Supplementary Information

H_2 Oxidation versus Organic Substrate Oxidation in Non-Heme Iron Mediated Reactions with H_2O_2

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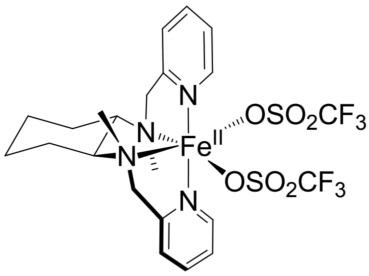
Materials and methods: All reagents were purchased from Aldrich and used as received unless noted otherwise. High purity deuterium and hydrogen gases were purchased from Linde and Air Liquide respectively. Iron(II) complex [(α-BPMCN)Fe(OTf)$_2$] (BPMCN =N,N'-bis(2-pyridylmethyl)-1,2-diaminocyclohexane, OTF = trifluoromethanesulfonate anion) was synthesized by procedures reported elsewhere.[1] CH_3CN solvent was distilled over CaH_2 before use. GC product analyses were performed on a CP-3800 Varian gas chromatograph (AT-1701 column, 30 m) with a flame ionization detector. The products were identified by comparison of their GC retention times. ^{2}D-NMR spectra were carried out on a Bruker DRX-500 spectrometer on CH_3CN solutions. Natural deuterium content of acetonitrile solvent served as internal standard. Quantification of deuterium content in CH_3CN was determined by calibration with controlled amounts of D_2O (0.1 mM, 1 mM and 10 mM).



Molecular structure of iron(II) complex [Fe(CF_3SO_3)$_2$(BPMCN)]

Reaction conditions for catalytic oxidation of organic substrates at ambient pressure. In a typical catalysis experiment, a total of 0.29 mL of a 70 mM H_2O_2 solution (diluted from a 35% H_2O_2 solution) in CH_3CN was delivered by syringe pump over 30 min at 25 °C in air to a CH_3CN solution (2.0 mL) containing iron 1 mM catalyst and 1M organic substrate. In various experiments, acetic acid (1.5 M) was added to the initial solution. The solution was stirred for another 10 min after syringe pump addition was complete.

After this procedure, naphthalene (1mM) as an internal standard was added to the solution. When methyl phenyl sulfide was used as substrate, the solution was passed through a silica column and directly injected to a gas chromatograph.

When cyclohexane or cyclooctene were used as substrate, an aditional work up was carried out. Thus, the resulting solutions were treated with acetic anhydride (1 mL) together with 1-methylimidazole (0.1 mL) to esterify the diol or alcohol products.

Organic products were extracted with $CHCl_3$ and the solution was subjected to GC analysis. All experiments were run at least in triplictae, the reported data being the average of these reactions.

Catalytic reactions were carried out under an argon or H_2 atmosphere. For argon atmosphere experiments the solutions containing the iron catalyst and the organic substrate were subjected to three succesive frezze-vacuum-argon cycles. Analogously, for H_2 atmosphere reactions also three succesive frezze-vacuum-H_2 cycles were executed to replace air by H_2. In adition, catalytic reactions under a H_2 atmosphere were performed while bubling a controled flow of H_2 (200 cm^3 per minute) to the reaction flask.

The possible evaporation caused by the H_2 flow was analyzed by means of Gas Chromatography measurements that allowed comparing the amount of organic substrate before and after oxidation runs. In all cases the amount detected of substrate indicates that there is no significant loss of reactant during the reaction. The substrate (cyclohexane) is more volatile than the product, and thus is neither expected significant product loss. In fact, H_2 flow does not imply bubbling and is comparable to Ar flow usual in schlenck systems. Therefore, for experiments in presence of H_2 we performed a degasification process using H_2 instead of an inert gas, and later we maintained a positive pressure of H_2 in a similar way how is done in regular anaerobic experiments.

Reaction conditions at controlled pressures of H_2 or D_2. In order to perform catalytic reactions at controlled pressures of H_2 or D_2, a magnetically stirred thermostated teflon-lined steel reactor was used (Berghof BR 100). Injection of H_2O_2 under high pressure conditions was achieved by using a 307 Gilson HPLC pump. Tube of the reactor was charged with dry acetonitrile as a solvent, iron complex (1 mM) and cyclohexane (1 M). H_2 pressure was set to 10, 8, 6 or 4 atmospheres and a solution of 10 equiv H_2O_2 (final concentration: 10 mM) was injected over a period of 30 min under pressure and stirring for 30 additional minutes.

Analogous experiments were made by using D_2 instead of H_2, or adding acetic acid (1.5M) to the reaction media.

After finishing the reaction, an estherification work up was carried out and products analyzed by GC.

Alternatively, reactions performed at 10 atm of D_2, in absence of cyclohexane were also carried out, and the reaction mixture analyzed directly by ^{2}D-NMR without further treatment. As a control reaction, a reaction was performed at 10 atm of D_2, in absence of cyclohexane and in absence of iron catalyst. The reaction mixture was also directly analyzed.

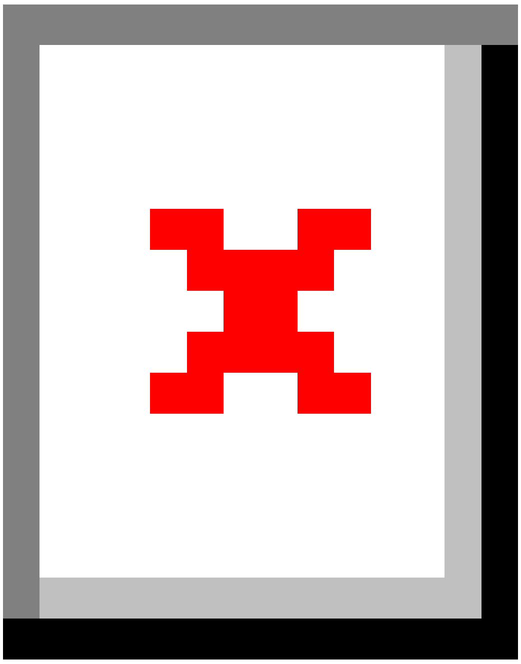


Figure SI.1. Replicate of the experiment shown in the main text: Reaction between α-[$Fe(CF_3SO_3)_2$(BPMCN)] 1mM in CH_3CN and 10 equivalents of H_2O_2, carried out at 10 atm of D_2, in absence of cyclohexane. The reaction mixture was analyzed directly by ^{2}D-NMR without further treatment (top). As a control reaction, a reaction run at 10 atm of D_2, in absence of cyclohexane and in absence of iron catalyst was performed, and the reaction mixture also directly analyzed (bottom).

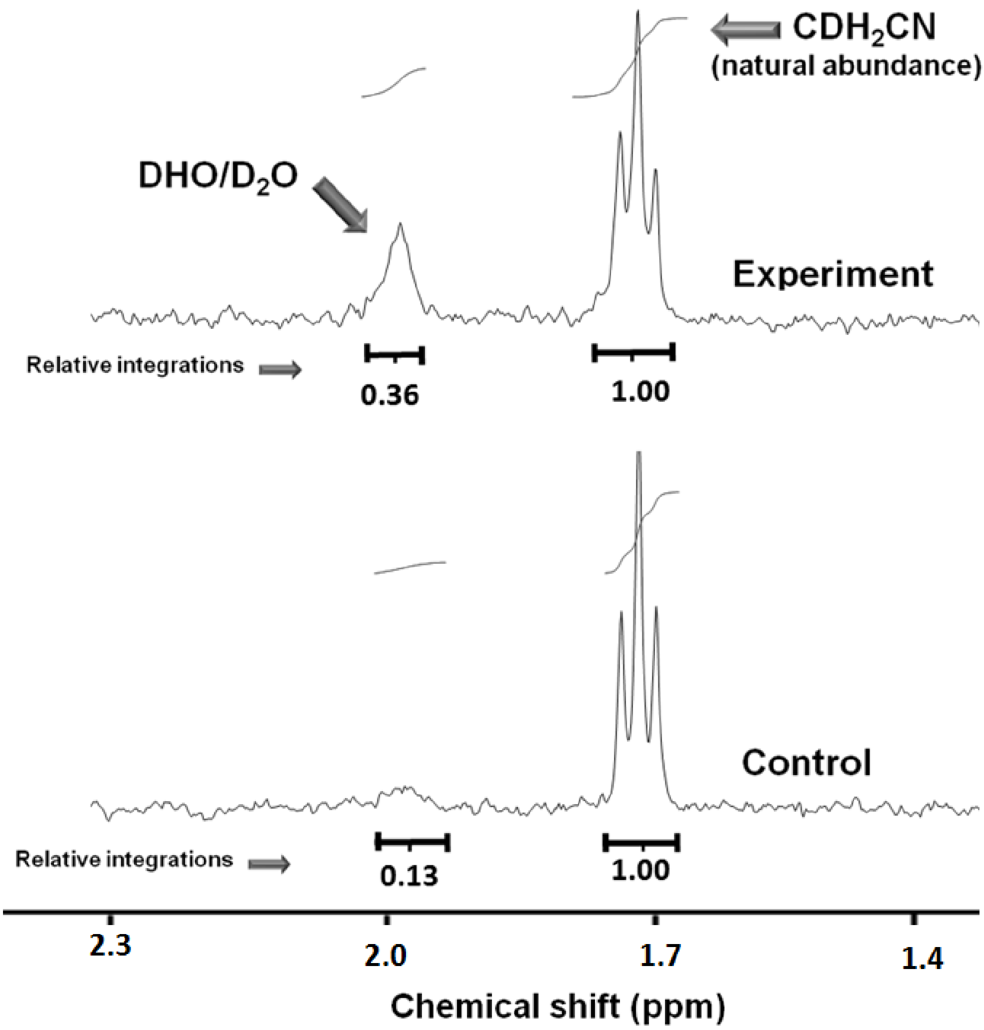


Figure SI.2. Reaction between α-[Fe(CF_3SO_3)$_2$(BPMCN)] 1mM in CH_3CN and 100 equivalents of H_2O_2, carried out at 10 atm of D_2, in absence of cyclohexane. The reaction mixture was analyzed directly by ^{2}D-NMR without further treatment (top). As a control reaction, reaction run at 10 atm of D_2, in absence of cyclohexane and in absence of iron catalyst was performed, and the reaction mixture also directly analyzed (down).

Control experiments.

Catalysis in absence of H_2O_2.

In order to check that air does not act as final oxidant, we performed control experiments using cyclohexane as a substrate in absence of H_2O_2 under an open (air) atmosphere. After 30 min of stirring, the sample was submitted to the workup procedure explained above. In such controls no oxidation products were detected by GC. It is worth to note that all experiments reported in the manuscript are done in absence of air, being degassed the reaction media in all the cases.

Catalytic reactions using iron(II) triflate as a catalyst

In order to check the catalytic activity of free iron cations that could potentially originate from catalyst decomposition, we performed control experiments using cyclohexane as a substrate, H_2O_2 as oxidant and $Fe(OTf)_2$ as catalyst, under the reaction conditions used in this work. In pure CH_3CN, 1.5 TON of cyclohexanone and 0.6 TON of cyclohexanol were detected. In CH_3CN/CH_3COOH 10:1, no oxidation products were detected. Thus, it is evident that catalytic results reported herein are not the result of catalyst decomposition.

Catalytic reactions at 10 atm of Ar.

In order to test if there is an effect of the pressure on the catalytic efficiency of the α-$[Fe(CF_3SO_3)_2(BPMCN)]/H_2O_2$ system, control experiments were performed using cyclohexane as a substrate and CH_3CN as solvent at 10 atm of argon. In such control experiments it is observed that the yield of cyclohexanol is reduced by 40% under 10 atm of Ar in comparison with the yield found at 1 atm of Argon (yields: 58% at 1 atm, 35% at 10 atm). It is worth to note that even though a significant effect of the pressure of an inert gas is observed, the effect of 10 atm of H_2 is the complete quenching of the reaction. Thus, the effect of different H_2 pressures is far beyond the decrease observed by adding pressure of an inert gas. Therefore, these results provide experimental evidence to conclude that H_2 is a competitive substrate.

Computational details

The density functional theory (DFT) study was carried out using the Gaussian09 software package[2] and the B3LYP hybrid exchange-correlation functional.[3] Optimizations were performed with the 6-31G(d,p) basis set for all atoms. Solvent effects were taken into account in geometry optimizations and energies ($G_{solv.}$ correction) through the SMD polarizable continuum model, with acetonitrile as implicit solvent.[4] Dispersion effects were also introduced with the Grimme-D_2 correction (G_{disp}).[5]

The energies were further refined by single-point calculations with the cc-pVTZ dunning basis set for all atoms. All calculations employed the spin-unrestricted formalism and spin-contaminated energies were systematically corrected ($E_{spin\ corr.}$) using the equations described in reference 6.

Thermal plus entropy corrections at 298.15 K were obtained from solvent phase frequency calculations at B3LYP/6-31G(d,p) level (G_{corr}). All calculated solvation free energies use a standard state liquid phase concentration of 1 mol·L^{-1}, but for acetonitrile itself a 19.1 M standard state was employed. The free energy change associated with moving from a standard-state gas phase pressure of 1 atm to a standard state gas phase concentration of 1 M (19.1 M for acetonitrile) was calculated. The value of $\Delta G^{o/*}$ at 298.15 K is 1.9 kcal·mol^{-1} for 1 M standard state solutes and 3.6 kcal·mol^{-1} for 19.1 M standard state acetonitrile.

The final free energy (G) was obtained by adding the previous corrections to the spin corrected potential energy $E_{spin\ corr.}$:

$$G = E_{spin\ corr.} + G_{solv..} + G_{corr.} + G_{disp.} + \Delta G^{o/*} \quad (1)$$

The nature of the located stationary points was established by frequency calculations in solvent phase, where transition states have only one imaginary frequency. Finally, the connectivity of all transition states respect to the associated minimums was confirmed through intrinsic reaction coordinate (IRC) calculations.[7]

Labels **I**, **TS** and **II** were used as short nomenclature of reactant complexes, transition states and products involved in the H-H bond breaking event. The **homo** and **heter** notations are related to the homolytic or heterolytic nature of the H-H bond cleavage. Labels **d**, **q** and **sext** are used to specify the doublet, quartet and sextuple spin state of the iron center.

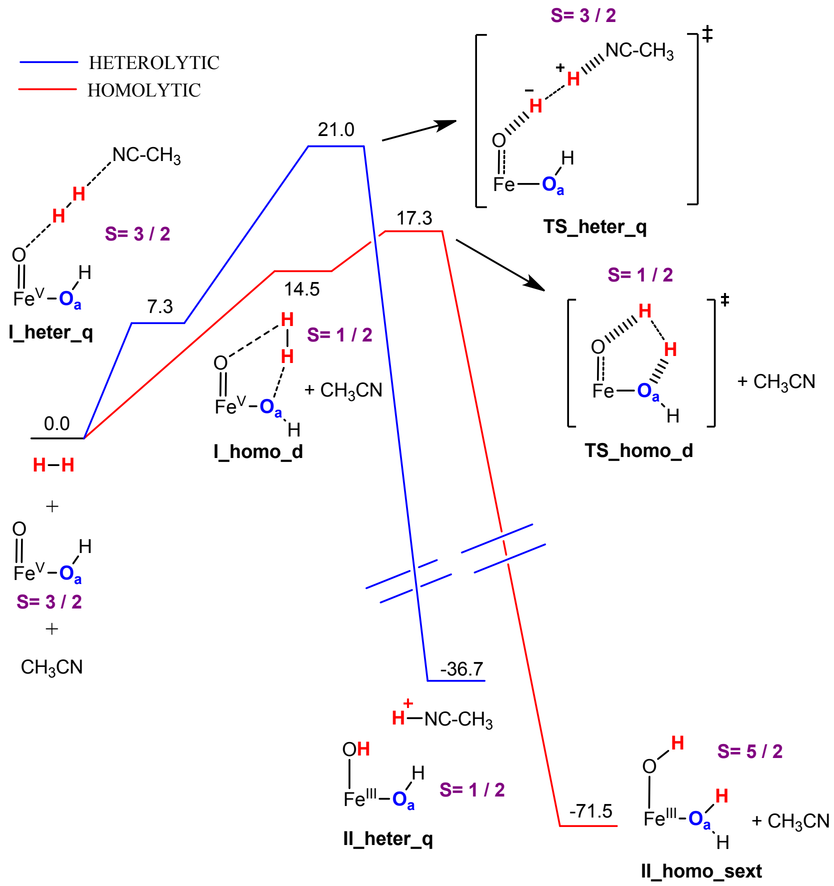


Figure SI.3. Homolytic *vs* heterolytic minimum free energy profiles for the H_2 oxidation by $[Fe^{V}(O)(OH)(BPMCN)]^{2+}$. All species are labeled with its ground spin state. Gibbs energy values are given in $kcal \cdot mol^{-1}$.

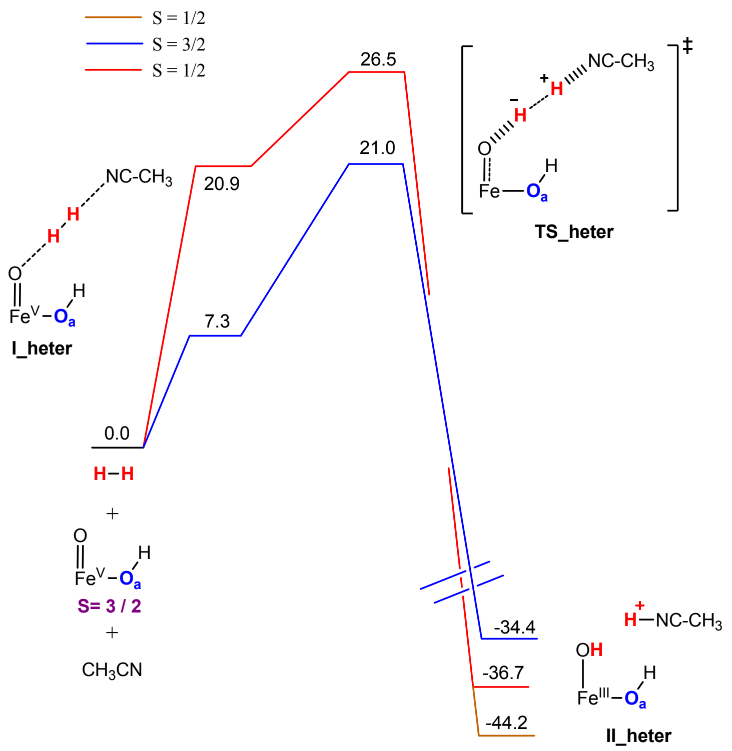


Figure SI.4. Heterolytic H_2 oxidation free energy profiles found for $[Fe^{V}(O)(OH)(BPMCN)]^{2+}$ in the S = 1/2 and 3/2 spin states. Gibbs energy values are given in kcal·mol^{-1}.

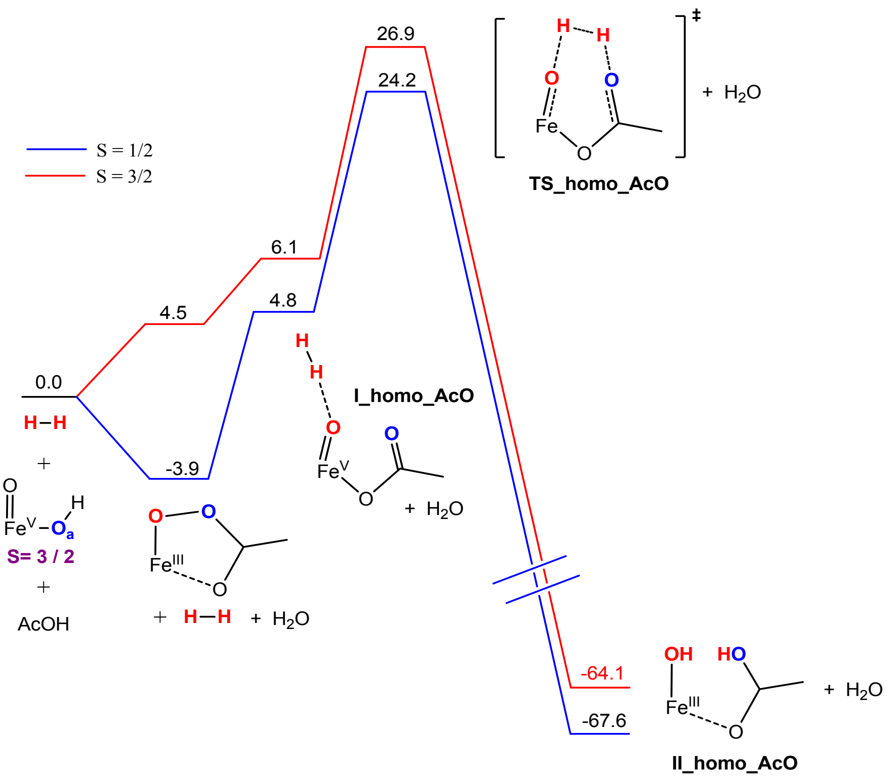
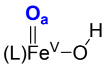
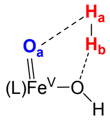
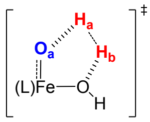
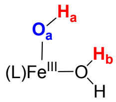


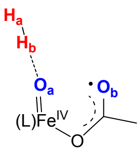
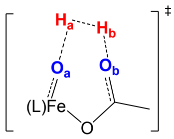
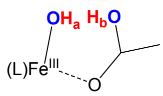
Figure SI.5. Homolytic H_2 oxidation free energy profiles found for $[Fe^{IV}(AcO\cdot)(BPMCN)]^{2+}$ in the S = 1/2 and 3/2 spin states. Gibbs energy values are given in kcal·mol^{-1}.

Table SI.1. Mulliken atomic spin populations, Fe-O_a and H_a-H_b bond distances for key species involved in the 2+3 homolytic H-H bond activation mechanism for $[Fe^{V}(O)(OH)(BPMCN)]^{2+}$ active species.

	 S = 3 / 2	 I_homo_d	 TS_homo_d	 II_homo_sext
ρ(Fe)[a]	2.13	0.77	1.48	4.24
ρ(O_a)[a]	0.85	0.42	-0.14	0.31
ρ(H_a)[a]	-	0.00	-0.03	0.01
ρ(H_b)[a]	-	0.00	-0.14	0.00
d(Fe-O_a)[b]	1.64	1.58	1.64	1.81
d(H_a-H_b)[b]	-	0.74	0.81	3.01

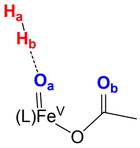
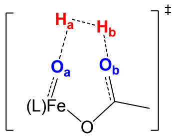
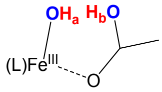
[a] All values are calculated at the B3LYP(SMD)/6-31G** level in acetonitrile as solvent. [b] Bond distances are in Å.

Table SI.2. Mulliken atomic spin populations, Fe-O_a and H_a-H_b bond distances for the S = 1/2 species involved in the 2+3 homolytic H-H bond activation mechanism for complex $[Fe^{IV}(O)(AcO\cdot)(BPMCN)]^{2+}$.

	 I_homo_AcO_d	 TS_homo_AcO_d	 II_homo_AcO_d
ρ(Fe)[a]	1.58	1.86	0.99
ρ(O_a)[a]	0.00	-0.46	0.09
ρ(O_b)[a]	-0.40	-0.05	0.00
ρ(H_a)[a]	0.00	-0.02	0.00
ρ(H_b)[a]	0.00	-0.13	0.00
d(Fe-O_a)[b]	1.63	1.68	1.81
d(H_a-H_b)[b]	0.74	0.78	2.31

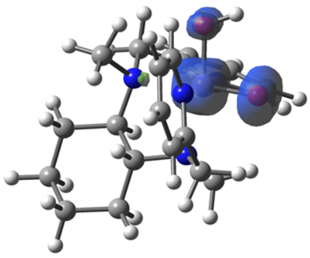
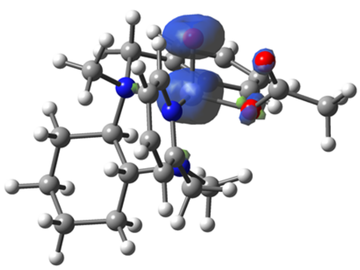
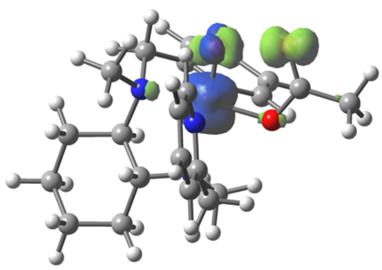
[a] All values are calculated at the B3LYP(SMD)/6-31G** level in acetonitrile as solvent. [b] Bond distances are in Å.

Table SI.3. Mulliken atomic spin populations, Fe-O_a and H_a-H_b bond distances for the S = 3/2 species involved in the 2+3 homolytic H-H bond activation mechanism for complex $[Fe^{IV}(O)(AcO\cdot)(BPMCN)]^{2+}$.

	 I_homo_AcO_q	 TS_homo_AcO_q	 II_homo_AcO_q
ρ(Fe)[a]	2.15	1.84	2.84
ρ(O_a)[a]	0.92	0.86	0.06
ρ(O_b)[a]	0.06	0.21	0.00
ρ(H_a)[a]	0.00	0.04	0.00
ρ(H_b)[a]	0.00	0.18	0.00
d(Fe-O_a)[b]	1.64	1.71	1.80
d(H_a-H_b)[b]	0.74	0.81	2.70

[a] All values are calculated at the B3LYP(SMD)/6-31G** level in acetonitrile as solvent. [b] Bond distances are in Å.

Table SI.4. Summary of the Mulliken atomic spin populations, for complex $[Fe^{V}(O)(OH)(BPMCN)]^{2+}$ (S=3/2), $[Fe^{V}(O)(AcO)(BPMCN)]^{2+}$ (S=3/2) and $[Fe^{IV}(O)(AcO\cdot)(BPMCN)]^{2+}$ (S=1/2).

			
ρ(Fe)[a]	2.13	2.15	1.58
ρ(O_{Oxo})[a]	0.85	0.92	0.00
ρ(O_b)[a]	0.16	0.06	-0.40
d(Fe-O_{oxo})[b]	1.64	1.64	1.63

[a] All values are calculated at the B3LYP(SMD)/6-31G** level in acetonitrile as solvent. [b] Bond distances are in Å.

Cartesian coordinates

In parenthesis are the free energies (in hartrees) and the spin state of each iron intermediate.

[Fe^{V}(O)(OH)(BPMCN)]$^{2+}$ (G = -2412.676640) (quartet)

26	0.028550000	-1.187031000	-0.034618000
6	-2.649450000	-1.658913000	1.162711000
1	-2.062738000	-2.137729000	1.935512000
7	-1.962026000	-1.102427000	0.147942000
7	-0.406316000	0.384202000	-1.340655000
6	-4.036415000	-1.609442000	1.200267000
7	0.399113000	0.387831000	1.344932000
7	2.001236000	-1.026129000	-0.205035000
8	-0.071348000	-2.293461000	-1.234084000
6	-4.720510000	-0.975145000	0.162442000
6	-3.998173000	-0.412026000	-0.889042000
1	-4.487094000	0.092972000	-1.714061000
6	-2.612860000	-0.502578000	-0.874778000
6	-1.718542000	0.014021000	-1.955054000
1	-1.534718000	-0.776832000	-2.688765000
1	-2.148131000	0.877605000	-2.468649000
6	0.608890000	0.501116000	-2.423835000
1	0.762146000	-0.489904000	-2.849777000
1	1.540801000	0.889652000	-2.016099000
6	-0.566601000	1.660658000	-0.531553000
6	0.489357000	1.681642000	0.562539000
6	-0.602985000	0.435285000	2.441395000
1	-0.708453000	-0.571206000	2.845826000
1	-1.558619000	0.785914000	2.052690000
6	1.734641000	0.069567000	1.923316000
1	1.602973000	-0.733180000	2.654919000
1	2.154240000	0.941733000	2.431977000
6	2.629886000	-0.412629000	0.825522000
6	4.013574000	-0.289222000	0.845306000
1	4.484970000	0.224735000	1.675085000
6	4.757148000	-0.831922000	-0.201016000
6	4.096774000	-1.485942000	-1.243168000
6	2.712950000	-1.569055000	-1.213696000
1	2.148288000	-2.064580000	-1.992974000
8	0.176070000	-2.312559000	1.332514000
1	-5.804020000	-0.917635000	0.172423000
1	-4.560068000	-2.062868000	2.033691000
1	5.838845000	-0.745993000	-0.203715000
1	4.637479000	-1.927750000	-2.071864000
1	-0.259541000	1.106619000	3.233190000
1	0.234545000	1.172894000	-3.200376000
1	0.207044000	-3.237125000	1.026891000
6	-0.517958000	2.932733000	-1.387899000
6	-0.667298000	4.173846000	-0.497954000
6	0.443003000	4.200131000	0.559365000
6	0.368614000	2.940236000	1.431212000
1	1.419910000	4.250348000	0.060435000
1	0.349704000	5.086053000	1.196438000
1	-0.628035000	5.071091000	-1.124808000
1	-1.645647000	4.158388000	0.000394000
1	0.448049000	2.990051000	-1.898687000
1	-1.304286000	2.893475000	-2.147984000
1	1.157209000	2.935719000	2.190212000
1	-0.597317000	2.933994000	1.945697000
1	1.472576000	1.686162000	0.083275000
1	-1.548493000	1.599838000	-0.055013000

[Fe^{V}(O)(OH)(BPMCN)]$^{2+}$ (G = -2412.651179) (doublet)

26	0.031626000	-1.194262000	-0.057828000
6	-2.658088000	-1.671084000	1.167399000
1	-2.088605000	-2.138770000	1.959598000
7	-1.961414000	-1.130963000	0.149022000
7	-0.415432000	0.389352000	-1.329956000
6	-4.044207000	-1.613122000	1.210095000
7	0.403061000	0.387475000	1.329492000
7	2.007343000	-1.044949000	-0.203216000
8	-0.075045000	-2.234140000	-1.291561000
6	-4.727159000	-0.974915000	0.174326000
6	-4.000717000	-0.412624000	-0.874001000
1	-4.486110000	0.104307000	-1.693760000
6	-2.615890000	-0.515455000	-0.862948000
6	-1.729922000	0.022968000	-1.940611000
1	-1.548077000	-0.750462000	-2.693115000
1	-2.170257000	0.893139000	-2.433330000
6	0.598766000	0.511113000	-2.416833000
1	0.747429000	-0.473887000	-2.857219000
1	1.534362000	0.889600000	-2.008475000
6	-0.568966000	1.667021000	-0.525662000
6	0.497542000	1.682687000	0.556565000
6	-0.602408000	0.438934000	2.423800000
1	-0.706288000	-0.564970000	2.833216000
1	-1.558344000	0.786438000	2.033259000
6	1.733877000	0.064638000	1.916589000
1	1.594740000	-0.727016000	2.657894000
1	2.155095000	0.939731000	2.418880000
6	2.632949000	-0.430884000	0.827580000
6	4.017053000	-0.309291000	0.858262000
1	4.482769000	0.205772000	1.690610000
6	4.768345000	-0.853520000	-0.181398000
6	4.113016000	-1.503955000	-1.228431000
6	2.728389000	-1.583123000	-1.207714000
1	2.171879000	-2.073121000	-1.996410000
8	0.200594000	-2.280889000	1.337261000
1	-5.810104000	-0.908441000	0.186939000
1	-4.567249000	-2.058226000	2.048318000
1	5.850199000	-0.769605000	-0.176253000
1	4.657720000	-1.944753000	-2.055119000
1	-0.260225000	1.115108000	3.211945000
1	0.224843000	1.194471000	-3.183188000
1	-0.336368000	-3.087432000	1.221510000
6	-0.524829000	2.939988000	-1.381350000
6	-0.662006000	4.179891000	-0.487870000
6	0.460297000	4.201313000	0.557018000
6	0.390411000	2.940923000	1.428378000
1	1.431674000	4.248411000	0.047079000
1	0.377441000	5.086898000	1.196021000
1	-0.627192000	5.078018000	-1.113702000
1	-1.634737000	4.166217000	0.021402000
1	0.436913000	2.996932000	-1.899894000
1	-1.317602000	2.904611000	-2.134895000
1	1.186423000	2.932977000	2.179537000
1	-0.570239000	2.938901000	1.952463000
1	1.476974000	1.683092000	0.069646000
1	-1.547365000	1.607693000	-0.041580000

I_heter_q (G = -2546.634697) (quartet)

26	0.262316000	-0.997734000	0.011107000
6	-2.389857000	-0.335981000	1.171861000
1	-2.044371000	-0.979854000	1.969665000
7	-1.530462000	-0.125686000	0.157640000
7	0.492251000	0.568653000	-1.350115000
6	-3.647291000	0.251104000	1.177480000
7	1.220840000	0.348192000	1.346798000
7	2.139697000	-1.636049000	-0.131207000
8	-0.260341000	-2.015956000	-1.157040000
6	-4.019682000	1.067195000	0.108637000
6	-3.126041000	1.267668000	-0.942006000
1	-3.372641000	1.892676000	-1.792602000
6	-1.886784000	0.644057000	-0.895106000
6	-0.857669000	0.723672000	-1.975303000
1	-1.000164000	-0.105610000	-2.675152000
1	-0.909026000	1.664848000	-2.528154000
6	1.471297000	0.235677000	-2.420897000
1	1.218121000	-0.747854000	-2.815712000
1	2.480947000	0.234016000	-2.013698000
6	0.849916000	1.833280000	-0.587425000
6	1.819240000	1.473204000	0.527577000
6	0.316503000	0.824648000	2.424960000
1	-0.171941000	-0.045000000	2.864459000
1	-0.428193000	1.502879000	2.009682000
6	2.319055000	-0.452480000	1.957567000
1	1.875448000	-1.114199000	2.707141000
1	3.045924000	0.199418000	2.449844000
6	2.956518000	-1.284706000	0.889890000
6	4.276645000	-1.715442000	0.928516000
1	4.910057000	-1.400171000	1.749789000
6	4.748322000	-2.544117000	-0.087967000
6	3.886104000	-2.921337000	-1.119767000
6	2.581869000	-2.450417000	-1.110678000
1	1.868973000	-2.709978000	-1.882609000
8	-0.052265000	-2.041098000	1.414606000
1	-4.995367000	1.540872000	0.093958000
1	-4.317418000	0.063397000	2.008087000
1	5.776058000	-2.891884000	-0.075749000

1	4.211106000	-3.569697000	-1.924973000
1	0.894078000	1.341183000	3.196372000
1	1.396193000	0.975541000	-3.221607000
1	-0.374663000	-2.918376000	1.141189000
6	1.410907000	2.945946000	-1.482530000
6	1.761023000	4.176493000	-0.635331000
6	2.778536000	3.799881000	0.448270000
6	2.200783000	2.706312000	1.355889000
1	3.701014000	3.439781000	-0.026098000
1	3.037268000	4.673789000	1.055667000
1	2.161635000	4.958963000	-1.288594000
1	0.852572000	4.571098000	-0.161388000
1	2.323757000	2.593618000	-1.972875000
1	0.681090000	3.193956000	-2.259326000
1	2.916106000	2.416930000	2.132266000
1	1.307183000	3.102785000	1.848409000
1	2.727954000	1.072418000	0.069437000
1	-0.078134000	2.188252000	-0.131042000
1	-3.524777000	-1.998895000	-1.284722000
1	-2.787808000	-2.075269000	-1.349633000
7	-6.077504000	-1.644025000	-0.916259000
6	-6.628868000	-0.987954000	-0.132546000
6	-7.313157000	-0.158063000	0.850637000
1	-8.195234000	-0.683614000	1.231126000
1	-6.635699000	0.059645000	1.682847000
1	-7.627391000	0.782420000	0.386317000

TS_heter_q (G = -2546.612813) (quartet)

26	-0.031073000	-0.854715000	0.058343000
6	-2.528438000	0.173246000	1.289491000
1	-2.273184000	-0.541459000	2.060514000
7	-1.684192000	0.245365000	0.242749000
7	0.381137000	0.660288000	-1.313755000
6	-3.654694000	0.981639000	1.364597000
7	1.152211000	0.291028000	1.340665000
7	1.694493000	-1.802982000	-0.176914000
8	-0.748609000	-1.856942000	-1.185292000
6	-3.918196000	1.877098000	0.327618000
6	-3.048138000	1.935178000	-0.759837000
1	-3.209835000	2.615801000	-1.587784000
6	-1.940109000	1.098426000	-0.775959000
6	-0.945193000	1.036434000	-1.890128000
1	-1.236577000	0.257739000	-2.600137000
1	-0.865530000	1.987114000	-2.423098000
6	1.258432000	0.186372000	-2.419387000
1	0.841695000	-0.746433000	-2.798062000
1	2.269516000	0.027178000	-2.047156000
6	0.958255000	1.845525000	-0.559232000
6	1.897291000	1.322061000	0.512988000
6	0.368642000	0.893078000	2.451074000
1	-0.243648000	0.109309000	2.896639000
1	-0.265378000	1.691379000	2.066042000
6	2.133800000	-0.678647000	1.906946000
1	1.621040000	-1.265069000	2.674431000
1	2.972236000	-0.150959000	2.369373000
6	2.592462000	-1.595375000	0.814832000
6	3.826816000	-2.232927000	0.811959000
1	4.528842000	-2.029359000	1.612440000
6	4.126924000	-3.118904000	-0.221696000
6	3.183187000	-3.342613000	-1.226140000
6	1.972264000	-2.667401000	-1.172674000
1	1.202133000	-2.798105000	-1.921691000
8	-0.466577000	-1.865295000	1.446312000
1	-4.790368000	2.521425000	0.364994000
1	-4.311046000	0.897052000	2.222232000
1	5.085167000	-3.627572000	-0.243779000
1	3.375584000	-4.025997000	-2.044913000
1	1.045942000	1.296231000	3.208629000
1	1.270048000	0.931073000	-3.219245000
1	-0.865419000	-2.701829000	1.148614000
6	1.651889000	2.869963000	-1.465232000
6	2.222930000	4.017711000	-0.621265000
6	3.206983000	3.469265000	0.418334000
6	2.499662000	2.465403000	1.339516000
1	4.042367000	2.975967000	-0.096122000
1	3.623124000	4.281612000	1.023564000
1	2.719391000	4.736710000	-1.281610000
1	1.406304000	4.544864000	-0.110300000
1	2.478643000	2.386400000	-1.994450000
1	0.943143000	3.242715000	-2.211384000
1	3.189001000	2.054001000	2.083312000
1	1.699965000	2.989230000	1.872247000
1	2.714173000	0.787060000	0.020266000
1	0.114328000	2.335237000	-0.065531000
1	-2.786177000	-1.477550000	-1.616451000
1	-1.879251000	-1.665387000	-1.437425000
7	-5.082062000	-0.950201000	-1.479174000
6	-5.382633000	-1.234359000	-0.393105000
6	-5.748850000	-1.587269000	0.971270000
1	-6.508299000	-2.376257000	0.960091000
1	-4.862590000	-1.942868000	1.506743000
1	-6.146779000	-0.706653000	1.485124000

II_heter_q (G = -2546.701201) (quartet)

26	-0.221911000	-0.720236000	0.211667000
6	-2.795776000	0.631195000	1.552550000
1	-2.480348000	0.024068000	2.394303000
7	-1.984574000	0.600069000	0.484439000
7	-0.000686000	0.734175000	-1.300220000
6	-3.962379000	1.389760000	1.569565000
7	1.120290000	0.465704000	1.294835000
7	1.738051000	-1.696135000	-0.152688000
8	-1.119656000	-1.931371000	-0.859025000
6	-4.285586000	2.142054000	0.435737000
6	-3.439986000	2.105678000	-0.674283000
1	-3.654815000	2.675951000	-1.571800000
6	-2.297083000	1.308873000	-0.612424000
6	-1.354773000	1.131410000	-1.775172000
1	-1.737679000	0.336854000	-2.424752000
1	-1.299463000	2.041068000	-2.381239000
6	0.768270000	0.188045000	-2.449047000
1	0.334656000	-0.773972000	-2.726868000
1	1.805867000	0.037532000	-2.153138000
6	0.679783000	1.929460000	-0.660783000
6	1.742480000	1.444532000	0.326993000
6	0.415536000	1.129613000	2.421737000
1	-0.172607000	0.367908000	2.934637000
1	-0.247680000	1.903332000	2.035085000
6	2.160349000	-0.438271000	1.854015000
1	1.690580000	-1.000082000	2.666860000
1	2.994735000	0.138553000	2.266068000
6	2.633275000	-1.415541000	0.808734000
6	3.883635000	-2.030239000	0.851687000
1	4.588336000	-1.767664000	1.633634000
6	4.193345000	-2.978797000	-0.122912000
6	3.249608000	-3.282412000	-1.108241000
6	2.028993000	-2.614405000	-1.085670000
1	1.250926000	-2.802008000	-1.818022000
8	-0.593288000	-1.685978000	1.708769000
1	-5.183805000	2.751549000	0.418249000
1	-4.597595000	1.393508000	2.448468000
1	5.159224000	-3.474563000	-0.115207000
1	3.454229000	-4.017366000	-1.879013000
1	1.131874000	1.577509000	3.117795000
1	0.724298000	0.866101000	-3.306861000
1	-1.204976000	-2.402756000	1.479880000
6	1.271798000	2.918418000	-1.675077000
6	1.948016000	4.094958000	-0.959379000
6	3.045695000	3.579964000	-0.021463000
6	2.443730000	2.624167000	1.015089000
1	3.809640000	3.054527000	-0.610503000
1	3.539216000	4.412983000	0.491408000
1	2.363820000	4.783082000	-1.703721000
1	1.202289000	4.650443000	-0.374826000
1	2.025806000	2.406475000	-2.282333000
1	0.484111000	3.272119000	-2.348153000
1	3.215141000	2.245644000	1.693706000
1	1.714541000	3.179846000	1.614486000
1	2.493112000	0.883720000	-0.237591000
1	-0.095819000	2.446128000	-0.088361000
1	-4.519697000	-0.652655000	-0.591679000
1	-1.339764000	-1.590392000	-1.738566000
7	-4.127760000	-1.583037000	-0.521686000
6	-3.582522000	-2.593124000	-0.462052000
6	-3.112537000	-3.951364000	-0.360583000
1	-3.979748000	-4.616466000	-0.447640000
1	-2.386057000	-4.131865000	-1.155833000
1	-2.629561000	-4.083445000	0.613355000

I_heter_d (G = -2546.613035) (doublet)

26	0.255878000	-0.997574000	-0.026745000
6	-2.417796000	-0.323800000	1.137333000
1	-2.095621000	-0.952317000	1.956690000
7	-1.543659000	-0.132473000	0.131175000
7	0.504293000	0.594966000	-1.341182000
6	-3.670424000	0.272322000	1.133101000
7	1.219275000	0.340307000	1.332246000
7	2.125094000	-1.667855000	-0.127822000

8	-0.238444000	-1.933580000	-1.247634000
6	-4.026366000	1.092771000	0.062341000
6	-3.115122000	1.293247000	-0.972333000
1	-3.342368000	1.929607000	-1.819953000
6	-1.882048000	0.657484000	-0.913280000
6	-0.837818000	0.762928000	-1.978346000
1	-0.969169000	-0.045692000	-2.704086000
1	-0.887333000	1.718541000	-2.505691000
6	1.500019000	0.268773000	-2.401958000
1	1.254564000	-0.709107000	-2.814530000
1	2.502487000	0.259265000	-1.977394000
6	0.865183000	1.850791000	-0.571201000
6	1.833208000	1.469292000	0.536186000
6	0.305523000	0.817901000	2.403220000
1	-0.189119000	-0.050704000	2.836089000
1	-0.433181000	1.499837000	1.983519000
6	2.301571000	-0.472786000	1.954934000
1	1.846765000	-1.117406000	2.711808000
1	3.034783000	0.174295000	2.444222000
6	2.935196000	-1.323987000	0.899474000
6	4.249859000	-1.770572000	0.958693000
1	4.875654000	-1.459475000	1.787438000
6	4.726812000	-2.607475000	-0.048150000
6	3.874873000	-2.972596000	-1.092262000
6	2.576804000	-2.483815000	-1.101491000
1	1.877090000	-2.731290000	-1.889456000
8	-0.044033000	-2.018174000	1.395380000
1	-4.998895000	1.572721000	0.037694000
1	-4.347925000	0.091427000	1.959044000
1	5.749855000	-2.968027000	-0.020470000
1	4.203389000	-3.623410000	-1.894131000
1	0.878752000	1.330764000	3.180163000
1	1.440375000	1.019357000	-3.193740000
1	-0.870779000	-2.527195000	1.297458000
6	1.430808000	2.971956000	-1.453449000
6	1.788894000	4.188590000	-0.589967000
6	2.807652000	3.790712000	0.484879000
6	2.224752000	2.689395000	1.380171000
1	3.725860000	3.430621000	0.002244000
1	3.074591000	4.654567000	1.103000000
1	2.191893000	4.978100000	-1.233188000
1	0.884023000	4.581255000	-0.107615000
1	2.341907000	2.622738000	-1.948858000
1	0.701998000	3.234690000	-2.226384000
1	2.939491000	2.385594000	2.151579000
1	1.335365000	3.087118000	1.878898000
1	2.739564000	1.066427000	0.075140000
1	-0.061497000	2.205222000	-0.111774000
1	-3.528000000	-2.032087000	-1.283351000
1	-2.795520000	-2.092986000	-1.397103000
7	-6.045773000	-1.748531000	-0.783990000
6	-6.613943000	-1.034016000	-0.066154000
6	-7.321648000	-0.132850000	0.834087000
1	-6.665844000	0.146917000	1.665120000
1	-7.622820000	0.769971000	0.292776000
1	-8.213888000	-0.628867000	1.230292000

TS_heter_d (G = -2546.604166) (doublet)

26	-0.029864000	-0.855953000	0.055900000
6	-2.534559000	0.165270000	1.280690000
1	-2.283849000	-0.554465000	2.048657000
7	-1.689808000	0.238177000	0.235137000
7	0.382827000	0.661105000	-1.315050000
6	-3.656158000	0.980183000	1.360071000
7	1.147605000	0.293305000	1.341125000
7	1.695894000	-1.804145000	-0.174929000
8	-0.733463000	-1.860275000	-1.214523000
6	-3.912984000	1.883651000	0.328672000
6	-3.041394000	1.942800000	-0.757732000
1	-3.197887000	2.629701000	-1.581498000
6	-1.938427000	1.099582000	-0.777978000
6	-0.943845000	1.035997000	-1.892154000
1	-1.234616000	0.254700000	-2.599318000
1	-0.863929000	1.985511000	-2.427079000
6	1.262252000	0.189617000	-2.419728000
1	0.846983000	-0.743225000	-2.800153000
1	2.272894000	0.031196000	-2.045810000
6	0.956842000	1.846742000	-0.558754000
6	1.894177000	1.324286000	0.515150000
6	0.359555000	0.894750000	2.448726000
1	-0.253745000	0.110648000	2.892523000
1	-0.273925000	1.692232000	2.061181000
6	2.127678000	-0.676459000	1.909818000
1	1.613341000	-1.262447000	2.676619000
1	2.965059000	-0.148780000	2.374148000
6	2.590198000	-1.594126000	0.819595000
6	3.825105000	-2.230666000	0.821434000
1	4.524427000	-2.025274000	1.623822000
6	4.129321000	-3.118018000	-0.209875000
6	3.189400000	-3.343794000	-1.217427000
6	1.978133000	-2.668832000	-1.168967000
1	1.212432000	-2.799683000	-1.923114000
8	-0.469869000	-1.871189000	1.432898000
1	-4.780861000	2.533559000	0.369342000
1	-4.313442000	0.894422000	2.216884000
1	5.088122000	-3.625776000	-0.228084000
1	3.385389000	-4.027489000	-2.035060000
1	1.033805000	1.298667000	3.208635000
1	1.274224000	0.934956000	-3.218973000
1	-0.874624000	-2.702813000	1.127411000
6	1.650388000	2.872796000	-1.462960000
6	2.218129000	4.020870000	-0.617233000
6	3.201275000	3.473258000	0.423672000
6	2.493844000	2.467945000	1.343211000
1	4.038224000	2.981461000	-0.089669000
1	3.615237000	4.285858000	1.030058000
1	2.714572000	4.741148000	-1.276194000
1	1.399779000	4.546347000	-0.107292000
1	2.478782000	2.390948000	-1.991202000
1	0.942191000	3.244862000	-2.209973000
1	3.182479000	2.056966000	2.087899000
1	1.692620000	2.990511000	1.874886000
1	2.712340000	0.789515000	0.024323000
1	0.111380000	2.335118000	-0.066412000
1	-2.801660000	-1.492126000	-1.591169000
1	-1.955820000	-1.664253000	-1.475362000
7	-5.068868000	-0.949622000	-1.468727000
6	-5.373938000	-1.237525000	-0.384922000
6	-5.746106000	-1.594483000	0.976746000
1	-6.505804000	-2.383114000	0.960137000
1	-4.862168000	-1.952061000	1.514729000
1	-6.145676000	-0.715132000	1.491483000

II_heter_d (G = -2546.704836) (doublet)

26	-0.348997000	-0.584192000	0.130344000
6	-2.524364000	1.006469000	1.410518000
1	-2.366298000	0.310751000	2.224498000
7	-1.719502000	0.848540000	0.341993000
7	0.326694000	0.769098000	-1.311180000
6	-3.493676000	2.000404000	1.470141000
7	1.145296000	0.250137000	1.311036000
7	1.066586000	-1.965590000	-0.110120000
8	-1.418734000	-1.434764000	-1.121909000
6	-3.637180000	2.866522000	0.383605000
6	-2.790634000	2.717367000	-0.714115000
1	-2.848337000	3.380367000	-1.570561000
6	-1.841118000	1.699563000	-0.701426000
6	-0.885679000	1.452999000	-1.835610000
1	-1.349326000	0.800248000	-2.580958000
1	-0.626436000	2.389382000	-2.339663000
6	1.008156000	0.070575000	-2.428240000
1	0.358338000	-0.747377000	-2.741249000
1	1.958797000	-0.332585000	-2.079384000
6	1.211351000	1.779496000	-0.620002000
6	2.058922000	1.047972000	0.414297000
6	0.582064000	1.050155000	2.425354000
1	-0.173460000	0.432682000	2.911143000
1	0.119140000	1.955038000	2.030687000
6	1.887963000	-0.907525000	1.879033000
1	1.275987000	-1.318097000	2.686063000
1	2.853601000	-0.595853000	2.289307000
6	2.048083000	-1.954679000	0.816023000
6	3.096849000	-2.868747000	0.784488000
1	3.875793000	-2.813955000	1.537394000
6	3.115860000	-3.836758000	-0.219387000
6	2.086078000	-3.856287000	-1.161936000
6	1.079181000	-2.900720000	-1.075175000
1	0.249320000	-2.852992000	-1.769793000
8	-0.932915000	-1.522394000	1.606677000
1	-4.384958000	3.653242000	0.397729000
1	-4.119432000	2.087055000	2.351206000
1	3.921992000	-4.562481000	-0.266136000
1	2.060755000	-4.593732000	-1.956701000
1	1.361415000	1.319913000	3.144882000
1	1.182657000	0.751399000	-3.267127000
1	-1.896485000	-1.598981000	1.569388000
6	2.079369000	2.610507000	-1.575745000
6	2.978008000	3.577044000	-0.792937000
6	3.863833000	2.796465000	0.185378000
6	2.989303000	2.006642000	1.166878000

1	4.506629000	2.106341000	-0.378002000
1	4.517722000	3.476541000	0.742658000
1	3.589836000	4.155291000	-1.494203000
1	2.356998000	4.288184000	-0.231102000
1	2.721524000	1.940253000	-2.156628000
1	1.437383000	3.150604000	-2.279432000
1	3.602688000	1.441182000	1.876310000
1	2.388427000	2.720342000	1.740026000
1	2.676084000	0.318966000	-0.120039000
1	0.538193000	2.456735000	-0.085058000
1	-4.805390000	0.237312000	-0.482226000
1	-2.057991000	-0.848731000	-1.548340000
7	-4.540121000	-0.737056000	-0.388568000
6	-4.180268000	-1.822716000	-0.294237000
6	-3.746446000	-3.185998000	-0.169618000
1	-4.525477000	-3.846742000	-0.566865000
1	-2.809327000	-3.265739000	-0.732758000
1	-3.569840000	-3.396711000	0.891977000

II_heter_sext (G = -2546.716803) (sextuplet)

26	-0.375988000	-0.837502000	0.279911000
6	-2.714096000	0.817050000	1.527189000
1	-2.478858000	0.161971000	2.358480000
7	-1.912282000	0.692788000	0.455466000
7	0.119192000	0.749421000	-1.322210000
6	-3.773135000	1.718408000	1.554188000
7	1.192704000	0.432274000	1.307218000
7	1.489998000	-1.887197000	-0.045096000
8	-1.310753000	-1.872110000	-0.970811000
6	-3.998156000	2.518008000	0.430106000
6	-3.157563000	2.392652000	-0.676924000
1	-3.292133000	3.000991000	-1.564871000
6	-2.123554000	1.459115000	-0.631354000
6	-1.205335000	1.201381000	-1.798398000
1	-1.637387000	0.398182000	-2.405542000
1	-1.128312000	2.092305000	-2.432304000
6	0.868673000	0.128554000	-2.434689000
1	0.376065000	-0.804123000	-2.714348000
1	1.884646000	-0.099341000	-2.110211000
6	0.861480000	1.883971000	-0.679460000
6	1.880320000	1.335081000	0.325335000
6	0.539854000	1.160890000	2.419101000
1	-0.097076000	0.453853000	2.952747000
1	-0.074135000	1.966863000	2.015271000
6	2.147248000	-0.557638000	1.857506000
1	1.648930000	-1.057775000	2.694428000
1	3.056333000	-0.074829000	2.234417000
6	2.483675000	-1.593396000	0.815564000
6	3.717754000	-2.236680000	0.751790000
1	4.501804000	-1.963592000	1.449820000
6	3.913703000	-3.219451000	-0.218556000
6	2.873320000	-3.529482000	-1.097855000
6	1.673088000	-2.837936000	-0.976540000
1	0.822942000	-3.027739000	-1.622113000
8	-0.813846000	-1.611236000	1.913161000
1	-4.812424000	3.236096000	0.419140000
1	-4.401802000	1.791292000	2.434626000
1	4.866812000	-3.734231000	-0.290529000
1	2.987136000	-4.287957000	-1.864376000
1	1.279000000	1.582250000	3.110184000
1	0.908602000	0.784308000	-3.312160000
1	-1.322982000	-2.435041000	1.892700000
6	1.527723000	2.829902000	-1.692302000
6	2.282362000	3.961785000	-0.985874000
6	3.340758000	3.374978000	-0.045218000
6	2.670689000	2.470792000	0.995291000
1	4.066012000	2.794427000	-0.631897000
1	3.893150000	4.173128000	0.463772000
1	2.746291000	4.615858000	-1.732939000
1	1.578066000	4.572118000	-0.404145000
1	2.247953000	2.265323000	-2.295058000
1	0.768107000	3.229755000	-2.372633000
1	3.411250000	2.044494000	1.680456000
1	1.984379000	3.084900000	1.588865000
1	2.588858000	0.709617000	-0.226782000
1	0.120292000	2.458975000	-0.115356000
1	-4.526752000	-0.242853000	-0.683539000
1	-1.301145000	-1.727968000	-1.926099000
7	-4.232383000	-1.207233000	-0.599935000
6	-3.773532000	-2.259222000	-0.530732000
6	-3.438967000	-3.654059000	-0.392159000
1	-4.368524000	-4.206881000	-0.211626000
1	-2.950680000	-3.993661000	-1.309076000
1	-2.750384000	-3.767482000	0.450049000

I_homo_d (G = -2413.831448) (doublet)

26	0.003470000	-1.182556000	0.081589000
6	2.659564000	-1.698083000	-1.140151000
1	2.072194000	-2.222090000	-1.882505000
7	1.972468000	-1.104386000	-0.147292000
7	0.417452000	0.463109000	1.328057000
6	4.044951000	-1.623971000	-1.202113000
7	-0.398259000	0.432928000	-1.312806000
7	-1.994341000	-1.068579000	0.182849000
8	0.094894000	-2.079624000	1.376544000
6	4.729940000	-0.918626000	-0.211838000
6	4.009974000	-0.312598000	0.817199000
1	4.500246000	0.247563000	1.605122000
6	2.626597000	-0.433415000	0.829655000
6	1.752597000	0.122879000	1.911280000
1	1.599310000	-0.633915000	2.686222000
1	2.194353000	1.009486000	2.372565000
6	-0.588910000	0.573370000	2.421389000
1	-0.712487000	-0.407745000	2.877710000
1	-1.537104000	0.919610000	2.012065000
6	0.545993000	1.737490000	0.523836000
6	-0.519220000	1.729296000	-0.556660000
6	0.627474000	0.479877000	-2.389930000
1	0.755546000	-0.529285000	-2.778066000
1	1.570004000	0.850802000	-1.989400000
6	-1.719769000	0.092240000	-1.910902000
1	-1.564284000	-0.675990000	-2.673959000
1	-2.152382000	0.968718000	-2.400442000
6	-2.620763000	-0.428202000	-0.832336000
6	-4.003659000	-0.295579000	-0.859956000
1	-4.466502000	0.239459000	-1.681259000
6	-4.757176000	-0.852917000	0.171302000
6	-4.103630000	-1.522162000	1.207057000
6	-2.719016000	-1.610756000	1.182300000
1	-2.162667000	-2.109007000	1.965979000
8	-0.115497000	-2.249350000	-1.320679000
1	5.811627000	-0.837768000	-0.242072000
1	4.567137000	-2.109313000	-2.018300000
1	-5.838403000	-0.761488000	0.169739000
1	-4.649727000	-1.968639000	2.029823000
1	0.285901000	1.137948000	-3.193798000
1	-0.229370000	1.279561000	3.173602000
1	-1.033222000	-2.500073000	-1.533625000
6	0.473133000	3.014940000	1.373255000
6	0.596748000	4.250128000	0.471971000
6	-0.520186000	4.247390000	-0.578835000
6	-0.427821000	2.981809000	-1.440389000
1	-1.494870000	4.284223000	-0.074527000
1	-0.446839000	5.128643000	-1.224896000
1	0.544421000	5.151736000	1.091503000
1	1.572414000	4.247757000	-0.031680000
1	-0.493218000	3.058909000	1.884032000
1	1.260757000	2.997075000	2.132659000
1	-1.221453000	2.956388000	-2.193425000
1	0.534635000	2.989245000	-1.960833000
1	-1.499330000	1.718125000	-0.070918000
1	1.526240000	1.699765000	0.041231000
1	0.127059000	-4.265099000	-0.150781000
1	0.152440000	-4.746511000	0.417555000

TS_homo_d (G = -2413.826956) (doublet)

26	0.016409000	-1.134914000	0.068655000
6	2.669031000	-1.642125000	-1.164911000
1	2.082215000	-2.155235000	-1.915276000
7	1.980475000	-1.055240000	-0.168256000
7	0.415702000	0.447922000	1.337885000
6	4.054978000	-1.579015000	-1.218126000
7	-0.397917000	0.404503000	-1.322466000
7	-1.980859000	-1.056825000	0.186727000
8	0.136755000	-2.177906000	1.334703000
6	4.739771000	-0.893330000	-0.213440000
6	4.019329000	-0.299007000	0.821967000
1	4.510370000	0.241830000	1.622828000
6	2.634805000	-0.408460000	0.824434000
6	1.757533000	0.127305000	1.914071000
1	1.618875000	-0.642139000	2.679935000
1	2.190198000	1.013441000	2.385071000
6	-0.579924000	0.544705000	2.440599000
1	-0.691335000	-0.443645000	2.886341000
1	-1.535155000	0.884680000	2.042044000
6	0.524472000	1.727895000	0.528446000
6	-0.536555000	1.704157000	-0.558307000
6	0.619107000	0.471756000	-2.407565000

1	0.760854000	-0.536470000	-2.795700000
1	1.558127000	0.856905000	-2.012317000
6	-1.715027000	0.049335000	-1.926774000
1	-1.548705000	-0.740120000	-2.666627000
1	-2.143908000	0.912338000	-2.442608000
6	-2.618350000	-0.452827000	-0.842903000
6	-4.003035000	-0.345118000	-0.874906000
1	-4.475729000	0.161251000	-1.708640000
6	-4.745769000	-0.892197000	0.169998000
6	-4.080558000	-1.528811000	1.218986000
6	-2.694214000	-1.593783000	1.196081000
1	-2.126512000	-2.072180000	1.983628000
8	-0.098880000	-2.373567000	-1.237287000
1	5.822280000	-0.820957000	-0.236499000
1	4.578514000	-2.057545000	-2.037486000
1	-5.828501000	-0.820147000	0.167322000
1	-4.619501000	-1.969199000	2.049753000
1	0.262318000	1.122650000	-3.210176000
1	-0.223641000	1.245987000	3.199035000
1	-1.017298000	-2.605856000	-1.471247000
6	0.433408000	3.003693000	1.375255000
6	0.537176000	4.241640000	0.474726000
6	-0.577325000	4.221132000	-0.578597000
6	-0.464218000	2.956734000	-1.440554000
1	-1.553483000	4.242319000	-0.076076000
1	-0.517031000	5.103974000	-1.223910000
1	0.469248000	5.142978000	1.093164000
1	1.513570000	4.255273000	-0.027532000
1	-0.533054000	3.031999000	1.887639000
1	1.221391000	2.998788000	2.134677000
1	-1.255808000	2.920281000	-2.195370000
1	0.498988000	2.979442000	-1.959681000
1	-1.517236000	1.675185000	-0.074614000
1	1.505807000	1.701723000	0.046737000
1	0.120545000	-3.755091000	-0.078001000
1	0.174328000	-3.617506000	0.721122000

II_homo_d (G = -2413.965275) (doublet)

26	0.004816000	-1.060893000	0.065101000
6	2.664667000	-1.623146000	-1.181702000
1	2.085623000	-2.089727000	-1.969303000
7	1.975086000	-1.047129000	-0.179235000
7	0.438877000	0.440730000	1.327043000
6	4.053100000	-1.610379000	-1.221275000
7	-0.414677000	0.404210000	-1.330100000
7	-1.982954000	-1.040947000	0.216214000
8	0.215588000	-2.281298000	1.387415000
6	4.749747000	-0.976182000	-0.191330000
6	4.034459000	-0.382569000	0.847588000
1	4.533262000	0.124411000	1.665914000
6	2.645996000	-0.446436000	0.828451000
6	1.770475000	0.102847000	1.912711000
1	1.609444000	-0.670070000	2.668245000
1	2.213047000	0.980428000	2.391719000
6	-0.550281000	0.548834000	2.432591000
1	-0.673144000	-0.446482000	2.857524000
1	-1.500359000	0.909897000	2.039734000
6	0.554938000	1.716472000	0.513558000
6	-0.523112000	1.705974000	-0.563090000
6	0.579043000	0.467462000	-2.434973000
1	0.707350000	-0.539565000	-2.833014000
1	1.530233000	0.838963000	-2.055428000
6	-1.744671000	0.056598000	-1.909230000
1	-1.593928000	-0.730621000	-2.655665000
1	-2.185588000	0.917676000	-2.419397000
6	-2.635264000	-0.448991000	-0.812140000
6	-4.021446000	-0.347567000	-0.839702000
1	-4.501704000	0.147071000	-1.676407000
6	-4.757280000	-0.883883000	0.215492000
6	-4.081795000	-1.498040000	1.271506000
6	-2.695003000	-1.553067000	1.239724000
1	-2.123224000	-2.000885000	2.042218000
8	-0.235210000	-2.487103000	-1.331290000
1	5.834458000	-0.941196000	-0.199385000
1	4.568787000	-2.084163000	-2.048486000
1	-5.840486000	-0.817278000	0.217542000
1	-4.613740000	-1.923765000	2.114530000
1	0.218353000	1.123578000	-3.232045000
1	-0.182590000	1.235267000	3.199881000
1	-1.146844000	-2.790281000	-1.497154000
6	0.496401000	2.996507000	1.355226000
6	0.595609000	4.234298000	0.454157000
6	-0.537980000	4.225172000	-0.579374000
6	-0.452659000	2.959536000	-1.442366000
1	-1.504482000	4.255210000	-0.058542000
1	-0.481669000	5.108822000	-1.224244000
1	0.548590000	5.137280000	1.072494000
1	1.562467000	4.238505000	-0.066797000
1	-0.459032000	3.036719000	1.887835000
1	1.298184000	2.983909000	2.100371000
1	-1.256068000	2.932203000	-2.185519000
1	0.501793000	2.973840000	-1.978303000
1	-1.496628000	1.686302000	-0.063723000
1	1.527935000	1.671626000	0.015955000
1	0.292385000	-3.290375000	-1.166001000
1	-0.424674000	-3.005536000	1.301440000

II_homo_q (G = -2413.960599) (quartet)

26	-0.008582000	-1.123038000	0.091868000
6	2.730369000	-1.641610000	-1.097115000
1	2.160244000	-2.160776000	-1.857547000
7	2.024904000	-1.032906000	-0.124912000
7	0.478748000	0.582003000	1.375703000
6	4.118112000	-1.601679000	-1.134412000
7	-0.424178000	0.346435000	-1.311132000
7	-2.004447000	-1.090581000	0.277447000
8	0.289303000	-2.419306000	1.301531000
6	4.795665000	-0.899329000	-0.136030000
6	4.062190000	-0.268524000	0.866715000
1	4.546313000	0.295256000	1.656563000
6	2.673677000	-0.364366000	0.852122000
6	1.809611000	0.242465000	1.925813000
1	1.662631000	-0.499441000	2.716984000
1	2.295923000	1.121311000	2.363347000
6	-0.507896000	0.704974000	2.472338000
1	-0.610877000	-0.274266000	2.944127000
1	-1.471128000	1.014173000	2.064407000
6	0.552979000	1.785862000	0.481461000
6	-0.545320000	1.679789000	-0.579252000
6	0.567551000	0.389513000	-2.420563000
1	0.709056000	-0.627036000	-2.788082000
1	1.512594000	0.785462000	-2.051025000
6	-1.756856000	-0.029372000	-1.875108000
1	-1.602811000	-0.826456000	-2.609611000
1	-2.205089000	0.816070000	-2.403446000
6	-2.647779000	-0.512005000	-0.767445000
6	-4.031252000	-0.386332000	-0.790873000
1	-4.507992000	0.093850000	-1.637752000
6	-4.770950000	-0.875008000	0.285200000
6	-4.104157000	-1.460569000	1.363270000
6	-2.719993000	-1.546549000	1.326485000
1	-2.161947000	-1.965978000	2.154766000
8	-0.170967000	-2.635323000	-1.533843000
1	5.879333000	-0.839139000	-0.142442000
1	4.647581000	-2.104793000	-1.935313000
1	-5.852617000	-0.787447000	0.289088000
1	-4.641028000	-1.838799000	2.225399000
1	0.196058000	1.016321000	-3.235828000
1	-0.177514000	1.433516000	3.220201000
1	-1.066504000	-2.855376000	-1.842086000
6	0.476675000	3.118725000	1.239618000
6	0.509976000	4.306330000	0.271188000
6	-0.649076000	4.196526000	-0.725883000
6	-0.536279000	2.889750000	-1.522339000
1	-1.602103000	4.218982000	-0.180335000
1	-0.645290000	5.043074000	-1.421089000
1	0.446270000	5.242064000	0.837447000
1	1.461650000	4.314469000	-0.277166000
1	-0.463294000	3.160545000	1.799720000
1	1.299226000	3.167473000	1.961105000
1	-1.351810000	2.802054000	-2.247129000
1	0.406906000	2.910133000	-2.077740000
1	-1.509043000	1.649358000	-0.061747000
1	1.519237000	1.735891000	-0.030314000
1	0.213135000	-3.474446000	-1.226722000
1	-0.499360000	-2.936223000	1.531274000

II_homo_sext (G = -2413.968425) (sextuplet)

26	0.003090000	-1.224321000	0.128468000
6	2.840739000	-1.629136000	-1.150053000
1	2.280744000	-2.163450000	-1.908161000
7	2.118703000	-1.072360000	-0.159624000
7	0.513371000	0.472229000	1.360754000
6	4.224909000	-1.519571000	-1.201059000
7	-0.483225000	0.388499000	-1.341358000

7	-2.139494000	-1.019049000	0.232837000
8	0.074736000	-2.526414000	1.387163000
6	4.878341000	-0.806304000	-0.193676000
6	4.128584000	-0.231299000	0.831695000
1	4.595885000	0.336601000	1.628597000
6	2.746523000	-0.391235000	0.823203000
6	1.856143000	0.147646000	1.912420000
1	1.721146000	-0.624931000	2.676715000
1	2.303911000	1.025904000	2.387832000
6	-0.470713000	0.576303000	2.469409000
1	-0.587713000	-0.416549000	2.907569000
1	-1.428159000	0.916072000	2.073802000
6	0.584630000	1.706818000	0.496195000
6	-0.534446000	1.679403000	-0.551689000
6	0.509605000	0.427216000	-2.445252000
1	0.637881000	-0.582057000	-2.841176000
1	1.467175000	0.782575000	-2.064616000
6	-1.829972000	0.093912000	-1.892564000
1	-1.734203000	-0.680332000	-2.662451000
1	-2.256902000	0.972587000	-2.386569000
6	-2.742932000	-0.392841000	-0.798294000
6	-4.123693000	-0.221722000	-0.843361000
1	-4.570036000	0.299143000	-1.683299000
6	-4.897935000	-0.719657000	0.203134000
6	-4.269062000	-1.365179000	1.270667000
6	-2.886996000	-1.493901000	1.248468000
1	-2.348715000	-1.966969000	2.061016000
8	-0.089380000	-2.602540000	-1.492654000
1	5.957785000	-0.693852000	-0.210312000
1	4.771921000	-1.979252000	-2.016265000
1	-5.976241000	-0.596326000	0.192342000
1	-4.833942000	-1.756917000	2.108882000
1	0.172047000	1.083675000	-3.253432000
1	-0.119076000	1.275201000	3.234398000
1	-0.652099000	-2.494067000	-2.278546000
6	0.551819000	3.007039000	1.312719000
6	0.623732000	4.234940000	0.398674000
6	-0.543223000	4.211646000	-0.595035000
6	-0.486160000	2.932861000	-1.438784000
1	-1.491750000	4.250385000	-0.042447000
1	-0.509262000	5.084771000	-1.255932000
1	0.597759000	5.145056000	1.008112000
1	1.572834000	4.232698000	-0.154194000
1	-0.386076000	3.053939000	1.875813000
1	1.375631000	3.001545000	2.033959000
1	-1.310262000	2.902834000	-2.158603000
1	0.451311000	2.937743000	-2.004598000
1	-1.489051000	1.670430000	-0.016822000
1	1.540568000	1.654638000	-0.033326000
1	-0.146535000	-3.537432000	-1.228406000
1	-0.594633000	-3.136551000	1.724725000

[Fe^{III}(OO)(OCH_3)(BPMCN)]$^{2+}$ (G = -2565.365982) (quartet)

26	0.037511000	-0.704927000	0.125734000
6	2.964660000	-0.993139000	-1.105628000
1	2.464684000	-1.588781000	-1.861533000
7	2.179307000	-0.441415000	-0.164095000
7	0.409440000	0.950485000	1.315743000
6	4.341923000	-0.806578000	-1.116389000
7	-0.554144000	0.612355000	-1.305508000
7	-2.069408000	-0.875843000	0.302053000
8	0.336864000	-1.878931000	1.472430000
6	4.917620000	-0.014860000	-0.119475000
6	4.101481000	0.551911000	0.858465000
1	4.506896000	1.173299000	1.649608000
6	2.732276000	0.304830000	0.811017000
6	1.782976000	0.803081000	1.870844000
1	1.736548000	0.067264000	2.680242000
1	2.125547000	1.752872000	2.291727000
6	-0.576357000	0.986938000	2.431003000
1	-0.576806000	0.010317000	2.919352000
1	-1.568226000	1.197672000	2.031926000
6	0.337692000	2.163869000	0.410800000
6	-0.772280000	1.951115000	-0.614023000
6	0.436761000	0.686292000	-2.418406000
1	0.659454000	-0.330558000	-2.744469000
1	1.346462000	1.172176000	-2.070929000
6	-1.848683000	0.108396000	-1.869895000
1	-1.612665000	-0.723581000	-2.541447000
1	-2.328372000	0.895518000	-2.457234000
6	-2.735027000	-0.384827000	-0.762576000
6	-4.123946000	-0.387574000	-0.821119000
1	-4.628071000	0.028901000	-1.686004000
6	-4.833034000	-0.932881000	0.249947000
6	-4.136905000	-1.452792000	1.344283000
6	-2.748021000	-1.403601000	1.335831000
1	-2.148147000	-1.779948000	2.156904000
8	0.114172000	-2.327892000	-1.030203000
1	5.988701000	0.160506000	-0.106063000
1	4.943306000	-1.266315000	-1.892434000
1	-5.918212000	-0.948476000	0.232716000
1	-4.656847000	-1.883438000	2.192363000
1	0.010495000	1.247003000	-3.254261000
1	-0.297969000	1.755249000	3.157457000
6	0.154203000	3.484384000	1.168368000
6	0.075517000	4.657823000	0.182157000
6	-1.075661000	4.441166000	-0.806582000
6	-0.868126000	3.134234000	-1.584754000
1	-2.025612000	4.397892000	-0.257385000
1	-1.139492000	5.275125000	-1.513700000
1	-0.064304000	5.590475000	0.739288000
1	1.020218000	4.740032000	-0.371742000
1	-0.779340000	3.447666000	1.739227000
1	0.978556000	3.616133000	1.876311000
1	-1.683760000	2.965566000	-2.294500000
1	0.064699000	3.214794000	-2.152246000
1	-1.721404000	1.860071000	-0.076957000
1	1.292432000	2.200002000	-0.121737000
6	0.360766000	-3.337402000	-0.331632000
8	0.512327000	-3.252619000	0.969426000
6	0.506214000	-4.706294000	-0.894842000
1	1.306388000	-4.680682000	-1.642573000
1	0.731374000	-5.442876000	-0.122494000
1	-0.429388000	-4.963854000	-1.403460000

I_homo_AcO_q (G = -2566.541447) (quartet)

26	0.371045000	0.635376000	0.297688000
6	-1.422962000	2.719484000	-0.850143000
1	-0.583523000	2.889865000	-1.511186000
7	-1.289205000	1.729862000	0.052401000
7	-1.003861000	-0.571667000	1.274055000
6	-2.584816000	3.476959000	-0.913284000
7	-0.012642000	-0.653305000	-1.342945000
7	1.912690000	-0.582215000	0.457844000
8	0.730286000	1.419612000	1.692680000
6	-3.622594000	3.203910000	-0.021062000
6	-3.468227000	2.182646000	0.915963000
1	-4.249378000	1.932128000	1.624372000
6	-2.278985000	1.466427000	0.936280000
6	-1.962677000	0.382175000	1.915885000
1	-1.471079000	0.808922000	2.794926000
1	-2.858363000	-0.153335000	2.240287000
6	-0.354065000	-1.386305000	2.339910000
1	0.249081000	-0.722136000	2.957546000
1	0.264656000	-2.157881000	1.884839000
6	-1.734138000	-1.417026000	0.241731000
6	-0.736845000	-1.873644000	-0.811124000
6	-0.743990000	0.022081000	-2.447082000
1	-0.234210000	0.959733000	-2.666446000
1	-1.772879000	0.213724000	-2.145260000
6	1.336732000	-1.051667000	-1.832720000
1	1.741682000	-0.221234000	-2.418551000
1	1.272979000	-1.933271000	-2.475930000
6	2.224489000	-1.292297000	-0.653403000
6	3.323595000	-2.140557000	-0.672110000
1	3.535922000	-2.708516000	-1.570643000
6	4.123613000	-2.235911000	0.465460000
6	3.804696000	-1.477971000	1.594334000
6	2.691911000	-0.652917000	1.557585000
1	2.399374000	-0.038489000	2.398314000
8	1.274593000	1.686197000	-0.880112000
1	-4.542549000	3.778105000	-0.055444000
1	-2.663495000	4.264153000	-1.653996000
1	4.986508000	-2.893907000	0.471511000
1	4.405352000	-1.518510000	2.495287000
1	-0.735534000	-0.608273000	-3.340239000
1	-1.126911000	-1.847941000	2.959020000
6	-2.486274000	-2.604171000	0.857377000
6	-3.185443000	-3.408764000	-0.246139000
6	-2.155890000	-3.905738000	-1.267068000
6	-1.419907000	-2.716076000	-1.897719000
1	-1.435365000	-4.565564000	-0.765779000
1	-2.643679000	-4.486505000	-2.057133000
1	-3.717777000	-4.250863000	0.208717000
1	-3.928751000	-2.778262000	-0.751570000
1	-1.775073000	-3.262001000	1.365821000
1	-3.205702000	-2.241159000	1.597744000
1	-0.671346000	-3.052173000	-2.621891000

1	-2.151804000	-2.099137000	-2.428484000
1	0.019140000	-2.492324000	-0.318459000
1	-2.462871000	-0.755479000	-0.234442000
6	2.405597000	2.381814000	-0.630979000
8	3.072628000	2.254703000	0.374683000
6	2.728786000	3.305393000	-1.780152000
1	1.909564000	4.020963000	-1.912680000
1	3.661684000	3.834857000	-1.576827000
1	2.817198000	2.725344000	-2.705041000
1	0.209675000	1.303959000	4.902941000
1	0.345751000	1.325548000	4.172062000

TS_homo_AcO_q (G = -2566.508244) (quartet)

26	-0.244925000	0.665514000	-0.454502000
6	1.630671000	2.685330000	0.678338000
1	0.774172000	2.961038000	1.278049000
7	1.462965000	1.650135000	-0.167209000
7	1.059069000	-0.686894000	-1.270780000
6	2.842405000	3.357224000	0.762522000
7	-0.076824000	-0.513461000	1.280301000
7	-1.878331000	-0.438066000	-0.627294000
8	-0.428167000	1.420079000	-1.978111000
6	3.902893000	2.948176000	-0.047690000
6	3.718325000	1.881300000	-0.926361000
1	4.514005000	1.526602000	-1.571484000
6	2.478698000	1.257860000	-0.970811000
6	2.137606000	0.137005000	-1.899656000
1	1.749408000	0.541683000	-2.838830000
1	3.005291000	-0.488751000	-2.122057000
6	0.413799000	-1.516703000	-2.327723000
1	-0.098012000	-0.846577000	-3.016979000
1	-0.291043000	-2.209180000	-1.870923000
6	1.658179000	-1.524539000	-0.146429000
6	0.570579000	-1.821906000	0.871275000
6	0.648447000	0.172677000	2.383044000
1	0.206039000	1.159747000	2.512950000
1	1.704418000	0.262730000	2.131776000
6	-1.476058000	-0.772457000	1.721738000
1	-1.838184000	0.108067000	2.257019000
1	-1.506573000	-1.620440000	2.411353000
6	-2.322089000	-1.019854000	0.512849000
6	-3.486398000	-1.776995000	0.531742000
1	-3.802072000	-2.238380000	1.460455000
6	-4.212814000	-1.927631000	-0.647850000
6	-3.748177000	-1.322814000	-1.817532000
6	-2.577379000	-0.582613000	-1.771881000
1	-2.180355000	-0.086239000	-2.646371000
8	-1.136761000	1.938105000	0.603646000
1	4.862246000	3.452376000	0.005294000
1	2.943261000	4.184033000	1.455807000
1	-5.125723000	-2.514068000	-0.656610000
1	-4.280812000	-1.416792000	-2.756533000
1	0.538013000	-0.397499000	3.309161000
1	1.183554000	-2.071054000	-2.869590000
6	2.336629000	-2.811769000	-0.636300000
6	2.893036000	-3.600202000	0.557572000
6	1.767960000	-3.929471000	1.545092000
6	1.117633000	-2.635384000	2.050728000
1	1.014479000	-4.553522000	1.046429000
1	2.156327000	-4.495629000	2.398307000
1	3.366805000	-4.516395000	0.189490000
1	3.664722000	-3.007986000	1.067086000
1	1.600881000	-3.438328000	-1.149298000
1	3.128365000	-2.561581000	-1.348766000
1	0.307526000	-2.848565000	2.755263000
1	1.878326000	-2.049351000	2.575681000
1	-0.207167000	-2.412396000	0.378673000
1	2.412490000	-0.893885000	0.331236000
6	-2.367235000	2.332668000	0.790162000
8	-3.277701000	2.243880000	-0.047807000
6	-2.622768000	2.936359000	2.148550000
1	-1.816316000	3.635607000	2.391798000
1	-3.589133000	3.443511000	2.167555000
1	-2.612495000	2.134484000	2.896490000
1	-1.831593000	2.055437000	-2.032493000
1	-2.513581000	2.201858000	-1.618105000

II_homo_AcO_q (G = -2566.653324) (quartet)

26	0.289449000	-0.607801000	-0.517982000
6	-1.443083000	-2.868925000	0.525948000
1	-0.547212000	-3.119218000	1.079846000
7	-1.383143000	-1.761638000	-0.237825000
7	-1.285899000	0.738951000	-1.239403000
6	-2.590449000	-3.648485000	0.600976000
7	0.081121000	0.486862000	1.236044000
7	1.872172000	0.617593000	-0.735163000
8	0.507979000	-1.501455000	-2.064812000
6	-3.713778000	-3.263430000	-0.132916000
6	-3.648263000	-2.115591000	-0.920159000
1	-4.498299000	-1.773657000	-1.500440000
6	-2.460532000	-1.390545000	-0.961229000
6	-2.289578000	-0.172569000	-1.830379000
1	-1.913126000	-0.489848000	-2.807661000
1	-3.248953000	0.335493000	-1.978572000
6	-0.753971000	1.647435000	-2.280200000
1	-0.214404000	1.041870000	-3.011049000
1	-0.070060000	2.365316000	-1.825457000
6	-1.838408000	1.445319000	-0.034893000
6	-0.686330000	1.764516000	0.918196000
6	-0.551013000	-0.297095000	2.331870000
1	-0.050503000	-1.263062000	2.391110000
1	-1.608214000	-0.439788000	2.111473000
6	1.477688000	0.837823000	1.638403000
1	1.922171000	-0.038331000	2.117578000
1	1.475170000	1.651054000	2.369208000
6	2.266242000	1.215564000	0.418896000
6	3.323227000	2.116728000	0.446659000
1	3.601902000	2.580194000	1.386213000
6	3.989831000	2.413103000	-0.741286000
6	3.564525000	1.818007000	-1.930895000
6	2.497904000	0.932103000	-1.891175000
1	2.120104000	0.468343000	-2.793869000
8	1.473301000	-2.010925000	0.672125000
1	-4.628605000	-3.845739000	-0.088211000
1	-2.597275000	-4.532690000	1.228087000
1	4.818789000	3.113620000	-0.742252000
1	4.042628000	2.038151000	-2.878215000
1	-0.439344000	0.225751000	3.285579000
1	-1.562432000	2.185997000	-2.785755000
6	-2.650852000	2.701091000	-0.379283000
6	-3.146001000	3.400957000	0.891790000
6	-1.954834000	3.766524000	1.784511000
6	-1.179006000	2.500938000	2.171419000
1	-1.293993000	4.458577000	1.245520000
1	-2.293264000	4.273710000	2.694646000
1	-3.714428000	4.296801000	0.618628000
1	-3.822553000	2.734696000	1.443925000
1	-2.015577000	3.401383000	-0.932232000
1	-3.485968000	2.420493000	-1.029916000
1	-0.328536000	2.744614000	2.816222000
1	-1.852449000	1.847778000	2.735542000
1	0.017429000	2.414007000	0.388786000
1	-2.501701000	0.733902000	0.466938000
6	2.634480000	-2.386050000	0.862331000
8	3.645993000	-2.014997000	0.091942000
6	3.015232000	-3.273413000	2.000265000
1	2.284619000	-4.083081000	2.079971000
1	4.024485000	-3.671035000	1.883181000
1	2.960587000	-2.679116000	2.920804000
1	1.374041000	-1.376062000	-2.484930000
1	3.333174000	-1.434696000	-0.629883000

$[Fe^{III}(OO)(OCH_3)(BPMCN)]^{2+}$ (G = -2565.379400) (doublet)

26	-0.357177000	-0.573198000	0.117778000
6	1.336482000	-2.684653000	-1.103747000
1	0.534282000	-2.750302000	-1.828098000
7	1.202018000	-1.755751000	-0.137350000
7	0.926498000	0.409791000	1.316850000
6	2.450567000	-3.510393000	-1.168228000
7	0.129839000	0.774792000	-1.329865000
7	-1.926986000	0.647864000	0.288198000
8	-0.951982000	-1.634411000	1.461969000
6	3.450319000	-3.369991000	-0.203557000
6	3.299251000	-2.417999000	0.804050000
1	4.048643000	-2.280801000	1.575346000
6	2.153313000	-1.632725000	0.815640000
6	1.828464000	-0.635972000	1.886749000
1	1.285443000	-1.143261000	2.690747000
1	2.727739000	-0.182636000	2.312300000
6	0.242243000	1.111395000	2.436370000
1	-0.427842000	0.400329000	2.920360000
1	-0.328330000	1.952961000	2.045310000
6	1.740937000	1.347744000	0.442143000
6	0.828142000	1.926196000	-0.631458000
6	0.941210000	0.191076000	-2.434260000
1	0.438398000	-0.709799000	-2.787201000
1	1.936918000	-0.055334000	-2.068881000

6	-1.169869000	1.239318000	-1.904284000
1	-1.534444000	0.456948000	-2.577111000
1	-1.028415000	2.154983000	-2.484814000
6	-2.151581000	1.431528000	-0.789659000
6	-3.224885000	2.312332000	-0.841573000
1	-3.359486000	2.936190000	-1.718031000
6	-4.100884000	2.367428000	0.241597000
6	-3.871055000	1.545379000	1.346279000
6	-2.770266000	0.698792000	1.337174000
1	-2.540830000	0.044523000	2.167963000
8	-1.515186000	-1.665731000	-1.014539000
1	4.336175000	-3.996123000	-0.234785000
1	2.527412000	-4.243690000	-1.962655000
1	-4.947995000	3.045682000	0.226203000
1	-4.527527000	1.557559000	2.208677000
1	1.016183000	0.903790000	-3.259627000
1	0.975744000	1.467630000	3.163941000
6	2.465934000	2.452623000	1.219445000
6	3.241371000	3.361383000	0.255865000
6	2.287316000	3.971425000	-0.778026000
6	1.592787000	2.859610000	-1.575730000
1	1.535362000	4.584457000	-0.263451000
1	2.831886000	4.625428000	-1.467552000
1	3.745871000	4.147462000	0.827962000
1	4.015314000	2.779231000	-0.262086000
1	1.731634000	3.065004000	1.752949000
1	3.132244000	2.001561000	1.961566000
1	0.904160000	3.276916000	-2.317261000
1	2.359765000	2.289606000	-2.110302000
1	0.041384000	2.501447000	-0.134485000
1	2.489753000	0.723099000	-0.053613000
6	-2.235884000	-2.403117000	-0.307038000
8	-2.089059000	-2.453379000	0.997307000
6	-3.305095000	-3.278327000	-0.858393000
1	-2.840923000	-3.985835000	-1.554401000
1	-3.829444000	-3.819073000	-0.069050000
1	-4.005137000	-2.651822000	-1.421036000

I_homo_AcO_d (G = -2566.543376) (doublet)

26	0.380657000	0.583112000	0.224682000
6	-1.304589000	2.704195000	-1.001732000
1	-0.480052000	2.805722000	-1.694757000
7	-1.192540000	1.742631000	-0.065381000
7	-0.962629000	-0.500514000	1.291515000
6	-2.428221000	3.516327000	-1.070008000
7	-0.065418000	-0.747027000	-1.341809000
7	1.925223000	-0.684065000	0.373749000
8	0.876384000	1.452631000	1.514223000
6	-3.457155000	3.327404000	-0.145595000
6	-3.328988000	2.336907000	0.827389000
1	-4.103074000	2.156744000	1.564478000
6	-2.174120000	1.565844000	0.848677000
6	-1.882778000	0.521962000	1.882330000
1	-1.365231000	0.983303000	2.728933000
1	-2.794513000	0.043070000	2.248019000
6	-0.320769000	-1.268901000	2.394800000
1	0.322887000	-0.589545000	2.952281000
1	0.263084000	-2.087673000	1.976856000
6	-1.748291000	-1.387785000	0.333678000
6	-0.797210000	-1.921730000	-0.725617000
6	-0.823449000	-0.107029000	-2.450504000
1	-0.300172000	0.805729000	-2.735945000
1	-1.834535000	0.126716000	-2.119639000
6	1.252855000	-1.204215000	-1.872361000
1	1.651455000	-0.411295000	-2.511345000
1	1.130172000	-2.107605000	-2.475661000
6	2.185582000	-1.428858000	-0.723151000
6	3.262534000	-2.306526000	-0.764705000
1	3.428130000	-2.899744000	-1.656955000
6	4.101085000	-2.397082000	0.344577000
6	3.834619000	-1.609408000	1.466017000
6	2.735917000	-0.761214000	1.446561000
1	2.482977000	-0.126953000	2.286038000
8	1.432741000	1.581943000	-1.006282000
1	-4.349341000	3.943965000	-0.182304000
1	-2.488059000	4.278175000	-1.838541000
1	4.948995000	-3.074382000	0.335536000
1	4.462514000	-1.646664000	2.348638000
1	-0.865478000	-0.779052000	-3.311683000
1	-1.090727000	-1.664661000	3.061183000
6	-2.506619000	-2.522358000	1.033935000
6	-3.253936000	-3.372499000	-0.002989000
6	-2.267450000	-3.942457000	-1.028174000
6	-1.532186000	-2.801884000	-1.744248000
1	-1.541686000	-4.587967000	-0.515936000
1	-2.791488000	-4.555467000	-1.769185000
1	-3.786023000	-4.179170000	0.512523000
1	-4.002733000	-2.757014000	-0.518868000
1	-1.794540000	-3.167561000	1.557897000
1	-3.196232000	-2.105251000	1.774213000
1	-0.817604000	-3.192064000	-2.475829000
1	-2.270859000	-2.197947000	-2.281280000
1	-0.037325000	-2.529950000	-0.226351000
1	-2.475598000	-0.733891000	-0.155204000
6	2.175450000	2.513500000	-0.517447000
8	2.223143000	2.802552000	0.702511000
6	3.030945000	3.282331000	-1.489144000
1	2.384435000	3.688965000	-2.273357000
1	3.572230000	4.084908000	-0.986412000
1	3.735532000	2.580528000	-1.948464000
1	0.677674000	1.472911000	4.744195000
1	0.718153000	1.468910000	4.001329000

TS_homo_AcO_d (G = -2566.512473) (doublet)

26	-0.238611000	0.695526000	-0.454776000
6	1.658228000	2.694547000	0.675394000
1	0.801090000	2.991481000	1.264194000
7	1.478034000	1.653882000	-0.160134000
7	1.046706000	-0.701090000	-1.277694000
6	2.885268000	3.337081000	0.769170000
7	-0.067275000	-0.506897000	1.268447000
7	-1.895686000	-0.401230000	-0.611721000
8	-0.406551000	1.375145000	-1.979032000
6	3.945582000	2.893404000	-0.022694000
6	3.746276000	1.823474000	-0.894588000
1	4.540528000	1.445550000	-1.528160000
6	2.492710000	1.229255000	-0.949570000
6	2.138751000	0.118405000	-1.889442000
1	1.762809000	0.536066000	-2.829535000
1	3.001528000	-0.513290000	-2.114366000
6	0.390476000	-1.515905000	-2.336624000
1	-0.118132000	-0.838453000	-3.021856000
1	-0.323124000	-2.199901000	-1.880152000
6	1.638928000	-1.548022000	-0.159531000
6	0.551370000	-1.829564000	0.857933000
6	0.677905000	0.169513000	2.365248000
1	0.251373000	1.163336000	2.496134000
1	1.733721000	0.240046000	2.108043000
6	-1.469507000	-0.747646000	1.725753000
1	-1.813806000	0.138099000	2.263777000
1	-1.495713000	-1.593401000	2.417613000
6	-2.328468000	-0.989871000	0.525704000
6	-3.495636000	-1.743221000	0.551286000
1	-3.801239000	-2.213579000	1.478906000
6	-4.237810000	-1.875428000	-0.620529000
6	-3.785450000	-1.256528000	-1.786693000
6	-2.608653000	-0.523084000	-1.747638000
1	-2.219329000	-0.017679000	-2.620500000
8	-1.094895000	1.959331000	0.616571000
1	4.916535000	3.373937000	0.038446000
1	2.998227000	4.167382000	1.456369000
1	-5.153322000	-2.457789000	-0.625401000
1	-4.330343000	-1.334753000	-2.720182000
1	0.560316000	-0.400021000	3.290703000
1	1.149264000	-2.079349000	-2.884510000
6	2.298899000	-2.842807000	-0.655044000
6	2.843201000	-3.642463000	0.536971000
6	1.713946000	-3.955505000	1.524851000
6	1.086348000	-2.652133000	2.036679000
1	0.949094000	-4.565054000	1.025699000
1	2.093696000	-4.530342000	2.376058000
1	3.301474000	-4.565509000	0.166483000
1	3.624828000	-3.064017000	1.047037000
1	1.554586000	-3.456849000	-1.170776000
1	3.094442000	-2.600122000	-1.365798000
1	0.275438000	-2.854699000	2.743143000
1	1.858474000	-2.080048000	2.560342000
1	-0.240169000	-2.402879000	0.367682000
1	2.403725000	-0.930309000	0.318180000
6	-2.362651000	2.301193000	0.784696000
8	-3.251177000	2.161061000	-0.052550000
6	-2.608062000	2.942590000	2.130338000
1	-2.030731000	3.872989000	2.188804000
1	-3.670807000	3.160315000	2.253591000
1	-2.257191000	2.284424000	2.932103000
1	-1.767864000	2.288848000	-2.210987000
1	-2.386872000	2.351263000	-1.739121000

II_homo_AcO_d (G = -2566.658852) (doublet)

26	0.234991000	-0.610036000	-0.434992000
6	-1.553879000	-2.746050000	0.654499000
1	-0.696576000	-2.998120000	1.264574000
7	-1.415194000	-1.687172000	-0.165203000
7	-1.093008000	0.673616000	-1.249191000
6	-2.735433000	-3.474242000	0.718358000
7	0.064745000	0.530982000	1.284622000
7	1.883109000	0.506707000	-0.616818000
8	0.456097000	-1.412645000	-2.047190000
6	-3.807566000	-3.093609000	-0.090206000
6	-3.659414000	-2.000843000	-0.943131000
1	-4.464798000	-1.666952000	-1.587829000
6	-2.444070000	-1.326103000	-0.963003000
6	-2.145065000	-0.178537000	-1.877850000
1	-1.736472000	-0.565594000	-2.814359000
1	-3.038553000	0.411481000	-2.098909000
6	-0.480203000	1.523533000	-2.303908000
1	0.055450000	0.863674000	-2.985004000
1	0.208595000	2.233022000	-1.846336000
6	-1.711467000	1.487000000	-0.126562000
6	-0.624521000	1.819810000	0.885573000
6	-0.640018000	-0.178472000	2.385422000
1	-0.175454000	-1.156568000	2.511323000
1	-1.691826000	-0.299538000	2.129050000
6	1.457660000	0.828506000	1.726954000
1	1.846112000	-0.053320000	2.245259000
1	1.472688000	1.664695000	2.431836000
6	2.295672000	1.119509000	0.517852000
6	3.414057000	1.945451000	0.538492000
1	3.700707000	2.427577000	1.466370000
6	4.134367000	2.136597000	-0.639094000
6	3.703519000	1.507608000	-1.808818000
6	2.569197000	0.708627000	-1.762107000
1	2.183347000	0.207457000	-2.640756000
8	1.278770000	-1.927759000	0.609465000
1	-4.745703000	-3.638154000	-0.055139000
1	-2.806726000	-4.318167000	1.394907000
1	5.012050000	2.774778000	-0.647052000
1	4.228616000	1.635123000	-2.748367000
1	-0.550893000	0.384615000	3.318615000
1	-1.257112000	2.063123000	-2.851541000
6	-2.443825000	2.749344000	-0.600187000
6	-3.011093000	3.521838000	0.598511000
6	-1.883723000	3.891121000	1.570011000
6	-1.182214000	2.620923000	2.067656000
1	-1.159502000	4.539137000	1.058223000
1	-2.278509000	4.447841000	2.426792000
1	-3.522488000	4.421271000	0.238773000
1	-3.754192000	2.904423000	1.121022000
1	-1.739703000	3.401955000	-1.125856000
1	-3.236079000	2.472827000	-1.302947000
1	-0.371582000	2.863805000	2.762395000
1	-1.915998000	2.012422000	2.605618000
1	0.131316000	2.430912000	0.382627000
1	-2.435618000	0.828284000	0.361174000
6	2.414835000	-2.396082000	0.774102000
8	3.429778000	-2.157859000	-0.033802000
6	2.727037000	-3.274634000	1.936447000
1	1.979670000	-4.072461000	1.986177000
1	3.731956000	-3.692404000	1.865299000
1	2.635872000	-2.673381000	2.848815000
1	1.355148000	-1.748333000	-2.187846000
1	3.168656000	-1.575075000	-0.772845000

H_2 (G = -1.180942) (singlet)

1	0.000000000	0.000000000	0.371752000
1	0.000000000	0.000000000	-0.371752000

H_2O (G = -76.464043) (singlet)

8	0.000000000	0.000000000	0.120388000
1	0.000000000	0.757559000	-0.481551000
1	0.000000000	-0.757559000	-0.481551000

CH_3CN (G = -132.797503) (singlet)

6	0.000000000	0.000000000	-1.180293000
1	0.000000000	1.030352000	-1.551272000
1	0.892311000	-0.515176000	-1.551272000
1	-0.892311000	-0.515176000	-1.551272000
6	0.000000000	0.000000000	0.277406000
7	0.000000000	0.000000000	1.438735000

AcOH (G = -229.160637) (singlet)

6	-0.474791000	0.519312000	0.056040000
8	0.706750000	0.459885000	0.332936000
8	-1.100852000	1.686135000	-0.217914000
1	-0.437405000	2.397464000	-0.142477000
6	-1.421770000	-0.646803000	-0.025526000
1	-2.240567000	-0.506779000	0.689666000
1	-1.862286000	-0.697403000	-1.027280000
1	-0.887461000	-1.572186000	0.194834000

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