

**Inhibition of Peroxidase-Catalyzed Iodination by Thioamides. Experimental and  
Theoretical Study of the induced Antithyroid Activity of thioamides**

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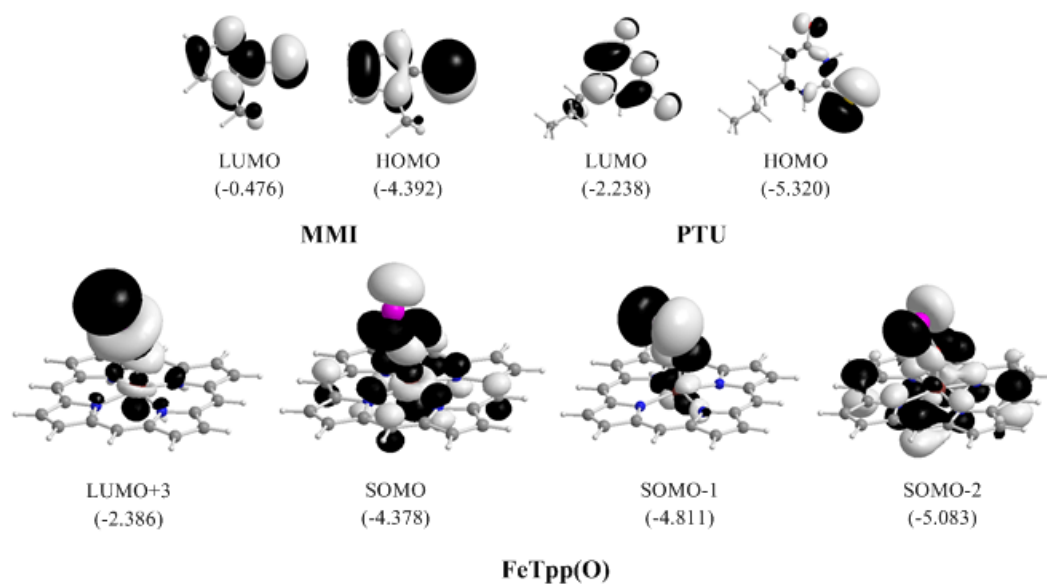
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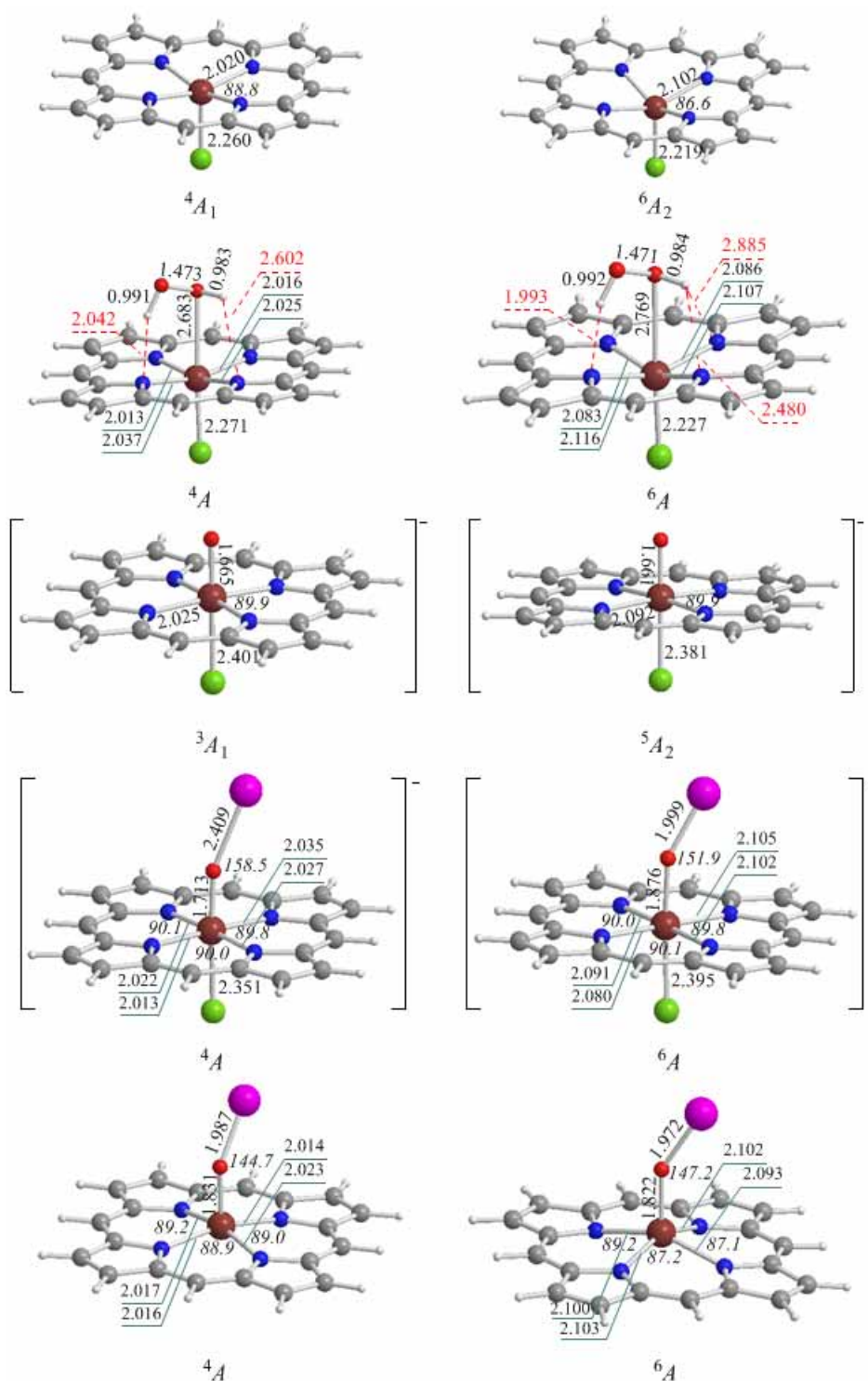
## Table of Contents

<b>Figure S1.</b>	The most relevant Frontier Molecular Orbitals (FMOs) of MMI, PTU and [FeTpp(OI)].	S3
<b>Figure S2.</b>	Equilibrium geometries of all stationary points located on the quartet and sextet potential energy surfaces of the inhibition of the catalytic activity of FeTppCl by the thioamide compounds computed at the UBP86/Def2-QZVPP(Fe,I) $\cup$ 6-31G(d,p)(E) level of theory.	S4
<b>Figure S3.</b>	3D isospin surfaces of total spin density of the stationary points located on the quartet and sextet potential energy surfaces of the inhibition of the catalytic activity of FeTppCl by the thioamide compounds computed at the UBP86/Def2-QZVPP(Fe,I) $\cup$ 6-31G(d,p)(E) level of theory (isospin of 0.002)	S5
<b>Table S1</b>	Cartesian Coordinates and energy data of all structures studied herein computed at the BP86/Def2-QZVPP(Fe,I) $\cup$ 6-31G(d,p)(E) level	<b>S6-S17</b>

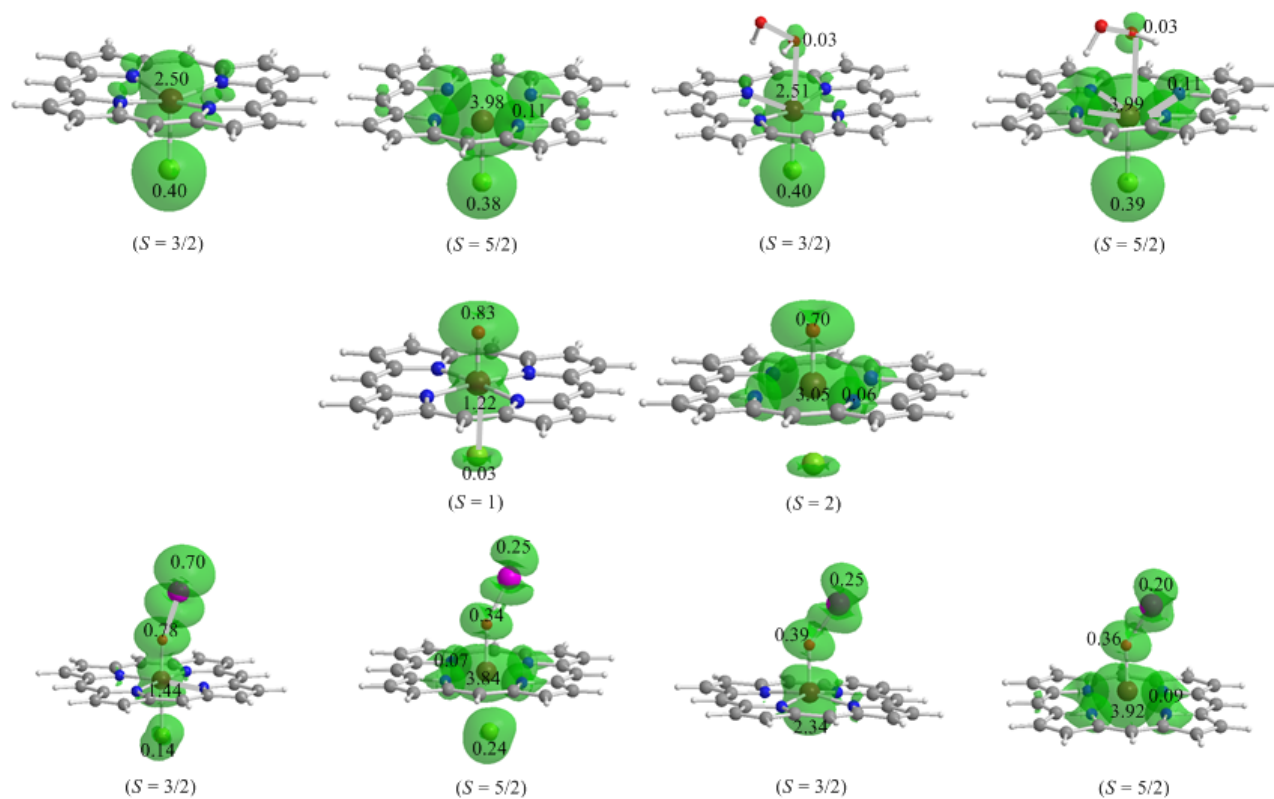


**Figure S1**

**Figure S1.** The most relevant Frontier Molecular Orbitals (FMOs) of MMI, PTU and [FeTpp(OI)].



**Figure S2.** Equilibrium geometries of all stationary points located on the quartet and sextet potential energy surfaces of the inhibition of the catalytic activity of FeTppCl by the thioamide compounds computed at the UBP86/Def2-QZVPP(Fe,I)∪6-31G(d,p)(E) level of theory.



**Figure S3.** 3D isospin surfaces of total spin density of the stationary points located on the quartet and sextet potential energy surfaces of the inhibition of the catalytic activity of FeTppCl by the thioamide compounds computed at the UBP86/Def2-QZVPP(Fe,I)  $\cup$  6-31G(d,p)(E) level of theory (isospin of 0.002).

**Table S1.**

**Cartesian Coordinates and energy data of all structures studied herein computed at the BP86/Def2-QZVPP(Fe,I)∪6-31G(d,p)(E) level**

**MMI**

C,0,-6.2106816142,-0.1470546739,-0.0021245903  
N,0,-7.5594692752,-0.4791612196,0.0009111114  
C,0,-8.350429114,0.6709379631,0.0039197304  
C,0,-7.509548668,1.7485344207,0.0028188356  
N,0,-6.2157381519,1.2378794035,-0.0006092001  
S,0,-4.8875731348,-1.18324144,-0.0061650599  
C,0,-8.0270498996,-1.8583821619,0.0009036661  
H,0,-9.4357140006,0.6207214799,0.0066070705  
H,0,-7.72112091,2.8135517534,0.0043388319  
H,0,-9.1265527789,-1.859560147,0.0005700626  
H,0,-7.6493382792,-2.3847756025,0.892342592  
H,0,-7.6487036343,-2.3845624267,-0.8903642558  
H,0,-5.3473805392,1.7645126511,-0.0022487945

Sum of electronic and zero-point Energies= -663.673721  
Sum of electronic and thermal Energies= -663.666696  
Sum of electronic and thermal Enthalpies= -663.665752  
Sum of electronic and thermal Free Energies= -663.706037

**MMI·I<sub>2</sub>**

C,0,-0.5106263608,-0.1877904262,0.1655801175  
N,0,0.455632041,0.7783169217,0.0051175088  
C,0,1.7175412996,0.1806530434,-0.0396168492  
C,0,1.5355638175,-1.1687300639,0.0941095382  
N,0,0.1675560471,-1.3737015412,0.2181810575  
S,0,-2.1980542697,0.0777049223,0.2726594329  
C,0,0.1615109529,2.2052808781,-0.0985710177  
H,0,2.6227672427,0.7685608142,-0.1617677467  
H,0,2.2497768471,-1.9863054179,0.111282934  
H,0,1.1071466623,2.7512276178,-0.220172031  
H,0,-0.3529227429,2.551926117,0.8119794004  
H,0,-0.4906019742,2.3943460879,-0.9662752083  
H,0,-0.3393664063,-2.2595870966,0.3360640367  
I,0,-2.9912438954,-2.6487950712,0.5765268117  
I,0,-3.6544792608,-5.4008067853,0.8726020153

Sum of electronic and zero-point Energies= -1259.399102  
Sum of electronic and thermal Energies= -1259.387726  
Sum of electronic and thermal Enthalpies= -1259.386782  
Sum of electronic and thermal Free Energies= -1259.442033

**MMI·I<sup>+</sup>**

C,0,1.3403812329,-0.2719702584,0.4437109203  
N,0,2.1519078656,0.6955352629,-0.0821499269  
C,0,3.2306058595,0.0988119508,-0.7076587107  
C,0,3.0924855358,-1.2668412434,-0.5660432309  
N,0,1.9296786941,-1.4651067377,0.1407675659  
S,0,-0.104443524,-0.0693158239,1.3985648457  
C,0,1.9148130816,2.1489155829,-0.0165708588  
H,0,4.0091676331,0.6815307301,-1.1945156252

H,0,3.7250086628,-2.0842248631,-0.9033887975  
H,0,1.6770048532,2.5256153551,-1.0226500204  
H,0,2.8189223192,2.641740767,0.3686365194  
H,0,1.0717978124,2.3363130464,0.6610732783  
H,0,1.5362044677,-2.3659410188,0.4195156525  
I,0,-1.872035494,-0.0290097499,-0.3020016118

Sum of electronic and zero-point Energies= -961.278483  
Sum of electronic and thermal Energies= -961.269741  
Sum of electronic and thermal Enthalpies= -961.268796  
Sum of electronic and thermal Free Energies= -961.316274

### MMI-I<sup>+</sup>-MMI

C,0,-7.3659914429,-0.6432600964,-0.1145061362  
N,0,-8.5069995665,-1.3676331727,-0.3312393979  
C,0,-9.5765876005,-0.7612090494,0.3304306635  
C,0,-9.0923367019,0.351487738,0.9611564248  
N,0,-7.7322121527,0.4052389032,0.6755535883  
S,0,-5.8076054045,-1.0427099359,-0.7446975345  
C,0,-8.5651156534,-2.5920867901,-1.1350474451  
H,0,-10.5798110579,-1.176152633,0.2901915583  
H,0,-9.5872154707,1.096825382,1.576450657  
H,0,-9.6085861754,-2.9306061781,-1.1799319161  
H,0,-7.9431488468,-3.3763870988,-0.6756693196  
H,0,-8.2010324083,-2.3882773354,-2.1541373686  
H,0,-7.0619071846,1.1112651606,0.9873343643  
I,0,-4.3298773258,1.0040030456,0.1883157972  
C,0,-1.4345467289,2.942756874,0.2023200851  
N,0,-0.3829832455,2.0760663874,0.3621778363  
C,0,0.593186787,2.3394964697,-0.5904346471  
C,0,0.1538580728,3.3936115375,-1.3527423447  
N,0,-1.0878999269,3.7410425448,-0.8533117693  
S,0,-2.8690388767,3.0797228429,1.1476345277  
C,0,-0.3173018506,1.0183512529,1.3772618149  
H,0,1.5129959848,1.7632968293,-0.6442730723  
H,0,0.6187493833,3.9121824537,-2.186374739  
H,0,0.7179078672,0.9312655491,1.735889056  
H,0,-0.6496257297,0.0598464617,0.9486920575  
H,0,-0.9810274554,1.2963784988,2.2079082361  
H,0,-1.6929472894,4.4882843588,-1.1913509767

Sum of electronic and zero-point Energies= -1625.001247  
Sum of electronic and thermal Energies= -1624.983624  
Sum of electronic and thermal Enthalpies= -1624.982680  
Sum of electronic and thermal Free Energies= -1625.053061

### PTU

N,0,-0.0154902177,0.5843406136,-0.5698146709  
H,0,0.5093011202,1.3673241128,-0.9591801003  
C,0,-1.3698196303,0.8332638892,-0.4001386972  
H,0,-3.0584037493,-0.1106739356,0.2610276497  
S,0,-2.061577953,2.3044716722,-0.7972465752  
H,0,0.371151453,-2.5987466238,0.4962949491  
N,0,-2.0552153698,-0.2410830629,0.1165929502  
H,0,2.3191009454,-0.3303361661,-1.5507999846  
C,0,-1.5371760956,-1.5253561299,0.4768537367  
H,0,2.4552201446,-1.6861049351,-0.4177970493  
O,0,-2.2924090479,-2.3852961862,0.9289425296  
H,0,2.7103139616,-0.0633319319,1.5004366416  
C,0,-0.102358703,-1.6489311149,0.2473416031

H,0,2.5736033753,1.3020089281,0.3874893607  
C,0,0.6247655933,-0.6082585025,-0.2640342629  
H,0,4.988759458,0.8318580869,0.8912653262  
C,0,2.1136101337,-0.6412365739,-0.5071935675  
H,0,4.6676737293,0.5328544641,-0.8354097443  
C,0,2.9225051561,0.2548997809,0.4638528102  
H,0,4.8150741407,-0.8371781455,0.2942454633  
C,0,4.4312445554,0.1922267606,0.1877996318

Sum of electronic and zero-point Energies= -855.601724  
Sum of electronic and thermal Energies= -855.590579  
Sum of electronic and thermal Enthalpies= -855.589635  
Sum of electronic and thermal Free Energies= -855.639824

### PTU·I<sub>2</sub>

N,0,-1.5722848786,0.5374963909,0.0018060221  
C,0,-2.4211011751,1.7007019073,0.0029821361  
C,0,-3.8394864288,1.3693476421,0.0016862474  
C,0,-4.2685049515,0.0701569839,-0.0005750299  
N,0,-3.3258914149,-0.9565392023,-0.0015068482  
C,0,-1.9729409884,-0.7659643576,-0.0003299721  
O,0,-1.9110890336,2.8172020561,0.0032443465  
S,0,-0.8523278286,-2.0521623238,-0.0016052842  
H,0,-0.5674896856,0.7278635836,0.0027729087  
H,0,-4.5443731164,2.199828809,0.0023729737  
H,0,-3.6292834693,-1.9456791577,-0.003190177  
C,0,-5.7060097063,-0.3943561519,-0.0026251452  
C,0,-6.7661623039,0.7181515061,-0.0029990774  
C,0,-8.1942979724,0.1513576443,0.004079391  
H,0,-5.8538179695,-1.0519557934,0.8778550803  
H,0,-5.8516555026,-1.0505274896,-0.8844929197  
H,0,-6.6250581053,1.3594936201,-0.8924391876  
H,0,-6.6191084669,1.365776596,0.8809101157  
H,0,-8.9390494236,0.963555573,-0.0054186502  
H,0,-8.3789792812,-0.4625293628,0.9025164913  
H,0,-8.3795028073,-0.4837075212,-0.8794278246  
I,0,-4.5352412227,-6.4163878455,0.000859172  
I,0,-2.6472442676,-4.3098231068,-0.0042747689

Sum of electronic and zero-point Energies= -1451.318863  
Sum of electronic and thermal Energies= -1451.303097  
Sum of electronic and thermal Enthalpies= -1451.302153  
Sum of electronic and thermal Free Energies= -1451.368252

### PTU·I<sup>+</sup>

N,0,-0.1027344232,-0.719606383,0.3203873396  
H,0,0.3911461395,-1.6061076258,0.4479156576  
C,0,-1.4381962044,-0.7412166162,0.0918186242  
H,0,-3.0723906053,0.4326049676,-0.257919761  
S,0,-2.2079810223,-2.3347747727,0.0591623558  
H,0,0.5727218245,2.6019237674,0.2468604965  
N,0,-2.0572705088,0.4255211284,-0.0842693781  
H,0,2.2722838935,-0.3065740847,1.5490562587  
C,0,-1.4133290719,1.7568999777,-0.0524177204  
H,0,2.5595673598,1.2826326393,0.8238894147  
O,0,-2.1107587552,2.735453765,-0.2317086394  
H,0,2.7051570763,0.2068509584,-1.4722605307  
C,0,0.0148822845,1.6651179712,0.2020333122  
H,0,2.4548108646,-1.3905983804,-0.7514661056  
C,0,0.6528130423,0.469187615,0.3838979189



H,0,4.895379452,-0.9844081645,-1.1217449492  
C,0,2.1256135878,0.2890007824,0.6261239257  
H,0,4.5775949584,-1.1151653672,0.626348384  
C,0,2.8770775365,-0.3853903288,-0.5560015439  
H,0,4.8396928282,0.4844036689,-0.1187388116  
C,0,4.381449883,-0.5068016063,-0.2728341792  
I,0,-4.5206301397,-1.8622539117,-0.3876320688

Sum of electronic and zero-point Energies= -1153.183169  
Sum of electronic and thermal Energies= -1153.169819  
Sum of electronic and thermal Enthalpies= -1153.168875  
Sum of electronic and thermal Free Energies= -1153.226661

### PTU-I<sup>+</sup>-PTU

N,0,-4.8783766667,-1.6846659262,0.435979538  
C,0,-6.0264395453,-0.8565667046,0.7803150635  
C,0,-5.7388786454,0.5681828917,0.6855416877  
C,0,-4.5097424661,1.0325120102,0.313063259  
N,0,-3.4978196363,0.1061372939,0.0116113162  
C,0,-3.6571388364,-1.2412691899,0.0623000678  
O,0,-7.0706451924,-1.4014902517,1.099761983  
S,0,-2.4099112792,-2.3780699142,-0.3215683351  
C,0,-4.1001714142,2.4790759266,0.1845622706  
C,0,-5.198738088,3.5105549155,0.4928485325  
C,0,-4.6906664171,4.9519597023,0.3346657596  
N,0,2.7914136574,-0.4837426963,0.6115644263  
C,0,3.7545315739,-0.7696305719,1.6666467331  
C,0,5.0802768313,-0.2455774942,1.3740639382  
C,0,5.3460583634,0.4403631579,0.2222006445  
N,0,4.3074061611,0.6422128311,-0.6997308737  
C,0,3.0309146003,0.1920150804,-0.5291351954  
O,0,3.3793934717,-1.3891006653,2.6501124858  
S,0,1.8618779592,0.5282773467,-1.7588145162  
C,0,6.6778891478,1.0201947852,-0.1873879317  
C,0,7.8338274591,0.7989363119,0.8033627082  
C,0,9.1472735887,1.411117704,0.2919410495  
H,0,-5.0462661476,-2.6938796928,0.486843872  
H,0,-6.5506815122,1.2545428819,0.9256051427  
H,0,-2.5709900869,0.4477272784,-0.269113053  
H,0,-3.7192167912,2.6376945216,-0.8451852351  
H,0,-3.231580029,2.6494129297,0.8535082668  
H,0,-5.5664378296,3.3566411091,1.5237366963  
H,0,-6.0577120473,3.3426242047,-0.1820372695  
H,0,-5.4922721877,5.6728529696,0.5594088613  
H,0,-4.3449797011,5.1473412126,-0.6950322329  
H,0,-3.8514000248,5.161742852,1.0199512644  
H,0,1.8430958609,-0.8437551542,0.775710988  
H,0,5.86002858,-0.4229562212,2.1142202572  
H,0,4.5098877756,1.1432638766,-1.5668133349  
H,0,6.5413651715,2.1072533535,-0.3622078436  
H,0,6.9485216707,0.591085559,-1.1740691438  
H,0,7.9693484112,-0.2851003415,0.9712319621  
H,0,7.5700036763,1.2442525232,1.7799679341  
H,0,9.9607659943,1.2441311833,1.0151942361  
H,0,9.0531802967,2.5001122718,0.1403495627  
H,0,9.455022445,0.9604909574,-0.6671184236  
I,0,-0.3045181518,-0.8919048179,-0.9996571185

Sum of electronic and zero-point Energies= -2008.824770  
Sum of electronic and thermal Energies= -2008.798245  
Sum of electronic and thermal Enthalpies= -2008.797300  
Sum of electronic and thermal Free Energies= -2008.888388

## I<sub>2</sub>

I,0,-3.4849097846,0.,0.

I,0,-0.7928902154,0.,0.

Sum of electronic and zero-point Energies= -595.705908  
Sum of electronic and thermal Energies= -595.703004  
Sum of electronic and thermal Enthalpies= -595.702060  
Sum of electronic and thermal Free Energies= -595.731663

## FeTppCl (<sup>4</sup>A<sub>1</sub>)

C,0,0.6856119544,4.2251903407,-0.2730840905  
C,0,-0.6856119544,4.2251903407,-0.2730840905  
C,0,1.1013302965,2.8427509898,-0.239002152  
C,0,2.4311401417,2.4311401417,-0.2386090409  
C,0,-1.1013302965,2.8427509898,-0.239002152  
C,0,4.2251903407,0.6856119544,-0.2730840905  
N,0,0.,1.9978617397,-0.2205513667  
C,0,2.8427509898,1.1013302965,-0.239002152  
C,0,-2.4311401417,2.4311401417,-0.2386090409  
C,0,4.2251903407,-0.6856119544,-0.2730840905  
N,0,1.9978617397,0.,-0.2205513667  
C,0,-2.8427509898,1.1013302965,-0.239002152  
C,0,-4.2251903407,0.6856119544,-0.2730840905  
C,0,2.8427509898,-1.1013302965,-0.239002152  
N,0,-1.9978617397,0.,-0.2205513667  
Fe,0,0.,0.,0.0759414223  
C,0,-4.2251903407,-0.6856119544,-0.2730840905  
C,0,2.4311401417,-2.4311401417,-0.2386090409  
C,0,-2.8427509898,-1.1013302965,-0.239002152  
N,0,0.,-1.9978617397,-0.2205513667  
C,0,1.1013302965,-2.8427509898,-0.239002152  
C,0,-2.4311401417,-2.4311401417,-0.2386090409  
C,0,-1.1013302965,-2.8427509898,-0.239002152  
C,0,0.6856119544,-4.2251903407,-0.2730840905  
C,0,-0.6856119544,-4.2251903407,-0.2730840905  
Cl,0,0.,0.,2.3357262546  
H,0,1.3685253834,5.0750236903,-0.2971023366  
H,0,-1.3685253834,5.0750236903,-0.2971023366  
H,0,3.2043846097,3.2043846097,-0.251444362  
H,0,5.0750236903,1.3685253834,-0.2971023366  
H,0,-3.2043846097,3.2043846097,-0.251444362  
H,0,5.0750236903,-1.3685253834,-0.2971023366  
H,0,-5.0750236903,1.3685253834,-0.2971023366  
H,0,-5.0750236903,-1.3685253834,-0.2971023366  
H,0,3.2043846097,-3.2043846097,-0.251444362  
H,0,-3.2043846097,-3.2043846097,-0.251444362  
H,0,1.3685253834,-5.0750236903,-0.2971023366  
H,0,-1.3685253834,-5.0750236903,-0.2971023366

Sum of electronic and zero-point Energies= -2712.402623  
Sum of electronic and thermal Energies= -2712.382807  
Sum of electronic and thermal Enthalpies= -2712.381863  
Sum of electronic and thermal Free Energies= -2712.450018

## FeTppCl (<sup>6</sup>A<sub>2</sub>)

C,0,0.6867108308,4.2567135319,-0.2939560762  
C,0,-0.6867108308,4.2567135319,-0.2939560762  
C,0,1.1067285493,2.8719238154,-0.2338245905  
C,0,2.4379681715,2.4379681715,-0.2402622626

C,0,-1.1067285493,2.8719238154,-0.2338245905  
C,0,4.2567135319,0.6867108308,-0.2939560762  
N,0,0.,2.0395351297,-0.193917083  
C,0,2.8719238154,1.1067285493,-0.2338245905  
C,0,-2.4379681715,2.4379681715,-0.2402622626  
C,0,4.2567135319,-0.6867108308,-0.2939560762  
N,0,2.0395351297,0.,-0.193917083  
C,0,-2.8719238154,1.1067285493,-0.2338245905  
C,0,-4.2567135319,0.6867108308,-0.2939560762  
C,0,2.8719238154,-1.1067285493,-0.2338245905  
N,0,-2.0395351297,0.,-0.193917083  
Fe,0,0.,0.,0.3158136252  
C,0,-4.2567135319,-0.6867108308,-0.2939560762  
C,0,2.4379681715,-2.4379681715,-0.2402622626  
C,0,-2.8719238154,-1.1067285493,-0.2338245905  
N,0,0.,-2.0395351297,-0.193917083  
C,0,1.1067285493,-2.8719238154,-0.2338245905  
C,0,-2.4379681715,-2.4379681715,-0.2402622626  
C,0,-1.1067285493,-2.8719238154,-0.2338245905  
C,0,0.6867108308,-4.2567135319,-0.2939560762  
C,0,-0.6867108308,-4.2567135319,-0.2939560762  
Cl,0,0.,0.,2.535088517  
H,0,1.3632790509,5.1111109792,-0.3374191197  
H,0,-1.3632790509,5.1111109792,-0.3374191197  
H,0,3.2114798955,3.2114798955,-0.2742115586  
H,0,5.1111109792,1.3632790509,-0.3374191197  
H,0,-3.2114798955,3.2114798955,-0.2742115586  
H,0,5.1111109792,-1.3632790509,-0.3374191197  
H,0,-5.1111109792,1.3632790509,-0.3374191197  
H,0,-5.1111109792,-1.3632790509,-0.3374191197  
H,0,3.2114798955,-3.2114798955,-0.2742115586  
H,0,-3.2114798955,-3.2114798955,-0.2742115586  
H,0,1.3632790509,-5.1111109792,-0.3374191197  
H,0,-1.3632790509,-5.1111109792,-0.3374191197

Sum of electronic and zero-point Energies= -2712.389434  
Sum of electronic and thermal Energies= -2712.369234  
Sum of electronic and thermal Enthalpies= -2712.368289  
Sum of electronic and thermal Free Energies= -2712.437610

### FeTppCl( $\kappa^1$ -O(H)OH) ( $^4A$ ) FeTppCl( $\kappa^1$ -O(H)OH) ( $^6A$ )

C,0,2.7541314955,3.3467487921,-0.0778535052  
C,0,1.5686352074,4.036325064,-0.0786806614  
C,0,2.4187374084,1.9412940566,-0.0503748023  
C,0,3.3592361729,0.9132887688,-0.0388343945  
C,0,0.5130090259,3.0493294528,-0.0569268711  
C,0,4.0395860886,-1.4984719896,0.0012059148  
N,0,1.0439025736,1.7685744675,-0.0391559939  
C,0,3.0497228,-0.4447596131,-0.0061477137  
C,0,-0.8463520567,3.3575882197,-0.0818653095  
C,0,3.3532655583,-2.6840405265,0.0490910655  
N,0,1.7711441604,-0.9763133852,0.0305766614  
C,0,-1.8723699684,2.4140838713,-0.1104194016  
C,0,-3.2774975245,2.7424272943,-0.1653015659  
C,0,1.946376896,-2.3503310103,0.0646215895  
N,0,-1.6932036996,1.0367465556,-0.1020261206  
Fe,0,0.0409926265,0.0367231632,0.2059135142  
C,0,-3.9618999006,1.5532450016,-0.1818357331  
C,0,0.9242360881,-3.2980544046,0.0973727008  
C,0,-2.9738100204,0.5009092479,-0.1340210917  
N,0,-0.9657835822,-1.7144685703,-0.0544934435

C,0,-0.4355984253,-2.9986269506,0.0544208424  
C,0,-3.2848894128,-0.8581303197,-0.1035714818  
C,0,-2.3487063043,-1.8882441229,-0.0445276835  
C,0,-1.4924516577,-3.9781398103,0.0982031777  
C,0,-2.679449888,-3.2893039289,0.0346044786  
Cl,0,-0.0436570119,0.0592085155,2.4756777533  
H,0,3.7712494568,3.7395819237,-0.0944941388  
H,0,1.4069009517,5.1146078573,-0.0973229562  
H,0,4.4165456286,1.1924137754,-0.0562982448  
H,0,5.1172556742,-1.3345568376,-0.0275486858  
H,0,-1.1278464554,4.4143648435,-0.0919257523  
H,0,3.7475214131,-3.7005763709,0.0665842955  
H,0,-3.6750544163,3.7576356723,-0.1873228531  
H,0,-5.0391806255,1.3880396657,-0.2190660735  
H,0,1.2107406773,-4.3519824663,0.1532306697  
H,0,-4.342839029,-1.135208539,-0.1108354265  
H,0,-1.3349069102,-5.0548047907,0.1696145443  
H,0,-3.6955806111,-3.6849706865,0.0443353042  
O,0,0.1250298644,0.1220603394,-2.4744082954  
O,0,-0.6593903564,-1.0318086378,-2.9463965939  
H,0,-0.7787833767,-1.4902454336,-2.0759471968  
H,0,-0.5760136646,0.810535466,-2.4412876614

Sum of electronic and zero-point Energies= -2863.933944  
Sum of electronic and thermal Energies= -2863.909613  
Sum of electronic and thermal Enthalpies= -2863.908669  
Sum of electronic and thermal Free Energies= -2863.988907

### FeTppCl( $\kappa^1$ -O(H)OH) ( $^6A$ )

C,0,4.3130912127,0.66793117,0.1713905007  
C,0,4.3086261265,-0.7060637587,0.146381771  
C,0,2.9298203098,1.0965270825,0.1126251512  
C,0,2.4969490832,2.4302176986,0.1345448057  
C,0,2.9219403593,-1.1213047564,0.0755053188  
C,0,0.7599214575,4.2701913435,0.1701414385  
N,0,2.0998553974,-0.0086572104,0.0483496565  
C,0,1.169269708,2.8803000367,0.1054645128  
C,0,2.4722713648,-2.4502752035,0.071631083  
C,0,-0.6126485103,4.2844579499,0.1239446553  
N,0,0.0551526549,2.0670874791,0.0188430806  
C,0,1.1356524867,-2.8767470842,0.0636644084  
C,0,0.6996265145,-4.2578607328,0.071828794  
C,0,-1.0450633917,2.9028214255,0.0358280494  
N,0,0.0332181193,-2.0351637592,0.0547439353  
Fe,0,0.0605321278,0.0247200173,-0.389157521  
C,0,-0.6747238641,-4.2439038651,0.0568441758  
C,0,-2.3812974258,2.4776423062,-0.0113421476  
C,0,-1.0841463884,-2.8545328361,0.0414576198  
N,0,-2.0099416454,0.0315227414,0.0482013936  
C,0,-2.8329689736,1.1505863003,-0.0300617737  
C,0,-2.4139891177,-2.408872325,-0.0020032566  
C,0,-2.8483744209,-1.0762467422,-0.0248733739  
C,0,-4.2147362738,0.7343885361,-0.1217030133  
C,0,-4.2242414755,-0.6417693356,-0.1190670709  
Cl,0,0.0367578886,-0.0036759647,-2.6161062226  
H,0,5.1712138644,1.3386772594,0.228983665  
H,0,5.1618835302,-1.3845351203,0.1814744396  
H,0,3.2747621269,3.1978823117,0.1953867158  
H,0,1.4419481177,5.118033432,0.2445347922  
H,0,3.2388349488,-3.2312164667,0.0894065093  
H,0,-1.2806515723,5.1460087297,0.1561258405  
H,0,1.365476481,-5.1216425209,0.0839446781

H,0,-1.3575025437,-5.0944813885,0.055609402  
H,0,-3.1474239665,3.2589345434,-0.0316467883  
H,0,-3.1898669495,-3.1799896399,-0.0360916953  
H,0,-5.0666243733,1.4126223875,-0.1842298851  
H,0,-5.0854782506,-1.3084366987,-0.1779429427  
O,0,0.1852857586,-0.0028193543,2.376462095  
O,0,-1.1878800233,-0.2078078655,2.8631241958  
H,0,-1.6667569872,-0.0404773776,2.0104470807  
H,0,0.464019515,-0.9357237447,2.2359569264

Sum of electronic and zero-point Energies= -2863.920233  
Sum of electronic and thermal Energies= -2863.895644  
Sum of electronic and thermal Enthalpies= -2863.894700  
Sum of electronic and thermal Free Energies= -2863.975582

### [FeTppCl(O)]<sup>-</sup> (<sup>3</sup>A<sub>1</sub>)

C,0,0.6853279239,4.2447502106,-0.1244609117  
C,0,-0.6853279239,4.2447502106,-0.1244609117  
C,0,1.0998057632,2.8531194782,-0.1283495084  
C,0,2.4308334602,2.4308334602,-0.12992076  
C,0,-1.0998057632,2.8531194782,-0.1283495084  
C,0,4.2447502106,0.6853279239,-0.1244609117  
N,0,0.,2.0244217629,-0.1279015121  
C,0,2.8531194782,1.0998057632,-0.1283495084  
C,0,-2.4308334602,2.4308334602,-0.12992076  
C,0,4.2447502106,-0.6853279239,-0.1244609117  
N,0,2.0244217629,0.,-0.1279015121  
C,0,-2.8531194782,1.0998057632,-0.1283495084  
C,0,-4.2447502106,0.6853279239,-0.1244609117  
C,0,2.8531194782,-1.0998057632,-0.1283495084  
N,0,-2.0244217629,0.,-0.1279015121  
Fe,0,0.,0.,-0.1908243959  
C,0,-4.2447502106,-0.6853279239,-0.1244609117  
C,0,2.4308334602,-2.4308334602,-0.12992076  
C,0,-2.8531194782,-1.0998057632,-0.1283495084  
N,0,0.,-2.0244217629,-0.1279015121  
C,0,1.0998057632,-2.8531194782,-0.1283495084  
C,0,-2.4308334602,-2.4308334602,-0.12992076  
C,0,-1.0998057632,-2.8531194782,-0.1283495084  
C,0,0.6853279239,-4.2447502106,-0.1244609117  
C,0,-0.6853279239,-4.2447502106,-0.1244609117  
Cl,0,0.,0.,2.2103057305  
H,0,1.3698193705,5.0951927558,-0.1191395958  
H,0,-1.3698193705,5.0951927558,-0.1191395958  
H,0,3.205242597,3.205242597,-0.1286656222  
H,0,5.0951927558,1.3698193705,-0.1191395958  
H,0,-3.205242597,3.205242597,-0.1286656222  
H,0,5.0951927558,-1.3698193705,-0.1191395958  
H,0,-5.0951927558,1.3698193705,-0.1191395958  
H,0,-5.0951927558,-1.3698193705,-0.1191395958  
H,0,3.205242597,-3.205242597,-0.1286656222  
H,0,-3.205242597,-3.205242597,-0.1286656222  
H,0,1.3698193705,-5.0951927558,-0.1191395958  
H,0,-1.3698193705,-5.0951927558,-0.1191395958  
O,0,0.,0.,-1.8554049806

Sum of electronic and zero-point Energies= -2787.674544  
Sum of electronic and thermal Energies= -2787.653686  
Sum of electronic and thermal Enthalpies= -2787.652742  
Sum of electronic and thermal Free Energies= -2787.721869

### [FeTppCl(O)]<sup>-</sup> (<sup>5</sup>A<sub>2</sub>)

C,0,-0.6872194776,4.2922775831,0.1147622604  
C,0,0.6872194776,4.2922775831,0.1147622604  
C,0,-1.1096095059,2.896590146,0.1095891167  
C,0,-2.4432309173,2.4432309173,0.1113867967  
C,0,1.1096095059,2.896590146,0.1095891167  
C,0,-4.2922775831,0.6872194776,0.1147622604  
N,0,0.,2.089818154,0.1026574691  
C,0,-2.896590146,1.1096095059,0.1095891167  
C,0,2.4432309173,2.4432309173,0.1113867967  
C,0,-4.2922775831,-0.6872194776,0.1147622604  
N,0,-2.089818154,0.,0.1026574691  
C,0,2.896590146,1.1096095059,0.1095891167  
C,0,4.2922775831,0.6872194776,0.1147622604  
C,0,-2.896590146,-1.1096095059,0.1095891167  
N,0,2.089818154,0.,0.1026574691  
Fe,0,0.,0.,0.1880280516  
C,0,4.2922775831,-0.6872194776,0.1147622604  
C,0,-2.4432309173,-2.4432309173,0.1113867967  
C,0,2.896590146,-1.1096095059,0.1095891167  
N,0,0.,-2.089818154,0.1026574691  
C,0,-1.1096095059,-2.896590146,0.1095891167  
C,0,2.4432309173,-2.4432309173,0.1113867967  
C,0,1.1096095059,-2.896590146,0.1095891167  
C,0,-0.6872194776,-4.2922775831,0.1147622604  
C,0,0.6872194776,-4.2922775831,0.1147622604  
Cl,0,0.,0.,-2.1929955439  
H,0,-1.3613900179,5.1514740343,0.1156998729  
H,0,1.3613900179,5.1514740343,0.1156998729  
H,0,-3.2183547321,3.2183547321,0.1159119877  
H,0,-5.1514740343,1.3613900179,0.1156998729  
H,0,3.2183547321,3.2183547321,0.1159119877  
H,0,-5.1514740343,-1.3613900179,0.1156998729  
H,0,5.1514740343,1.3613900179,0.1156998729  
H,0,5.1514740343,-1.3613900179,0.1156998729  
H,0,-3.2183547321,-3.2183547321,0.1159119877  
H,0,3.2183547321,-3.2183547321,0.1159119877  
H,0,-1.3613900179,-5.1514740343,0.1156998729  
H,0,1.3613900179,-5.1514740343,0.1156998729  
O,0,0.,0.,1.8487900824

Sum of electronic and zero-point Energies= -2787.644636  
Sum of electronic and thermal Energies= -2787.623158  
Sum of electronic and thermal Enthalpies= -2787.622214  
Sum of electronic and thermal Free Energies= -2787.693382

### [FeTppCl(OD)]<sup>-</sup> (<sup>4</sup>A)

C,0,-0.6047994655,4.3628433609,-0.7203456175  
C,0,0.5973500368,4.1403446797,-1.3398655361  
C,0,-1.1360670866,3.0605315202,-0.3653853626  
C,0,-2.3542389751,2.8578736678,0.2847600409  
C,0,0.7957476584,2.7034582036,-1.3600417971  
C,0,-4.1572680733,1.4232350852,1.2894112682  
N,0,-0.2717262882,2.0647488789,-0.764219225  
C,0,-2.8820888899,1.6124008475,0.6264176382  
C,0,1.9146523276,2.0761594671,-1.9091101204  
C,0,-4.3259986389,0.0710178173,1.4396585424  
N,0,-2.2840542224,0.3935913275,0.379198537  
C,0,2.1328786812,0.6975924929,-1.9374989985  
C,0,3.3085244093,0.0656515556,-2.508013132  
C,0,-3.1528110728,-0.5609352097,0.8690893778  
N,0,1.2750769432,-0.2537765488,-1.4357979964

Fe,0,-0.4898073537,0.0742426076,-0.4813180156  
C,0,3.148502603,-1.2845462216,-2.3382470173  
C,0,-2.9502241728,-1.9404548907,0.8262716753  
C,0,1.8751815781,-1.4706570756,-1.6669354563  
N,0,-0.7583327344,-1.9263222736,-0.2944268201  
C,0,-1.8291726691,-2.5701360639,0.2828982949  
C,0,1.3423528014,-2.7134038237,-1.3207294337  
C,0,0.1163369916,-2.9171450919,-0.6859191292  
C,0,-1.6315073349,-4.0073526827,0.2520422546  
C,0,-0.4193806222,-4.2230321372,-0.349784924  
Cl,0,-1.5240674892,-0.0671219346,-2.5875744883  
H,0,-1.1022726659,5.3117485436,-0.5126716492  
H,0,1.3003556007,4.8672625956,-1.7502961073  
H,0,-2.9426319045,3.7438967295,0.5440258142  
H,0,-4.8235050572,2.2333160335,1.5910888789  
H,0,2.6862435647,2.7174022152,-2.3472360206  
H,0,-5.1602343637,-0.4682285163,1.8918002848  
H,0,4.1387455075,0.6038872544,-2.9684277691  
H,0,3.8188251697,-2.0948810935,-2.6295179516  
H,0,-3.730121243,-2.5781575612,1.254799439  
H,0,1.9338339971,-3.6007486454,-1.5678889192  
H,0,-2.3385206126,-4.7381998204,0.6482612432  
H,0,0.0838010418,-5.1694058298,-0.554969282  
O,0,0.3445074902,0.1360114627,1.0136210288  
I,0,2.1438405334,-0.1424349255,2.5880644508

Sum of electronic and zero-point Energies= -3085.521816  
Sum of electronic and thermal Energies= -3085.499406  
Sum of electronic and thermal Enthalpies= -3085.498462  
Sum of electronic and thermal Free Energies= -3085.574697

### [FeTppCl(OD)]<sup>-</sup> (<sup>6</sup>A)

C,0,-0.5970741572,4.4193762919,-0.7255609209  
C,0,0.6143849821,4.1949993871,-1.3365299909  
C,0,-1.1407946551,3.1140447979,-0.3727518851  
C,0,-2.3690431296,2.8761397038,0.2763893533  
C,0,0.8172353747,2.75194572,-1.3595179454  
C,0,-4.1953297287,1.4348485862,1.3178375859  
N,0,-0.2632615895,2.1378105918,-0.771877591  
C,0,-2.9234866016,1.631984341,0.6372141753  
C,0,1.9393451097,2.0891070964,-1.8958657536  
C,0,-4.3575041444,0.0784175199,1.4794471479  
N,0,-2.3449735552,0.4070512852,0.4003250229  
C,0,2.1887157374,0.7012809459,-1.9397631185  
C,0,3.3570278473,0.0612751459,-2.5324293693  
C,0,-3.1862729748,-0.5617301994,0.8982912793  
N,0,1.354294105,-0.2638479888,-1.4376768294  
Fe,0,-0.5015438881,0.0772598713,-0.5054833023  
C,0,3.1929839902,-1.2946298726,-2.3721432313  
C,0,-2.9503770252,-1.9495610949,0.8487866069  
C,0,1.9232834758,-1.4880546941,-1.6821295566  
N,0,-0.7624329301,-1.9964530657,-0.285807463  
C,0,-1.8333225365,-2.6163432709,0.3041559157  
C,0,1.3548086918,-2.7294821429,-1.3290221064  
C,0,0.1229911639,-2.9673205971,-0.6857112481  
C,0,-1.6271110263,-4.0593719009,0.2763763808  
C,0,-0.4159666718,-4.2764300385,-0.3375673915  
Cl,0,-1.4868705019,-0.0888224679,-2.68177551  
H,0,-1.08451232,5.3763696836,-0.5281648544  
H,0,1.3135280878,4.9326195785,-1.7360114759  
H,0,-2.9606872572,3.7619800393,0.5348222377  
H,0,-4.8700324164,2.2349075957,1.6294446869

H,0,2.7111996611,2.7309875427,-2.3362614321  
H,0,-5.1907509524,-0.4483300218,1.9492803873  
H,0,4.1879789288,0.5870951824,-3.0072942179  
H,0,3.8625030776,-2.0959680683,-2.691329824  
H,0,-3.7259741293,-2.5864257495,1.289820139  
H,0,1.9405707297,-3.6186297803,-1.5896682335  
H,0,-2.3216637832,-4.8010706071,0.6761738306  
H,0,0.0761634903,-5.2306333418,-0.5368050292  
O,0,0.3441507082,0.1576418143,1.1667452633  
I,0,1.8957468133,-0.1937618184,2.3772262675

Sum of electronic and zero-point Energies= -3085.497653  
Sum of electronic and thermal Energies= -3085.473549  
Sum of electronic and thermal Enthalpies= -3085.472605  
Sum of electronic and thermal Free Energies= -3085.553740

### FeTpp(OI) (<sup>4</sup>A)

C,0,2.4333927603,3.4384606307,-0.2798006591  
C,0,3.4178134309,2.4855095153,-0.2430079866  
C,0,1.1715902751,2.7344479273,-0.2309588196  
C,0,-0.0713187419,3.3623077649,-0.2573891763  
C,0,2.7531594988,1.2038233791,-0.169974513  
C,0,-2.5738847252,3.3558973619,-0.3186771445  
N,0,1.375235164,1.3642886644,-0.1698029165  
C,0,-1.2931138626,2.6950478117,-0.241250624  
C,0,3.4193820606,-0.0173398054,-0.1136283072  
C,0,-3.5289883418,2.3716120832,-0.2956538825  
N,0,-1.4537696365,1.3158392305,-0.1713524714  
C,0,2.7895451623,-1.2584928272,-0.0599142368  
C,0,3.4931000205,-2.5193520884,-0.0157792432  
C,0,-2.8282853346,1.1130142675,-0.2043264896  
N,0,1.4174527243,-1.4614219117,-0.0514206921  
Fe,0,-0.0221234107,-0.0640764011,0.1459796553  
C,0,2.5384204798,-3.502896059,0.0268526753  
C,0,-3.4582732143,-0.1284647807,-0.1755696778  
C,0,1.2563188145,-2.8382942742,0.0052017205  
N,0,-1.4137078497,-1.5072849002,-0.0782347783  
C,0,-2.7913356967,-1.3498335341,-0.124582546  
C,0,0.0334048629,-3.5056265103,0.0197074221  
C,0,-1.2088062731,-2.8801764789,-0.0314673108  
C,0,-3.4538756868,-2.6344735029,-0.1176835411  
C,0,-2.4693919598,-3.5862595142,-0.0581412431  
H,0,2.5340989547,4.5227209664,-0.338365282  
H,0,4.4997700783,2.620203076,-0.2643506009  
H,0,-0.0891258456,4.4546415272,-0.30913942  
H,0,-2.7088019402,4.435892317,-0.3870546145  
H,0,4.5130151464,-0.0018677833,-0.1163295731  
H,0,-4.6138560668,2.4726232509,-0.3415703501  
H,0,4.578832831,-2.6215647918,-0.0176159795  
H,0,2.673547429,-4.5843229969,0.0652102209  
H,0,-4.5513636155,-0.1455482613,-0.2065155018  
H,0,0.0515271901,-4.5984810257,0.0608523136  
H,0,-4.5350085553,-2.7720925108,-0.1557421236  
H,0,-2.5700096348,-4.6718995502,-0.0366472102  
O,0,0.0471170924,-0.0384421447,1.9759893829  
I,0,-0.9258835819,0.4789818791,3.6298535235

Sum of electronic and zero-point Energies= -2625.196748  
Sum of electronic and thermal Energies= -2625.175175  
Sum of electronic and thermal Enthalpies= -2625.174231  
Sum of electronic and thermal Free Energies= -2625.249521



## FeTpp(OI) ( $^6A$ )

C,0,-1.231286286,-4.2462486723,-0.6672901384  
C,0,-2.4714344312,-3.7814123282,-0.3039496008  
C,0,-0.3832042277,-3.0840840489,-0.8463719537  
C,0,0.9614422789,-3.1220311922,-1.2408280582  
C,0,-2.382460481,-2.3349596882,-0.2620908366  
C,0,3.1560125938,-2.0887449665,-1.9471136614  
N,0,-1.1017417266,-1.9291050507,-0.594815895  
C,0,1.7914154287,-2.0164957405,-1.4675965316  
C,0,-3.4428754127,-1.4727489801,0.04698107  
C,0,3.6037573457,-0.7962305233,-2.0758605659  
N,0,1.4183774908,-0.6914544033,-1.2972519786  
C,0,-3.4007925425,-0.0715639776,0.0457748978  
C,0,-4.5250554003,0.7941332468,0.341517552  
C,0,2.5141592748,0.0693213855,-1.67434983  
N,0,-2.2842541387,0.6882586034,-0.2552711697  
Fe,0,-0.3022369931,-0.0031435125,-0.3246215072  
C,0,-4.0757063842,2.0864044547,0.218539626  
C,0,2.5520608671,1.4697939011,-1.6926792568  
C,0,-2.6766536079,2.0112168462,-0.1525252641  
N,0,0.2351158302,1.924138685,-0.9695679651  
C,0,1.4931823519,2.3319519767,-1.3770958016  
C,0,-1.8494963576,3.1176127043,-0.3928236232  
C,0,-0.5050158066,3.0801741306,-0.7844170865  
C,0,1.5476183912,3.7789297598,-1.4485775257  
C,0,0.308626826,4.2428315737,-1.0800186536  
H,0,-0.9121459407,-5.2793800897,-0.8106389946  
H,0,-3.3731616668,-4.3568739293,-0.0905918552  
H,0,1.398635191,-4.1106982665,-1.4122161508  
H,0,3.6911452843,-3.013778243,-2.1655778237  
H,0,-4.400962693,-1.9378712202,0.299517831  
H,0,4.5792137176,-0.4506974936,-2.4205929077  
H,0,-5.5258753521,0.4489146054,0.6040896298  
H,0,-4.634219221,3.0126459961,0.3597151207  
H,0,3.49177284,1.9345317912,-2.0071561286  
H,0,-2.3034011264,4.1070751489,-0.2786957454  
H,0,2.4233839778,4.3557215017,-1.7488484887  
H,0,-0.0351985234,5.276217737,-1.019184867  
O,0,0.0942495096,0.0360859068,1.4530015599  
I,0,1.49520912,0.1471623716,2.8367825781

Sum of electronic and zero-point Energies=	-2625.181980
Sum of electronic and thermal Energies=	-2625.160002
Sum of electronic and thermal Enthalpies=	-2625.159058
Sum of electronic and thermal Free Energies=	-2625.235751