230574	-0.312816
C	-2.967705	-1.747213	-0.311764
H	-3.917061	-2.306115	-0.312523
C	-3.008504	-0.359819	-0.312538
C	-2.456256	1.774892	-0.312443
C	-3.886260	1.715798	-0.311714
H	-5.239634	-0.050389	-0.311924
H	-4.557452	2.586446	-0.310842
N	-1.894784	0.490722	-0.313026
C	-4.230425	0.385498	-0.312247
C	-1.747464	2.968140	-0.311708
H	-2.306274	3.917556	-0.310149
Fe	-0.000026	0.000006	-0.311031

[Fe^{III}P]⁺ S=5/2

C	-0.352383	3.051863	-0.290891
C	0.397442	4.280897	-0.294154
C	1.729083	3.935780	-0.293606
C	1.787503	2.497243	-0.290084
N	0.506209	1.959265	-0.285576
H	-0.028813	5.293811	-0.291166
H	2.593739	4.614091	-0.290151
C	2.973796	1.750926	-0.291644
H	3.924233	2.310442	-0.294916
C	3.050666	0.351531	-0.290266
C	2.497384	-1.788867	-0.291126
C	3.935789	-1.729383	-0.294022
H	5.292751	0.029456	-0.290079
H	4.614668	-2.593580	-0.291041
N	1.958537	-0.507940	-0.286075
C	4.280113	-0.397547	-0.293476
C	1.751661	-2.975539	-0.292767
H	2.311130	-3.925944	-0.295670
C	0.352224	-3.051755	-0.290817
C	-1.787759	-2.497171	-0.291765
C	-1.729182	-3.935617	-0.292847
H	0.028776	-5.293671	-0.287313
H	-2.593824	-4.613915	-0.289191
N	-0.506470	-1.959093	-0.288154
C	-0.397557	-4.280763	-0.292010
C	-2.974155	-1.751069	-0.293737
H	-3.924688	-2.310402	-0.296769
C	-3.050611	-0.351628	-0.291328
C	-2.497261	1.788674	-0.290779
C	-3.935634	1.729367	-0.291412
H	-5.292650	-0.029433	-0.287239
H	-4.614341	2.593710	-0.286251
N	-1.958437	0.507700	-0.288109
C	-4.280003	0.397507	-0.291923
C	-1.751765	2.975450	-0.292392
H	-2.311494	3.925769	-0.295493
Fe	0.000357	0.000156	-0.579443

$[\text{Fe}^{\text{III}} \text{P} - \text{O}_2]^+ \ S = 3/2$

C	2.81712100	-0.94213200	-0.08369400
C	3.68472200	-2.00072700	0.34303500
C	2.87863200	-2.98767800	0.85757700
C	1.53129100	-2.50320900	0.78617200
N	1.48375800	-1.23991200	0.19245000
H	4.77947500	-2.00840300	0.24546100
H	3.18455600	-3.96010200	1.26859700
C	0.44044600	-3.18330500	1.31543700
H	0.60035400	-4.17795600	1.76272400
C	-0.82890000	-2.61680300	1.37687500
C	-2.51822400	-1.21056600	1.23625500
C	-2.97679600	-2.33233000	2.00024900
H	-1.91473600	-4.20827600	2.55029600
H	-3.98370400	-2.44483300	2.42570600
N	-1.18346100	-1.37161100	0.85388600
C	-1.93253900	-3.22335800	2.06216200
C	-3.33256300	-0.13968600	0.88341100
H	-4.36491500	-0.11190700	1.26766600
C	-2.92764900	0.84698400	-0.00953600
C	-1.76036700	2.04241400	-1.44447100
C	-3.09194100	2.57317400	-1.44806200
H	-4.86720600	1.97387900	-0.25056900
H	-3.44046400	3.41457800	-2.06404000
N	-1.64950900	0.96544700	-0.56210500
C	-3.81194200	1.84623100	-0.53020100
C	-0.71513100	2.59146900	-2.18053500
H	-0.92638900	3.44111000	-2.84971600
C	0.59868800	2.16088700	-2.03617800
C	2.40515200	1.11921800	-1.33013400
C	2.84910200	2.18180900	-2.18469300
H	1.65941200	3.66367900	-3.34087800
H	3.89651500	2.41378400	-2.42354900
N	1.01524900	1.10220300	-1.22580100
C	1.71971600	2.81162400	-2.64941900
C	3.26771600	0.19869300	-0.74179200
H	4.35331400	0.33558000	-0.87334800
Fe	-0.05839500	-0.06338000	-0.07357000
O	0.30737800	1.06432600	1.68417100
O	1.45011500	1.45837000	1.92799800

$[\text{Fe}^{\text{III}}\text{P} - \text{O}_2]^+ \ S=5/2$

C	2.78389300	-1.07337800	-0.31045500
C	3.65291900	-2.10075900	0.17608500
C	2.87916200	-2.95748100	0.92151300
C	1.54224900	-2.44882700	0.88323200
N	1.46587600	-1.27714200	0.11909300
H	4.73076000	-2.17058400	-0.02903400
H	3.19706900	-3.86857900	1.44829900
C	0.47873600	-3.06737000	1.52554000
H	0.66700100	-3.99124900	2.09532100
C	-0.81239100	-2.56012800	1.48143000
C	-2.58901100	-1.32683200	1.05383200
C	-3.02644600	-2.41512500	1.87371900
H	-1.86563200	-4.10626100	2.73616700
H	-4.06062200	-2.58313900	2.20672000
N	-1.21323200	-1.40360300	0.79986400
C	-1.91895100	-3.18348200	2.14090400
C	-3.44478500	-0.34045400	0.58374700
H	-4.51239700	-0.39281800	0.85028000
C	-3.00150300	0.71646300	-0.19911500
C	-1.75501400	2.10643600	-1.37082500
C	-3.09110200	2.61741500	-1.40585600
H	-4.94899800	1.81234000	-0.48333400
H	-3.40842400	3.53040300	-1.92986600
N	-1.68278600	0.92249400	-0.62483500
C	-3.86832200	1.75037300	-0.67583100
C	-0.69035900	2.72826100	-2.00794700
H	-0.87680400	3.65871300	-2.56745500
C	0.60191800	2.22438700	-1.95963100
C	2.37277600	0.97610300	-1.55353000
C	2.81468500	2.07525000	-2.35664200
H	1.65942800	3.78125700	-3.19735200
H	3.84700400	2.23690500	-2.69839400
N	0.99762900	1.05477200	-1.29781700
C	1.71123600	2.85430100	-2.60859000
C	3.22392500	-0.02449100	-1.10575100
H	4.28968500	0.02266000	-1.38027700
Fe	-0.11829000	-0.20423400	-0.29390400
O	0.59920700	1.72251200	2.67816100
O	1.80228700	1.90440200	2.74322000

[Fe^{III}P – CO]⁺ S = 1/2

C	-0.32909500	2.97088600	-0.05903300
C	0.41110900	4.20716100	-0.13766200
C	1.68214200	3.87971400	-0.52536500
C	1.73062000	2.43813600	-0.61879500
N	0.47241000	1.88865200	-0.36161700
H	-0.00133900	5.21052500	0.03667400
H	2.52405600	4.55806700	-0.72268900
C	2.89495300	1.71017700	-0.80049700
H	3.83292300	2.25837500	-0.98634000
C	2.96421000	0.31953700	-0.61282100
C	2.44457400	-1.74113700	-0.04453400
C	3.88470800	-1.68674300	-0.13742500
H	5.20328300	-0.00431700	-0.73658400
H	4.56704600	-2.53067300	0.03492800
N	1.88546600	-0.49321200	-0.33731600
C	4.20520000	-0.41644700	-0.53250800
C	1.71698600	-2.90259200	0.15877500
H	2.25965500	-3.83507600	0.38471800
C	0.32899600	-2.97097200	-0.05802300
C	-1.73027900	-2.43776800	-0.61888100
C	-1.68227300	-3.87938400	-0.52513700
H	0.00091100	-5.21065600	0.03712900
H	-2.52424100	-4.55732200	-0.72345500
N	-0.47206500	-1.88866100	-0.36110500
C	-0.41145900	-4.20720800	-0.13689600
C	-2.89441000	-1.70985300	-0.80148900
H	-3.83240500	-2.25815900	-0.98694600
C	-2.96378800	-0.31921500	-0.61408400
C	-2.44473700	1.74118700	-0.04493000
C	-3.88486500	1.68623800	-0.13658100
H	-5.20320200	0.00373500	-0.73566400
H	-4.56756800	2.52965900	0.03663500
N	-1.88524900	0.49379300	-0.33873900
C	-4.20503800	0.41605200	-0.53223600
C	-1.71706900	2.90258500	0.15810500
H	-2.25945000	3.83512500	0.38468900
Fe	0.00008500	0.00020600	-0.17928500
C	-0.00035400	-0.00006100	1.51347800
O	-0.00033000	-0.00036400	2.67793800

$[\text{Fe}^{\text{III}}\text{P} - \text{CO}]^+ \ S = 3/2$

C	-0.35926900	3.01183400	-0.37136900
C	0.38627200	4.23525100	-0.40484700
C	1.71671000	3.89084000	-0.40349800
C	1.77469400	2.45932800	-0.36978300
N	0.49178500	1.90150900	-0.34674400
H	-0.04999700	5.24397800	-0.43376000
H	2.58765400	4.56119900	-0.43083000
C	2.96748100	1.74731900	-0.36952200
H	3.91702200	2.30641700	-0.38316800
C	3.01123700	0.35889100	-0.37021300
C	2.45899700	-1.77520400	-0.37087100
C	3.89050600	-1.71686200	-0.40432500
H	5.24359800	0.04976500	-0.43143500
H	4.56107500	-2.58761700	-0.43259400
N	1.90104000	-0.49230900	-0.34661000
C	4.23482800	-0.38639300	-0.40381600
C	1.74735100	-2.96821700	-0.37089400
H	2.30639600	-3.91783200	-0.38558700
C	0.35884500	-3.01182300	-0.37031400
C	-1.77510400	-2.45922800	-0.36972000
C	-1.71711500	-3.89073300	-0.40405400
H	0.04959900	-5.24394200	-0.43338600
H	-2.58810100	-4.56098500	-0.43270400
N	-0.49217800	-1.90159600	-0.34571700
C	-0.38667500	-4.23521500	-0.40443200
C	-2.96783900	-1.74710300	-0.36991200
H	-3.91751700	-2.30605000	-0.38474100
C	-3.01155300	-0.35861900	-0.37003600
C	-2.45946900	1.77538500	-0.37097300
C	-3.89100200	1.71707200	-0.40478500
H	-5.24390400	-0.04973100	-0.43290600
H	-4.56164900	2.58772600	-0.43331200
N	-1.90155400	0.49264700	-0.34585000
C	-4.23519700	0.38657800	-0.40442600
C	-1.74769500	2.96833300	-0.37171300
H	-2.30660600	3.91798400	-0.38681600
Fe	-0.00013200	0.00001500	-0.17381200
C	0.00120400	0.00003700	2.14148100
O	0.00450700	-0.00113500	3.28570500

[Fe^{III}P – CO]⁺ S=5/2

C	-0.35580200	3.05076000	-0.38469600
C	0.39510300	4.27636900	-0.43090100
C	1.72914000	3.93071300	-0.43011500
C	1.79039100	2.49468500	-0.38388800
N	0.50603900	1.95753400	-0.34335100
H	-0.03040200	5.28933100	-0.46904700
H	2.59307000	4.60957200	-0.46747000
C	2.97733900	1.75303000	-0.38765200
H	3.92754400	2.31244400	-0.41398400
C	3.04976400	0.35535300	-0.38486000
C	2.49456500	-1.79115100	-0.38474300
C	3.93050400	-1.72920900	-0.43321600
H	5.28830400	0.03084000	-0.47239000
H	4.60969200	-2.59276100	-0.47202500
N	1.95707000	-0.50705300	-0.34243400
C	4.27563900	-0.39509700	-0.43324900
C	1.75342900	-2.97838200	-0.38737200
H	2.31286100	-3.92859600	-0.41428600
C	0.35573300	-3.05055300	-0.38262500
C	-1.79050000	-2.49465200	-0.38361600
C	-1.72912000	-3.93068100	-0.43056100
H	0.03073500	-5.28895600	-0.46818200
H	-2.59302100	-4.60942200	-0.46954000
N	-0.50629200	-1.95753200	-0.34113800
C	-0.39506900	-4.27616600	-0.42981500
C	-2.97725600	-1.75285100	-0.38870200
H	-3.92757800	-2.31207500	-0.41598600
C	-3.04957400	-0.35510600	-0.38540700
C	-2.49463800	1.79131800	-0.38481400
C	-3.93064200	1.72933500	-0.43147000
H	-5.28826800	-0.03096300	-0.47015700
H	-4.61006200	2.59273300	-0.46863900
N	-1.95688600	0.50733200	-0.34380400
C	-4.27556900	0.39513800	-0.43209800
C	-1.75350100	2.97855300	-0.38810200
H	-2.31297500	3.92871800	-0.41452600
Fe	-0.00009400	0.00015700	-0.01152400
C	0.000086100	-0.00088500	2.21325400
O	-0.00004200	-0.00059300	3.35638400

[Fe^{III}P – NO]⁺ S=0

C	-0.349537	2.999452	-0.432153
C	0.394466	4.229522	-0.429847
C	1.713671	3.890559	-0.295916
C	1.766153	2.454968	-0.241745
N	0.494514	1.895471	-0.337693
H	-0.041279	5.234271	-0.519488
H	2.583972	4.559947	-0.257545
C	2.952240	1.737808	-0.163217
H	3.899120	2.295081	-0.083941
C	3.003686	0.353044	-0.247737
C	2.452874	-1.761140	-0.437753
C	3.889438	-1.707122	-0.441363
H	5.241075	0.047124	-0.272566
H	4.556234	-2.575667	-0.533571
N	1.897142	-0.487377	-0.341503
C	4.233382	-0.389156	-0.307695
C	1.735448	-2.947939	-0.494784
H	2.292929	-3.894839	-0.569074
C	0.349817	-2.999607	-0.432010
C	-1.765893	-2.455064	-0.240996
C	-1.713447	-3.890611	-0.296225
H	0.041343	-5.234320	-0.521655
H	-2.583820	-4.559941	-0.259025
N	-0.494208	-1.895720	-0.337000
C	-0.394289	-4.229630	-0.430650
C	-2.952030	-1.737958	-0.162394
H	-3.898843	-2.295284	-0.083047
C	-3.003445	-0.353201	-0.246736
C	-2.452567	1.760939	-0.437609
C	-3.889086	1.706964	-0.440885
H	-5.240743	-0.047190	-0.270911
H	-4.555894	2.575379	-0.533715
N	-1.896888	0.487155	-0.341375
C	-4.233077	0.389077	-0.306578
C	-1.735153	2.947748	-0.494825
H	-2.292618	3.894681	-0.568735
FE	0.000059	0.000046	-0.006138
N	-0.000758	0.000773	1.593098
O	-0.002187	0.001639	2.751578

[^{III}P – NO]⁺ S=I

C	-0.378717	2.952724	-0.014603
C	0.351729	4.188442	-0.116641
C	1.631254	3.859807	-0.493661
C	1.689753	2.423189	-0.554782
N	0.452177	1.872032	-0.279427
H	-0.064987	5.193373	0.039693
H	2.466801	4.542929	-0.700067
C	2.872953	1.693543	-0.730909
H	3.807706	2.249782	-0.906591
C	2.943990	0.313163	-0.570029
C	2.407449	-1.755861	-0.042307
C	3.842552	-1.715714	-0.141379
H	5.176937	-0.032596	-0.710187
H	4.519675	-2.567535	0.011801
N	1.861477	-0.515815	-0.309111
C	4.174707	-0.435314	-0.508410
C	1.669406	-2.934728	0.164125
H	2.223478	-3.865508	0.367822
C	0.298162	-3.011858	-0.051948
C	-1.736070	-2.458175	-0.681109
C	-1.688343	-3.901389	-0.645183
H	-0.030170	-5.253754	-0.057425
H	-2.518433	-4.574018	-0.903424
N	-0.520378	-1.918936	-0.320019
C	-0.435321	-4.244058	-0.209613
C	-2.908251	-1.718602	-0.895768
H	-3.832491	-2.266321	-1.143096
C	-2.992633	-0.345911	-0.678440
C	-2.489223	1.701330	-0.048412
C	-3.923867	1.653991	-0.193253
H	-5.224373	-0.010869	-0.877775
H	-4.611811	2.495216	-0.032271
N	-1.925987	0.473014	-0.330708
C	-4.232681	0.391226	-0.627039
C	-1.757941	2.873227	0.183777
H	-2.310066	3.803485	0.394352
Fe	-0.030665	-0.020380	-0.045058
N	0.129128	0.067329	1.668226
O	0.733676	0.539465	2.545558

[Fe^{III}P – NO]⁺ S=2

C	0.551724	2.907953	-0.482761
C	1.615069	3.885027	-0.636317
C	2.791990	3.190552	-0.572818
C	2.441786	1.790548	-0.391081
N	1.058688	1.651706	-0.324217
H	1.484562	4.966316	-0.783129
H	3.811314	3.593604	-0.654906
C	3.359206	0.749991	-0.331455
H	4.428927	1.011022	-0.379608
C	3.032854	-0.635399	-0.273186
C	1.907584	-2.519054	-0.215392
C	3.316169	-2.876870	-0.279750
H	5.106564	-1.577439	-0.388435
H	3.720997	-3.898389	-0.307328
N	1.767815	-1.135113	-0.195849
C	4.016896	-1.703073	-0.319948
C	0.861889	-3.432314	-0.201002
H	1.123286	-4.502993	-0.205267
C	-0.524975	-3.107487	-0.232907
C	-2.416626	-1.995615	-0.285331
C	-2.763322	-3.407307	-0.334662
H	-1.448379	-5.189509	-0.344415
H	-3.779636	-3.820487	-0.402621
N	-1.036651	-1.844504	-0.206169
C	-1.584094	-4.099459	-0.308527
C	-3.331524	-0.953071	-0.349175
H	-4.400726	-1.215555	-0.400966
C	-3.001468	0.430567	-0.414870
C	-1.879252	2.318432	-0.487951
C	-3.283921	2.661303	-0.649240
H	-5.067349	1.348581	-0.702720
H	-3.688567	3.673118	-0.793160
N	-1.739160	0.944128	-0.332387
C	-3.981031	1.485020	-0.607159
C	-0.833995	3.231514	-0.530595
H	-1.094042	4.296085	-0.650220
Fe	0.004974	-0.073834	0.252893
N	-0.084072	0.252214	1.955930
O	-0.252276	0.889864	2.918782

[M⁻ – Fe^{III} P]⁺ S=I/2

C	-0.350921	3.004069	-0.107880
C	0.399147	4.230396	-0.140345
C	1.707341	3.884391	-0.359898
C	1.752275	2.446822	-0.423665
N	0.483697	1.896455	-0.269645
H	-0.020795	5.237993	-0.009882
H	2.575439	4.553224	-0.444397
C	2.934186	1.722318	-0.541082
H	3.879311	2.277059	-0.660162
C	2.992212	0.339236	-0.401658
C	2.456975	-1.765064	-0.062018
C	3.893124	-1.703266	-0.072963
H	5.233958	0.040058	-0.382110
H	4.569304	-2.556046	0.080667
N	1.894519	-0.501514	-0.251410
C	4.227269	-0.394597	-0.306471
C	1.737223	-2.949709	0.056445
H	2.291522	-3.891462	0.202645
C	0.352031	-3.003803	-0.060526
C	-1.747400	-2.451191	-0.403493
C	-1.705145	-3.887038	-0.306171
H	0.018328	-5.234154	0.085609
H	-2.573470	-4.556506	-0.382523
N	-0.479861	-1.899041	-0.252133
C	-0.399116	-4.229407	-0.070188
C	-2.928385	-1.729409	-0.545487
H	-3.871802	-2.286880	-0.665690
C	-2.988587	-0.344432	-0.427776
C	-2.455694	1.764597	-0.109292
C	-3.891942	1.703878	-0.144008
H	-5.229894	-0.041917	-0.452183
H	-4.569383	2.559934	-0.014289
N	-1.892055	0.497551	-0.271127
C	-4.223942	0.392330	-0.365348
C	-1.737604	2.951880	-0.004090
H	-2.293795	3.896335	0.116748
Fe	0.002329	-0.002777	-0.439003
N	0.011942	-0.020887	-2.336238
C	0.580189	-0.985762	-3.159296
C	-0.538665	0.910933	-3.121903
C	0.368317	-0.629366	-4.469500
H	1.095290	-1.858197	-2.747900
H	-1.061846	1.798923	-2.760575
H	-0.653814	1.102531	-5.216319
N	-0.338097	0.568026	-4.411355
C	0.751902	-1.284791	-5.756211
H	-0.148147	-1.541201	-6.355974
H	1.401896	-0.618823	-6.364148
H	1.309805	-2.220660	-5.555034

[MI – Fe^{III} P]⁺ S=3/2

C	-0.357724	3.018457	-0.197585
C	0.388538	4.244925	-0.163728
C	1.717204	3.900270	-0.174639
C	1.773340	2.466171	-0.213797
N	0.493299	1.915269	-0.236127
H	-0.046068	5.254064	-0.125041
H	2.587668	4.571047	-0.149855
C	2.965094	1.749302	-0.215491
H	3.914705	2.308063	-0.199114
C	3.012651	0.359333	-0.203622
C	2.462178	-1.771361	-0.161534
C	3.895968	-1.713444	-0.108875
H	5.247248	0.051465	-0.106107
H	4.566775	-2.581985	-0.046977
N	1.910594	-0.492905	-0.227768
C	4.238947	-0.384922	-0.137368
C	1.745401	-2.963609	-0.141256
H	2.303746	-3.911986	-0.087926
C	0.355130	-3.011947	-0.161555
C	-1.774874	-2.459329	-0.204765
C	-1.719297	-3.892746	-0.138870
H	0.042479	-5.245656	-0.047412
H	-2.590207	-4.562615	-0.108942
N	-0.495057	-1.909229	-0.227786
C	-0.391277	-4.237556	-0.109389
C	-2.967125	-1.743174	-0.217101
H	-3.916400	-2.302586	-0.201936
C	-3.015872	-0.353296	-0.215347
C	-2.464885	1.778123	-0.198869
C	-3.899434	1.720741	-0.167374
H	-5.251603	-0.043961	-0.154914
H	-4.571282	2.590255	-0.130372
N	-1.913117	0.498782	-0.236620
C	-4.242667	0.391677	-0.178286
C	-1.748376	2.970956	-0.197363
H	-2.307215	3.920517	-0.170753
Fe	-0.001212	0.003229	-0.417063
N	0.003881	-0.009260	-2.555332
C	0.575270	-0.978054	-3.365249
C	-0.534205	0.899951	-3.363425
C	0.379682	-0.649321	-4.688688
H	1.089183	-1.847578	-2.943099
H	-1.063826	1.796523	-3.034414
H	-0.636622	1.068796	-5.470924
N	-0.326582	0.546087	-4.656665
C	0.781405	-1.330071	-5.957733
H	-0.107373	-1.594987	-6.570598
H	1.446791	-0.681689	-6.568168
H	1.330388	-2.264934	-5.726534

[MI – Fe^{III} P]⁺ S=5/2

C	-0.329976	3.019482	-0.225256
C	0.419606	4.249987	-0.189528
C	1.750618	3.905291	-0.190302
C	1.810241	2.465822	-0.218972
N	0.529913	1.931275	-0.270191
H	-0.007533	5.262341	-0.155233
H	2.615485	4.582885	-0.154575
C	2.995413	1.723918	-0.163113
H	3.944918	2.283869	-0.130832
C	3.068104	0.327508	-0.085811
C	2.512855	-1.806779	0.050828
C	3.947899	-1.740811	0.167305
H	5.303760	0.018665	0.127948
H	4.621315	-2.598182	0.307301
N	1.983391	-0.535773	-0.124651
C	4.293937	-0.412954	0.077720
C	1.771008	-2.992252	0.105128
H	2.326951	-3.935161	0.236381
C	0.376199	-3.070044	0.023640
C	-1.758743	-2.522339	-0.134138
C	-1.705308	-3.954660	0.017234
H	0.045879	-5.300229	0.257672
H	-2.572031	-4.629944	0.053217
N	-0.477986	-1.990874	-0.157145
C	-0.376871	-4.295027	0.119836
C	-2.944839	-1.781224	-0.206612
H	-3.894833	-2.340868	-0.185553
C	-3.019912	-0.384332	-0.242692
C	-2.469270	1.756848	-0.228363
C	-3.908935	1.695427	-0.195176
H	-5.262647	-0.065229	-0.180870
H	-4.588507	2.558667	-0.155629
N	-1.932621	0.478167	-0.280204
C	-4.251062	0.364056	-0.208866
C	-1.728263	2.944813	-0.227581
H	-2.288623	3.893931	-0.198682
Fe	0.038385	-0.045467	-0.635525
N	0.005438	-0.008751	-2.730841
C	0.518884	-0.928961	-3.633394
C	-0.563398	0.961063	-3.449846
C	0.258308	-0.509956	-4.918383
H	1.043988	-1.832713	-3.309121
H	-1.062081	1.838907	-3.033259
H	-0.771920	1.268745	-5.529623
N	-0.428505	0.689370	-4.769020
C	0.582466	-1.109148	-6.248150
H	-0.342506	-1.323092	-6.826867
H	1.220858	-0.426168	-6.850223
H	1.131441	-2.062210	-6.112643

$[\text{MI} - \text{Fe}^{\text{III}}\text{P} - \text{O}_2]^+$ $S=3/2$

C	-0.34102800	3.00744300	-0.55118900
C	0.39144900	4.24329200	-0.44676800
C	1.68599000	3.90916200	-0.14118200
C	1.74797500	2.47287000	-0.11030300
N	0.49294000	1.91221200	-0.34810800
H	-0.03987700	5.24790700	-0.55895100
H	2.53130600	4.58511800	0.04630100
C	2.92985200	1.75586500	0.05655900
H	3.86436600	2.30909900	0.24171000
C	2.98627900	0.37194900	-0.08725900
C	2.44654400	-1.72327900	-0.48836200
C	3.88035000	-1.67887700	-0.36361800
H	5.21103800	0.03778900	0.10824900
H	4.55209200	-2.54481100	-0.44692700
N	1.89185800	-0.45880000	-0.32787100
C	4.21274700	-0.37827100	-0.08426900
C	1.72702800	-2.90502600	-0.64595200
H	2.28318100	-3.84633000	-0.77629600
C	0.34243200	-2.96320500	-0.50869600
C	-1.75998800	-2.42346300	-0.14192400
C	-1.70019000	-3.86002500	-0.16774800
H	0.03676600	-5.20304000	-0.51596600
H	-2.55235800	-4.53456200	-0.00671800
N	-0.49621800	-1.86715400	-0.34052300
C	-0.39545900	-4.19650300	-0.42499100
C	-2.94777800	-1.70524600	-0.02748600
H	-3.89016500	-2.25725300	0.11806800
C	-2.99943700	-0.32171500	-0.17939800
C	-2.44565000	1.76962400	-0.58489200
C	-3.88434900	1.72444400	-0.52738800
H	-5.23197700	0.01151300	-0.09264800
H	-4.55197600	2.58886100	-0.65084800
N	-1.89649000	0.50796500	-0.37827900
C	-4.22632900	0.42688600	-0.24465400
C	-1.71894800	2.94677900	-0.73814900
H	-2.26911800	3.88593000	-0.90216600
Fe	0.00014800	0.02211000	-0.50839000
O	0.11722500	-0.26349100	2.79220800
O	-0.47976100	0.75082300	3.10514000
N	0.00947700	0.00453800	-2.39833100
C	0.97362800	0.56913300	-3.22516000
C	-0.91622400	-0.55874800	-3.18091000
C	0.62280300	0.34118200	-4.53404400
H	1.83541100	1.09692100	-2.81282000
H	-1.79944600	-1.08230800	-2.81551400
H	-1.09921300	-0.70019600	-5.27628600
C	1.27747100	0.71544700	-5.82504500
H	1.50743900	-0.18752100	-6.43233100
H	0.61978400	1.38008100	-6.42777400
H	2.22571300	1.25191000	-5.63165200
N	-0.57162500	-0.37204900	-4.47214000

[MI – Fe^{III}P – O₂]⁺ S=5/2

C	-0.371616	3.046924	-0.427522
C	0.364418	4.276402	-0.330533
C	1.682544	3.937226	-0.151558
C	1.746734	2.502653	-0.170208
N	0.481220	1.948327	-0.351314
H	-0.073233	5.283335	-0.378046
H	2.541943	4.609585	-0.021151
C	2.935276	1.789427	-0.044366
H	3.874310	2.346390	0.098266
C	2.985408	0.400288	-0.114324
C	2.440056	-1.724974	-0.302905
C	3.869563	-1.672959	-0.174340
H	5.209293	0.081624	0.098846
H	4.538886	-2.544536	-0.173895
N	1.891439	-0.444720	-0.289838
C	4.207806	-0.349661	-0.037959
C	1.726494	-2.918158	-0.372447
H	2.286213	-3.865709	-0.391845
C	0.336477	-2.967166	-0.321709
C	-1.791800	-2.416359	-0.183152
C	-1.729013	-3.850153	-0.126434
H	0.034272	-5.202120	-0.229613
H	-2.594444	-4.519792	-0.022932
N	-0.518271	-1.867063	-0.314562
C	-0.403889	-4.194220	-0.229095
C	-2.985575	-1.701414	-0.144064
H	-3.931686	-2.256271	-0.042391
C	-3.031216	-0.313369	-0.239517
C	-2.477135	1.808684	-0.446789
C	-3.911022	1.758323	-0.386836
H	-5.263386	0.009078	-0.144680
H	-4.579757	2.629216	-0.436285
N	-1.930201	0.529230	-0.376821
C	-4.255742	0.437248	-0.241466
C	-1.759451	2.998716	-0.525583
H	-2.315853	3.945932	-0.595819
Fe	-0.016678	0.037916	-0.513359
O	0.269923	-0.521208	3.134735
O	-0.340851	0.520425	2.972222
N	0.003484	-0.001375	-2.659194
C	0.977867	0.552160	-3.472978
C	-0.906197	-0.545041	-3.461431
C	0.653109	0.339616	-4.795326
H	1.845371	1.065414	-3.048886
H	-1.805295	-1.063186	-3.128096
H	-1.068675	-0.678015	-5.568630
C	1.334907	0.716364	-6.072348
H	1.593510	-0.184804	-6.671032
H	0.686373	1.370536	-6.695921
H	2.271154	1.265955	-5.855157
N	-0.547508	-0.358981	-4.757457

[MI – Fe^{III} P – CO]⁺ S=I/2

C	-0.31866300	2.96806400	0.07795500
C	0.43502900	4.19960200	0.03334200
C	1.68584900	3.88076500	-0.42772500
C	1.71353100	2.44564900	-0.60250000
N	0.47631100	1.90734900	-0.31213900
H	0.04923000	5.19451100	0.29202700
H	2.53223600	4.55986700	-0.59807100
C	2.87957000	1.70498500	-0.82692400
H	3.81393500	2.25684000	-1.01856000
C	2.96380200	0.32283500	-0.62083400
C	2.44102600	-1.71868800	0.03464600
C	3.88284300	-1.65736900	-0.02903300
H	5.20885400	0.01051800	-0.65227300
H	4.56854200	-2.48177700	0.20704200
N	1.89556300	-0.50178600	-0.32866200
C	4.20609300	-0.40151100	-0.47436500
C	1.69890300	-2.88449900	0.26531700
H	2.24111100	-3.80522100	0.53491300
C	0.31942500	-2.96802400	0.03411700
C	-1.71978100	-2.43462800	-0.61958400
C	-1.68845500	-3.87253000	-0.47547500
H	-0.04451500	-5.19899200	0.20359500
H	-2.53498700	-4.54958800	-0.65403800
N	-0.48041000	-1.90052300	-0.32721400
C	-0.43312300	-4.19928600	-0.03117600
C	-2.88775700	-1.69070700	-0.82476300
H	-3.82376300	-2.23987200	-1.01622800
C	-2.96957400	-0.31171700	-0.60053400
C	-2.44003500	1.71897800	0.07836000
C	-3.88258500	1.65766400	0.03407700
H	-5.21555900	-0.00145900	-0.59626400
H	-4.56504000	2.47809600	0.29246600
N	-1.89840400	0.50901400	-0.31090200
C	-4.21095300	0.40895400	-0.42608500
C	-1.69546700	2.88056300	0.32186200
H	-2.23423800	3.79556900	0.61693000
Fe	-0.00076700	0.00267100	-0.29942000
C	0.00062600	-0.00402600	1.45384200
O	0.00026300	-0.01252800	2.61326200
N	-0.00393200	0.00696700	-2.32913700
C	0.53508300	-0.91311900	-3.12699300
C	-0.56924200	0.97042900	-3.15368300
H	1.05805900	-1.80532800	-2.77871100
C	-0.36745400	0.62453100	-4.47103900
H	-1.08108000	1.84418900	-2.74451500
H	0.64587100	-1.10460800	-5.23005100
C	-0.76181400	1.29423100	-5.74794500
H	0.13166100	1.55164100	-6.35693300
H	-1.42220700	0.63857800	-6.35577500
H	-1.31215600	2.23089100	-5.52991600
N	0.33363300	-0.57154800	-4.42335000

[MI – Fe^{III}P – CO]⁺ S=3/2

C	-0.34030100	2.98938800	0.07684800
C	0.42402800	4.22667900	0.04853500
C	1.66863500	3.90985200	-0.40656200
C	1.70132000	2.46248800	-0.58470100
N	0.46095200	1.92385900	-0.32585400
H	0.03695400	5.21865200	0.31677300
H	2.51804900	4.58658800	-0.57299200
C	2.86819500	1.73309900	-0.80313000
H	3.80368200	2.28272300	-0.99271100
C	2.95970100	0.33937100	-0.58566300
C	2.41915300	-1.72352600	0.02767000
C	3.84376000	-1.66770600	-0.06205100
H	5.17984000	0.02709800	-0.65287400
H	4.53120700	-2.49832100	0.14496400
N	1.87017200	-0.50311000	-0.28922300
C	4.17499500	-0.38012600	-0.48023400
C	1.66648400	-2.91131700	0.25805800
H	2.21355900	-3.83116600	0.51923600
C	0.30418200	-2.98834800	0.02491000
C	-1.73446700	-2.44999300	-0.64715400
C	-1.70063300	-3.89624900	-0.50936100
H	-0.07234700	-5.22159700	0.19428000
H	-2.54540700	-4.57155100	-0.70296900
N	-0.49929700	-1.91214100	-0.34210800
C	-0.45807100	-4.22190800	-0.04687500
C	-2.89227400	-1.71129300	-0.87481700
H	-3.82836300	-2.25177300	-1.08617200
C	-2.96993000	-0.32015900	-0.61044700
C	-2.45362800	1.71938900	0.10719800
C	-3.86001700	1.65890900	0.08076400
H	-5.20431800	-0.01591100	-0.56517400
H	-4.54685300	2.47397400	0.34176400
N	-1.89928600	0.48948300	-0.31876300
C	-4.19657900	0.38878900	-0.40072400
C	-1.69294400	2.89729600	0.35515800
H	-2.23439600	3.80089400	0.67744800
Fe	-0.02330900	-0.00063100	-0.31748200
C	0.05908500	0.05672500	1.46374000
O	0.18599700	0.11638300	2.61124800
N	-0.00751800	-0.01016400	-2.33126900
C	0.53924600	-0.93558600	-3.11777400
C	-0.56174200	0.95288000	-3.16370000
H	1.06094100	-1.82371800	-2.75750200
C	-0.34566600	0.60024700	-4.47669800
H	-1.08038000	1.82660500	-2.76361900
H	0.67909300	-1.13094700	-5.21713400
C	-0.72624200	1.26475500	-5.76029500
H	0.17239900	1.49633400	-6.37207400
H	-1.40032000	0.61649600	-6.36100400
H	-1.25646800	2.21540800	-5.55287100
N	0.35298200	-0.59748400	-4.41610500

[MI – Fe^{III} P – CO]⁺ S=5/2

C	-0.33729800	3.07426700	-0.16677900
C	0.42044500	4.29919500	-0.11539100
C	1.74948500	3.95079200	-0.19221100
C	1.80153700	2.51326200	-0.27942500
N	0.51749800	1.98939400	-0.28853600
H	-0.000005500	5.31036700	-0.02389100
H	2.61828600	4.62409100	-0.17917600
C	2.98908600	1.76785900	-0.31926500
H	3.93943500	2.32671500	-0.31506600
C	3.06418200	0.36761600	-0.31149200
C	2.51209300	-1.77718900	-0.25901400
C	3.95187900	-1.71314000	-0.22853600
H	5.30654300	0.04904500	-0.25197400
H	4.63131800	-2.57513200	-0.17254800
N	1.98050200	-0.49861000	-0.33036000
C	4.29479200	-0.38083000	-0.26637700
C	1.76965000	-2.96681600	-0.23924000
H	2.32818300	-3.91642000	-0.19345500
C	0.36925700	-3.03663200	-0.25682900
C	-1.77280500	-2.47395100	-0.30484500
C	-1.71859700	-3.91336300	-0.25764000
H	0.03361600	-5.27613600	-0.16557100
H	-2.58681900	-4.58757800	-0.24066900
N	-0.48868400	-1.94980100	-0.32859000
C	-0.38799200	-4.26279200	-0.22226800
C	-2.95887500	-1.72579600	-0.30546800
H	-3.91002100	-2.28309000	-0.29435500
C	-3.03094600	-0.32550100	-0.26508300
C	-2.47887100	1.81619400	-0.15722800
C	-3.91693800	1.75018000	-0.08972700
H	-5.27102200	-0.01159800	-0.13841500
H	-4.59470800	2.60939600	0.00979600
N	-1.94837500	0.54129900	-0.28540700
C	-4.26013900	0.41958700	-0.16339400
C	-1.73661000	3.00464100	-0.11277600
H	-2.29239700	3.95183300	-0.02162800
Fe	0.01305100	0.02239100	-0.62474400
N	0.00523300	0.00821800	-2.71802500
C	0.55684800	-0.91340000	-3.50586800
C	-0.58619900	0.94970700	-3.54551900
H	1.09988100	-1.79209100	-3.15901200
C	-0.38981900	0.59263100	-4.86089000
H	-1.11089900	1.81725700	-3.13636600
H	0.65266800	-1.12706000	-5.60703300
C	-0.80117200	1.22986500	-6.15037000
H	0.08659200	1.49182600	-6.76711000
H	-1.44701000	0.54681700	-6.74470900
H	-1.36986100	2.15780300	-5.95030100
N	0.33658100	-0.59175800	-4.80373800
C	0.04363100	-0.01061100	2.86795100
O	0.05096400	-0.00864100	4.01742200

[MI – Fe^{III}P – NO]⁺ S=0

C	-0.34738500	3.01898300	-0.11773600
C	0.40320600	4.25170800	-0.14234200
C	1.71314700	3.91475100	-0.35693800
C	1.76956200	2.47408600	-0.43025200
N	0.50109400	1.94182800	-0.29011300
H	-0.02330500	5.25610400	-0.02307600
H	2.57822900	4.58638800	-0.44058300
C	2.95677400	1.74951500	-0.53922900
H	3.90116400	2.30841400	-0.63551200
C	3.01785100	0.35959900	-0.44051800
C	2.46824800	-1.76122000	-0.15283100
C	3.91028800	-1.70374200	-0.19867900
H	5.25655100	0.03854800	-0.48730900
H	4.58259700	-2.56657100	-0.10305900
N	1.93823700	-0.49253100	-0.29701200
C	4.24993400	-0.39120900	-0.39611400
C	1.73788600	-2.94698000	-0.04378300
H	2.29293100	-3.88966500	0.08696700
C	0.34657100	-3.01042100	-0.15134700
C	-1.77482700	-2.46191900	-0.43789500
C	-1.71596400	-3.90357900	-0.39382000
H	0.02501000	-5.24996100	-0.10160000
H	-2.58006900	-4.57534800	-0.48497200
N	-0.50583500	-1.93145600	-0.29463800
C	-0.40338200	-4.24346700	-0.19700400
C	-2.96048100	-1.73409700	-0.53833600
H	-3.90721200	-2.28881700	-0.63530100
C	-3.01827100	-0.34436300	-0.42956600
C	-2.46725300	1.77113900	-0.11751300
C	-3.90936200	1.71327600	-0.14340400
H	-5.25762800	-0.02580000	-0.44223100
H	-4.58065700	2.57357100	-0.02429400
N	-1.93746900	0.50620800	-0.28829500
C	-4.25048100	0.40429800	-0.35785100
C	-1.73632900	2.95403200	0.01040400
H	-2.28945800	3.89365500	0.16571300
Fe	-0.00031900	0.00491600	-0.22831200
N	-0.00159400	0.00297200	-2.24600700
C	0.53954900	-0.92154800	-3.04041000
C	-0.56901500	0.96624600	-3.07045400
H	1.06417900	-1.81433100	-2.70282000
C	-0.36688400	0.61656700	-4.38517900
H	-1.08257100	1.84365100	-2.67236300
H	0.64801100	-1.11568400	-5.13947600
C	-0.76703000	1.29195400	-5.65773200
H	0.12265800	1.55043900	-6.27218100
H	-1.43178500	0.64073500	-6.26599500
H	-1.31468800	2.22909300	-5.43267900
N	0.33626200	-0.58008700	-4.33442000
N	0.00437500	-0.00560500	1.39113200
O	0.01270200	-0.02509300	2.54096100

[MI – Fe^{III} P – NO]⁺ S=1

C	-0.313136	2.955394	0.092825
C	0.435930	4.187227	0.022600
C	1.697448	3.857092	-0.399216
C	1.735745	2.419198	-0.530137
N	0.492417	1.882614	-0.240672
H	0.039560	5.188412	0.238617
H	2.546207	4.533292	-0.569825
C	2.908605	1.688318	-0.740197
H	3.838723	2.251370	-0.923755
C	2.999030	0.299473	-0.577423
C	2.475929	-1.772648	-0.049241
C	3.916961	-1.717700	-0.140535
H	5.242666	-0.019171	-0.679431
H	4.601749	-2.559109	0.030802
N	1.935298	-0.530689	-0.301699
C	4.240964	-0.435244	-0.505213
C	1.735879	-2.948195	0.139791
H	2.285390	-3.881810	0.345054
C	0.348548	-3.024685	-0.047473
C	-1.717436	-2.477045	-0.574540
C	-1.677704	-3.919307	-0.500392
H	0.004879	-5.264811	0.035558
H	-2.527677	-4.593460	-0.673326
N	-0.475063	-1.949517	-0.300429
C	-0.398868	-4.257966	-0.136349
C	-2.887979	-1.724370	-0.738397
H	-3.831662	-2.264624	-0.921195
C	-2.958015	-0.343830	-0.530492
C	-2.432479	1.708020	0.091631
C	-3.873009	1.651146	0.019902
H	-5.199673	-0.025793	-0.573112
H	-4.555895	2.484087	0.234357
N	-1.885647	0.482812	-0.240949
C	-4.196593	0.387755	-0.401330
C	-1.693389	2.876175	0.310603
H	-2.238107	3.801872	0.558299
Fe	0.009859	-0.016926	-0.205360
N	-0.001181	0.001587	-2.323954
C	0.532997	-0.913631	-3.129929
C	-0.565758	0.967529	-3.144002
H	1.057410	-1.809786	-2.792033
C	-0.369536	0.631120	-4.465766
H	-1.077471	1.842548	-2.735461
H	0.639640	-1.096277	-5.236485
C	-0.769653	1.315125	-5.733204
H	0.119383	1.579972	-6.345896
H	-1.434500	0.669185	-6.346856
H	-1.318025	2.250558	-5.501921
N	0.329806	-0.566751	-4.426160
N	-0.019807	0.031231	1.563009
O	-0.423391	0.718534	2.421757

[MI – Fe^{III} P – NO]⁺ S=3

C	-0.387700	3.074519	-0.159966
C	0.372019	4.308014	-0.113676
C	1.699724	3.958509	-0.135702
C	1.757826	2.510380	-0.189152
N	0.480943	1.996142	-0.202387
H	-0.044552	5.323447	-0.062849
H	2.561087	4.639951	-0.111603
C	2.944497	1.742396	-0.199040
H	3.892922	2.306098	-0.177028
C	3.048892	0.332875	-0.213160
C	2.497871	-1.814146	-0.215994
C	3.945710	-1.750194	-0.202272
H	5.302835	0.000867	-0.192340
H	4.631713	-2.608505	-0.185292
N	1.980533	-0.533530	-0.223283
C	4.287681	-0.419512	-0.202411
C	1.731520	-2.999752	-0.220674
H	2.293821	-3.949736	-0.189104
C	0.318388	-3.099006	-0.271678
C	-1.812902	-2.532846	-0.351770
C	-1.767210	-3.982170	-0.349260
H	-0.024715	-5.352681	-0.273849
H	-2.631547	-4.660741	-0.376792
N	-0.538904	-2.028998	-0.303180
C	-0.437782	-4.335152	-0.297656
C	-2.998359	-1.755667	-0.365895
H	-3.950934	-2.314030	-0.383002
C	-3.099239	-0.346914	-0.338342
C	-2.563944	1.790405	-0.225675
C	-4.012936	1.727780	-0.227872
H	-5.357187	-0.033428	-0.316782
H	-4.702147	2.581137	-0.173920
N	-2.039004	0.526590	-0.289738
C	-4.345737	0.396049	-0.301267
C	-1.792459	2.978698	-0.148153
H	-2.351082	3.928412	-0.086637
Fe	-0.009581	0.000327	-0.208570
N	0.027908	-0.005805	-2.434149
C	0.525347	-0.937700	-3.240389
C	-0.540524	0.955243	-3.255348
H	1.045419	-1.840169	-2.919395
C	-0.382853	0.602270	-4.577364
H	-1.030121	1.844569	-2.846285
H	0.584400	-1.149020	-5.347190
C	-0.804607	1.279729	-5.842101
H	0.069502	1.514572	-6.488355
H	-1.506186	0.645645	-6.427718
H	-1.321487	2.232605	-5.606727
N	0.300134	-0.605319	-4.538515
N	0.048668	0.022230	1.686417
O	0.763341	0.423765	2.518151

