Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


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

Mohammad Aarabi[a], Reza Omidyan[a,*] Satchin Soorkia[b], Gilles Grégoire[b], Michel Broquier [b,c] Maria-Elisa Crestoni[d], Aurélien de la Lande[e], Benoît Soep[f], Niloufar Shafizadeh [b,*]

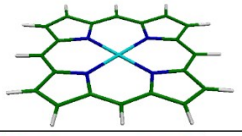
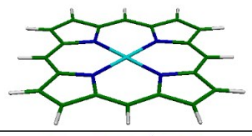
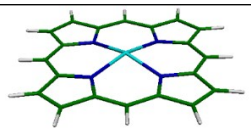
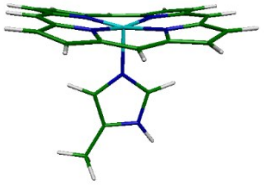
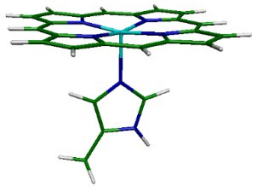
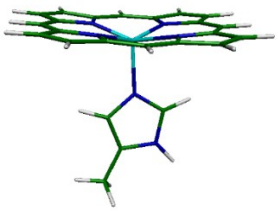
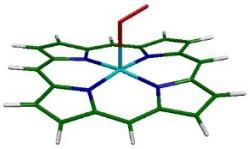
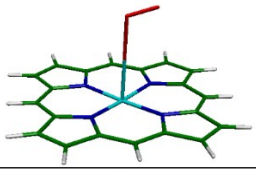
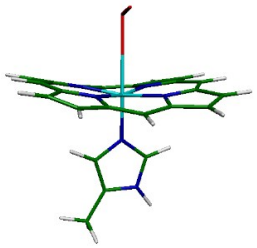
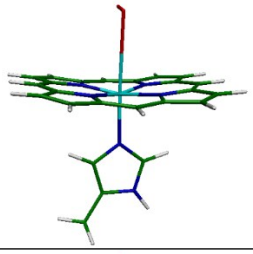
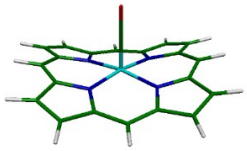
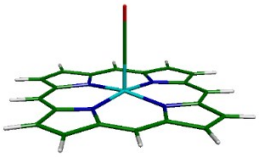
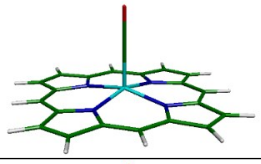
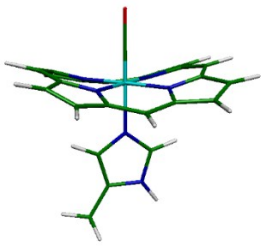
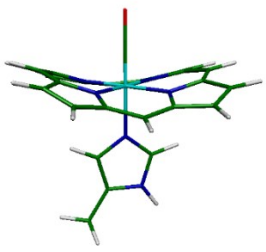
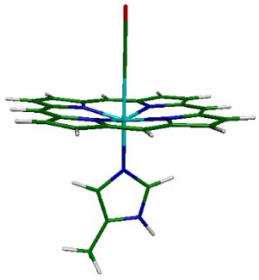
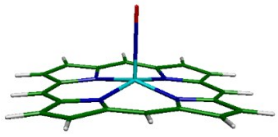
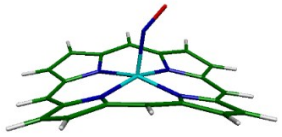
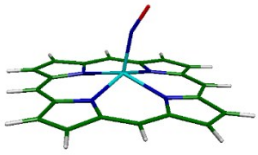
[a] *Department of Chemistry, University of Isfahan, 81746-73441 Isfahan, Iran.*
[b] *Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS, Univ. Paris Sud, Université Paris-Saclay, F-91405 Orsay, France*
[c] *Centre Laser de l'Université Paris-Sud (CLUPS/LUMAT), Univ. Paris-Sud, CNRS, IOGS, Université Paris-Saclay, F-91405 Orsay, France*
[d] *Dipartimento di Chimica e Tecnologie del Farmaco, Università degli Studi di Roma "La Sapienza", P.le A. Moro 5, 00185 Roma, Italy*
[e] *Laboratoire de Chimie-Physique, Université Paris Sud, CNRS, UMR 8000.batiment 349 Univ. Paris-Sud, Université Paris-Saclay, F-91405 Orsay, France*
[f] *LIDYL, CEA, CNRS, Université Paris-Saclay, UMR 9222 CEA Saclay, F-91191 Gif-sur-Yvette, France.*

## 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.*

| Complex | LS | IS | HS |
|---|---|---|---|
| $[Fe^{III}P]^+$ |  |  |  |
| $[MI - Fe^{III}P]^+$ |  |  |  |
| $[Fe^{III}P - O_2]^+$ | * |  |  |
| $[MI - Fe^{III}P - O_2]^+$ | * |  |  |
| $[Fe^{III}P - CO]^+$ |  |  |  |
| $[MI - Fe^{III}P - CO]^+$ |  |  |  |
| $[Fe^{III}P - NO]^+$ |  |  |  |

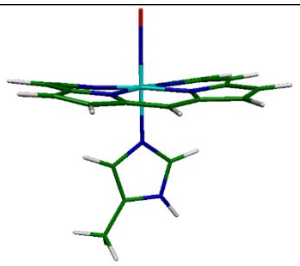
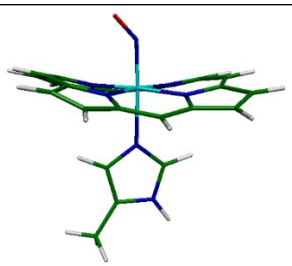
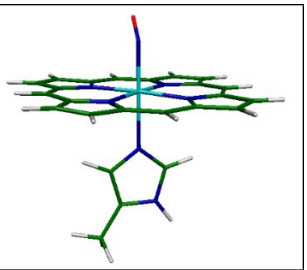
| | | | |
|---|---|---|---|
| $[MI - Fe^{III} P - NO]^{+}$ |  |  |  |

**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 Figure3C of the article.* [a] *Average value of the four Fe-Np bond lengths* [b] *Experimental 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 | - |
| $[MI\text{-}Fe^{III}P]^+$ | 1/2 | - | - | −0.178 | - | 1.967 | 1.897 |
| | 3/2 | - | - | −0.185 | - | 1.984 | 2.138 |
| | **5/2** | **-** | **-** | **−0.428** | **-** | **2.070** | **2.096** |
| $[Fe^{III}P\text{-}O_2]^+$ | 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** | **-** |
| $[MI\text{-}Fe^{III}P\text{-}O_2]^+$ | 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 | * | | | | | |
| $[Fe^{III}P\text{-}CO]^+$ | 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 | - |
| $[MI\text{-}Fe^{III}P\text{-}CO]^+$ | 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** |
| $[Fe^{III}P\text{-}NO]^+$ | **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 | - |
| $[MI\text{-}Fe^{III}P\text{-}NO]^+$ | **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 | |
| $[Fe^{III}P]^+$ | 1/2 | 6.81 | 7.09 | 3/2[2] |
| | **3/2** | ***0.00*** | ***0.00*** | |
| | 5/2 | 12.07 | 12.42 | |
| $[MI\text{-}Fe^{III}P]^+$ | 1/2 | 10.65 | 10.93 | 5/2[3] |
| | 3/2 | 0.00 | 0.00 | |
| | 5/2 | 5.52 | 5.18 | |
| $[Fe^{III}P\text{-}O_2]^+$ | 1/2 | * | * | - |
| | 3/2 | 23.17 | 24.66 | |
| | **5/2** | ***0.00*** | ***0.00*** | |
| $[MI\text{-}Fe^{III}P\text{-}O_2]^+$ | 3/2 | 10.86 | 11.27 | - |
| | **5/2** | ***0.00*** | ***0.00*** | |
| | 7/2 | * | * | |
| $[Fe^{III}P\text{-}CO]^+$ | 1/2 | 13.20 | 13.93 | 3/2[4] |
| | **3/2** | ***0.00*** | ***0.00*** | |
| | 5/2 | 10.74 | 10.34 | |
| $[MI\text{-}Fe^{III}P\text{-}CO]^+$ | 1/2 | 0.83 | 2.01 | - |
| | 3/2 | 42.40 | 43.57 | |
| | **5/2** | ***0.00*** | ***0.00*** | |
| $[Fe^{III}P\text{-}NO]^+$ | **0** | 0.00 | * | 0[5] |
| | 1 | 7.82 | * | |
| | 2 | 2.04 | * | |
| $[MI\text{-}Fe^{III}P\text{-}NO]^+$ | **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-O2]$^{+}$ and [MI-Fe$^{III}$P-O2]$^{+}$: Spin-up and spin-down densities are shown as white and blue, respectively.*

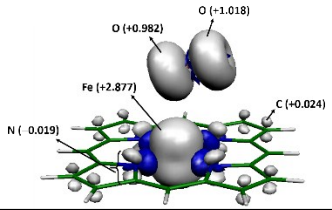
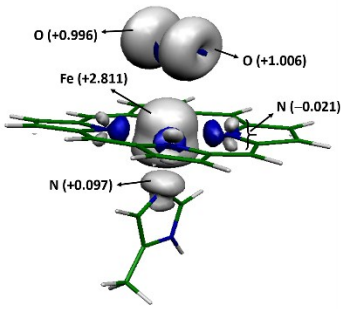
| Molecule | Spin | Spin-density plot (isosurfaces=0.0025) |
|---|---|---|
| [Fe$^{III}$P-O$_2$]$^{+}$ | 5/2 |   |
| [MI-Fe$^{III}$P-O$_2$]$^{+}$ | 5/2 |   |

**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


1. A. B. McQuarters, J. W. Kampf, E. E. Alp, M. Hu, J. Zhao and N. Lehnert, Inorg. Chem. **56** (17), 10513-10528 (2017).
2. M. Fang, S. R. Wilson and K. S. Suslick, J. Am. Chem. Soc. **130** (4), 1134-1135 (2008).
3. W. R. Scheidt, D. K. Geiger, Y. J. Lee, C. A. Reed and G. Lang, J. Am. Chem. Soc. **107** (20), 5693-5699 (1985).
4. S. Dillinger, J. Lang and G. Niedner-Schatteburg, J. Phys. Chem. A. **121** (38), 7191-7196 (2017).
5. A. P. Hunt and N. Lehnert, Acc. Chem. Res. **48** (7), 2117-2125 (2015).

**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 |

$[Fe^{III}P - O_2]^+$ $S = 3/2$

| | | | |
|---|---|---|---|
| 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 |

$[Fe^{III}P - O_2]^+$ *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 |

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

| | | | |
|---|---|---|---|
| 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 | 0.00086100 | -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 |

$[^{III}P - NO]^{+}$ $S=1$

| | | | |
|---|---|---|---|
| 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 |

$[MI - Fe^{III} P]^{+}$ *S=1/2*

| | | | |
|---|---|---|---|
| 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 |

$[MI - Fe^{III}P - O_2]^+$ *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 |

$[MI - Fe^{III}P - O_2]^+$ *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=1/2*

| | | | |
|---|---|---|---|
| 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 | -0.00005500 | 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 |