Electronic Supplementary Information

Heme compound II models in chemoselectivity and disproportionation reactions

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Experimental Section

Materials. Commercially available chemicals were used without further purification unless otherwise indicated. Solvents were dried according to the literature procedures and redistilled under Ar before use.[1] Iodosylbenzene (PhIO) was synthesized by a literature method.[2] *meta*-Chloroperoxybenzoic acid (*m*-CPBA; 77%) purchased from Aldrich Chemical Co. was purified by washing with phosphate buffer (pH 7.5) and then dried under reduced pressure.[3] $TPFPPH_2$ (*meso*-tetrakis(pentafluorophenyl)porphyrin) and $TMPH_2$ (*meso*-tetrakis(2,4,6-trimethylphenyl)porphyrin) were purchased from PorphyChem. Fe^{III}(TPFPP)(Cl) and Fe^{III}(TMP)(Cl) were prepared using established literature protocol.[4] $H_2{}^{18}O$ (95% ^{18}O-enriched) was purchased from Berry & Associates/ICON Isotopes (Dexter, MI, USA).

Instrumentation. UV-vis spectra were recorded on a Hewlett Packard Agilent 8453 UV-vis spectrophotometer equipped with an UNISOKU cryostat system (USP-203; UNISOKU, Japan). Coldspray ionization time-of-flight mass (CSI-MS) data were collected on a JMS-T100CS (JEOL) mass spectrometer equipped with a CSI source. Typical measurement conditions were as follows: needle voltage = 2.2 kV, orifice 1 current = 50-500 nA, orifice 1 voltage = 0 to 20 V, ring lens voltage = 10 V, ion source temperature = 278 K, and spray temperature = 233 K. Resonance Raman scattering was dispersed by a single polychromator (MC-100DG, Ritsu Oyo Kogaku) and was detected by a liquid-nitrogen-cooled CCD detector (model 7375-0001, Roper scientific). Raman spectra were collected with backscattering geometry at an excitation wavelength (λ_{ex}) of 405 nm (NT242, EKSPLA) using a spinning sample cell (NMR tube with 5 mm OD), which was placed in a thermostated quarts Dewar at 233 K by flashing cold nitrogen gas. The laser power at a measuring point in front of a quartz Dewar was adjusted to 20 mW. Raman shifts were calibrated using indene (accurate to within ± 1 cm^{-1}). X-band electron paramagnetic resonance (EPR) spectra were recorded at 5 K using an X-band Bruker EMX-plus spectrometer equipped with a dual mode cavity (ER 4116DM). Low temperatures were achieved and controlled with an Oxford Instruments ESR900 liquid Helium quartz cryostat fitted with an Oxford Instruments ITC503 temperature and gas flow controller. The experimental parameters for EPR spectra were as follows: microwave frequency = 9.647 GHz, microwave power = 1.0 mW, modulation amplitude = 10 G, gain = 1×10^4, modulation frequency = 100 kHz, time constant = 40.96 ms, and conversion time = 81.00 ms. Product analysis was performed with Agilent Technologies 6890N gas chromatograph (GC). Quantitative analysis were made on the basis of comparison of peak integration between products and authentic samples.

X-ray Absorption Spectroscopy. The Fe K-edge X-ray absorption spectra of **1** and **1a** were measured at the Stanford Synchrotron Radiation Lightsource (SSRL) on the unfocussed 20-pole 2 T wiggler side-station beam line 7-3 under standard ring conditions of 3 GeV and ~500 mA. A Si(220) double crystal monochromator was used for energy selection. The monochromator was detuned 30% to eliminate contributions from higher harmonics. The complexes were measured as solutions, which were transferred into 2 mm delrin XAS cells with 70 μm Kapton tape windows under synthesis conditions and were immediately frozen in cassettes after preparation and stored under liquid N_2. During data collection, samples were maintained at a constant temperature of ~10 K using a Cryo Industries closed cycle cryocooler. Data were measured to k = 14 $Å^{-1}$ (fluorescence mode) using a Canberra Ge 30-element array detector. Internal energy calibration was accomplished by simultaneous measurement of the absorption of a Fe-foil placed between two ionization chambers situated after the sample. The first inflection point of the foil spectrum was fixed at 7111.2 eV. The samples were monitored for photoreduction and no shift in the rising edge energy position was observed over successive scans, although a very small decrease in the pre-edge intensity was apparent, indicating insignificant levels of X-ray dose related photoreduction of the Fe center. Data presented here are 12-scan average for **1a** and were processed by fitting a second-order polynomial to the pre-edge region and subtracting this from the entire spectrum as background. A four-region spline of orders 2, 3, 3 and 3 was used to model the smoothly decaying post-edge region. The data were normalized by subtracting the cubic spline and assigning the edge jump to 1.0 at 7150 eV using the Pyspline program.[5]

Theoretical EXAFS signals $\chi(k)$ were calculated by using FEFF version 7.[6-8] Starting structural models were obtained by modifying DFT structures for related compounds and visualized in Avogadro.[9] Improvement of input structure was not required since the model provided accurate theoretical EXAFS signals. Data fitting was performed in EXAFSPAK.[10] The structural parameters varied during the fitting process were the bond distance (R) and the bond variance σ^2, which is related to the Debye-Waller factor resulting from thermal motion, and static disorder of the absorbing and scattering atoms. The non-structural parameter ΔE_0 (E_0 = the energy at which k is 0) was also allowed to vary but was restricted to a common value for every component in a given fit. Coordination numbers was systematically varied in the course of the fit but were fixed within a given fit.

Generation of Intermediate 1a. $[Fe^{IV}(O)(TPFPP)(Cl)]^-$ (**1a**) was generated by adding *meta*-chloroperoxybenzoic acid (*m*-CPBA, 4.0 equiv., 2.0 mM) into a UV-vis cuvette containing a

MeCN solution of Fe^{III}(TPFPP)(Cl) (**1**) (0.50 mM, containing 15 μL H_2O) at 283 K. Formation of **1a** was confirmed by monitoring UV-vis spectral changes at 545nm due to the formation of **1a** and 500 nm due to the decay of **1**. **1a** can also be generated by adding PhIO (4.0 equiv., 0.40 mM) into a UV-vis cuvette containing a MeCN solution of **1** (0.10 mM, containing 15 μL H_2O) at 283 K. The ^{18}O-labeled complex $[Fe^{IV}(^{18}O)(TPFPP)(Cl)]^-$ (**1a**-^{18}O) was generated by adding $PhI^{18}O$ (4.0 equiv., 0.40 mM) into a UV-vis cuvette containing a MeCN solution of **1** (0.10 mM, containing a small amount of $H_2{}^{18}O$) at 283 K.

Generation of Intermediate 2a. $[Fe^{IV}(O)(TMP)(Cl)]^-$ (**2a**) was generated by adding PhIO (3.0 equiv., 0.30 mM) into a UV-vis cuvette containing a butyronitrile solution of Fe^{III}(TMP)(Cl) (**2**) (0.10 mM) at 253 K. Formation of **2a** was confirmed by monitoring UV-vis spectral changes at 545 nm due to the formation of **2a** and 505 nm due to the decay of **2**.

Kinetic Studies and Product Analysis. All reactions were performed in a 1.0 cm quartz cuvette and followed by monitoring UV-vis spectral changes of **1a** in CH_3CN at 283 K and **2a** in butyronitrile at 253 K. The kinetic experiments were run at least in triplicate, and the data reported here represent the average values of these reactions. Rate constants were determined under pseudo-first-order conditions (*i.e.*, [substrate]/[intermediate] > 10) by fitting the changes in absorbance at 545 nm due to the decay of **1a** or **2a**. The second-order rate constants in the oxidation of cyclohexene by **2a** were determined by a least-squares curve fit of the second-order plot ($[substrate]^{-1}$ *vs.* time). Kinetic isotope effect was determined by comparing the rate constants obtained in the oxidation of cyclohexene-h_{10} and cyclohexene-d_{10} by **1a** or **2a**. Reactions were run at least in triplicate, and the data reported represent the average of these reactions.

Products formed in the oxidation of cyclohexene were analyzed by GC and GC-MS. The decay product of **1a** and **2a** was analyzed with UV-vis and EPR spectroscopies. In both the reactions, Fe^{III} species were produced.

Computational Details. Density functional theory (DFT)[11] geometry optimizations and frequency calculations were done at the UB3LYP/Def2-SVP level[12-17] using the Gaussian 09 package.[18] Solvent effects (butyronitrile) were included in the geometry optimizations by use of the conductor-like polarizable continuum model (CPCM) implementation[19] in Gaussian 09. Vibrational frequency analysis was performed to ascertain the stationary points. The transition states (TS) had one imaginary frequency, whereas the ground states had all positive frequencies. The continuity on the potential energy surface was confirmed by intrinsic

reaction coordinate (IRC) calculations on the TSs. Single point energy evaluations were carried out at the UB3LYP/Def2-TZVPP level[16,17] including the solvent. Dispersion effects were included by evaluating its effects at the converged geometries by use of the DFT-D3 program using the Becke-Johnson damping.[20] The free energies were also evaluated at 253 K. The free energy ΔG include the following terms: the electronic energy (ΔE), zero-point vibrational energy (ΔZ_0), enthalpy ($\Delta E_{\text{thermal}}$), entropy ($-T\Delta S$), dispersion effect ($\Delta$Disp) and correction for change of standard state in solution upon complexation (ΔG_{corr}).[21-22] However, the calculations performed in solvent make the thermal contributions inaccurate, because the standard solvent models have been parameterized to give good solvation free energies and not any other properties. This means that thermal effects are already included to a certain extent in the obtained electronic energies, therefore possibly double-counting the thermal contributions.[23] The same consideration applies to the dispersion correction as well. On the other hand, gas-phase frequency calculations on the optimized structure in solvation may not be meaningful since the structure may be not in a stationary point in the gas-phase. Based on the above description, the free energy barrier is not deemed to be reliable due to possible double counting of effects. In our repeated and consistent experience, the calculated electronic energies (ΔE) are actually closer to the experimentally measured rate constants, when using the Eyring equation to convert between these two formats (as can be seen in this study). We attribute this to the empirical parametrization of B3LYP and the solvation scheme. Thus, the electronic energies are mainly discussed in the main text, but free energies are also provided in the SI.

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Table S1 EXAFS least square fitting results for $[Fe^{IV}(O)(TPFPP)(Cl)]^-$ (**1a**).

complex	coordination/path	R(Å)[a]	σ^2(Å^2)[b]	ΔE_0 (eV)	F [c]
	1 Fe-O	1.65	103		
	4 Fe-N	2.00	185		
	1 Fe-Cl	2.24	941		
1a	8 Fe-C	3.03	223	–2.3	0.42
	16 Fe-C-N	3.27	[d]/223		
	16 Fe-C-N	4.31	552		
	16 Fe-C-N	4.98	392		

[a] The estimated standard deviations for the distances are in the order of ± 0.02 Å. [b] The σ^2 values are multiplied by 10^5. [c] Error is given by $\Sigma[(\chi_{obsd} - \chi_{calcd})^2 k^6]/\Sigma[(\chi_{obsd})^2 k^6]$. The S_0^2 factor was set at 0.9. [d] '/' represents that the parameter was locked to the parent single scattering path.

Table S2 Relative energies (in kcal mol^{-1}) of $[Fe^{IV}(O)(TPFPP)(Cl)]^-$ (**1a**) and $[Fe^{IV}(O)(TMP)(Cl)]^-$ (**2a**).

	ΔDef2-SVP	ΔDef2-TZVPP	$\Delta \boldsymbol{E}^a$	ΔZ_0	$\Delta E_{thermal}{}^b$	$-T\Delta S^b$	ΔDisp	$\Delta \boldsymbol{G}^c$
1a								
^{1}**1a**	9.23	+0.02	**9.26**	−0.03	+0.01	+0.62	−0.01	**9.86**
^{3}**1a**	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
^{5}**1a**	11.63	+1.08	**12.71**	−1.54	+0.36	−1.45	+0.62	**10.63**
^{7}**1a**[d]	28.85	+0.33	**29.19**	−2.54	+0.71	−2.22	+0.53	**25.67**
^{7}**1a**[e]	46.14	+2.74	**48.88**	−3.83	+0.52	−1.18	+0.54	**44.92**
2a								
^{1}**2a**	9.12	−0.05	**9.07**	+0.03	−0.54	+1.89	+0.05	**10.51**
^{3}**2a**	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
^{5}**2a**	12.46	+0.68	**13.14**	−1.30	+0.22	−1.08	+0.62	**11.60**
^{7}**2a**[d]	29.37	−0.72	**28.65**	−2.30	+0.53	−1.83	−2.11	**22.94**
^{7}**2a**[e]	44.42	+4.66	**46.09**	−3.42	+0.48	−1.76	+0.65	**42.03**

[a] Sum of the two previous columns. [b] T = 298.15 K. [c] $\Delta \boldsymbol{G}$ = Sum of the five previous columns. However, these values are not deemed to be reliable due to possible double counting of effects, as described in "Computational details" section in the main text. [d] A septet state with an electronic configuration of $d_{xy}{}^1,\pi^*_{xz}{}^1,\pi^*_{yz}{}^1,\sigma^*_{x2\text{-}y2}{}^1,\sigma^*_{z2}{}^1,a_{2u}{}^1$. [e] A septet state with an electronic configuration of $d_{xy}{}^1,\pi^*_{xz}{}^1,\pi^*_{yz}{}^1,\sigma^*_{x2\text{-}y2}{}^1,\sigma^*_{z2}{}^0,a_{2u}{}^1,e_{2g}{}^1$.

Table S3 Key bond lengths (Å) of $[Fe^{IV}(O)(TPFPP)(Cl)]^-$ (**1a**) and $[Fe^{IV}(O)(TMP)(Cl)]^-$ (**2a**) calculated at the B3LYP/Def2-SVP level.

	Fe-O	Fe-N1	Fe-N2	Fe-N3	Fe-N4	Fe-Cl
1a						
^{1}**1a**	1.63	2.03	2.03	2.03	2.03	2.44
^{3}**1a**	1.63	2.03	2.03	2.03	2.03	2.45
^{5}**1a**	1.63	2.09	2.09	2.09	2.09	2.43
^{7}**1a**[a]	1.95	2.09	2.11	2.11	2.09	2.45
^{7}**1a**[b]	1.63	2.10	2.11	2.11	2.10	2.42
2a						
^{1}**2a**	1.63	2.03	2.03	2.03	2.03	2.52
^{3}**2a**	1.63	2.03	2.03	2.03	2.03	2.52
^{5}**2a**	1.63	2.09	2.09	2.09	2.09	2.49
^{7}**2a**[a]	1.95	2.08	2.10	2.10	2.08	2.53
^{7}**2a**[b]	1.62	2.10	2.10	2.10	2.10	2.45

[a] A septet state with an electronic configuration of $d_{xy}^1,\pi^*_{xz}{}^1,\pi^*_{yz}{}^1,\sigma^*_{x2\text{-}y2}{}^1,\sigma^*_{z2}{}^1,a_{2u}{}^1$. [b] A septet state with an electronic configuration of $d_{xy}^1,\pi^*_{xz}{}^1,\pi^*_{yz}{}^1,\sigma^*_{x2\text{-}y2}{}^1,\sigma^*_{z2}{}^0,a_{2u}{}^1,e_{2g}{}^1$.

Table S4 Mulliken spin density distribution of the oxidation of cyclohexene by $[Fe^{IV}(O)(TPFPP)(Cl)]^{-}$ (**1a**) calculated at the B3LYP/Def2-TZVPP//Def2-SVP level.

	Fe	O	4 × N	TPFPP − 4 × N	Cl	H/C	CHE – H/C
$S = 0$							
^{3}**1a**+CHE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
^{1}**RC**	0.01	−0.01	0.00	0.00	0.00	0.00	0.00
$^{1\alpha}$**TS**$_{H}$	0.86	−0.46	−0.09	0.02	0.00	0.05	−0.43
$^{1\alpha}$**TS**$_{Ep}$	0.84	−0.42	−0.08	0.02	0.00	0.12	−0.49
$S = 1$							
^{3}**1a**+CHE	1.32	0.76	−0.06	−0.03	0.00	0.00	0.00
^{3}**RC**	1.32	0.76	−0.06	−0.03	0.00	0.00	0.00
$^{3\alpha}$**TS**$_{H}$	2.35	0.17	−0.12	0.01	0.06	0.04	−0.50
$^{3\alpha}$**IM**$_{H}$	2.74	0.25	−0.13	0.04	0.09	0.01	−0.99
$^{3\beta}$**TS**$_{H}$	1.05	0.58	−0.05	−0.02	0.00	−0.04	0.48
$^{3\beta}$**IM**$_{H}$	0.99	0.07	−0.08	0.01	0.00	0.00	1.00
$^{3\alpha}$**TS**$_{Ep}$	2.25	0.20	−0.11	0.00	0.05	0.12	−0.50
$^{3\alpha}$**IM**$_{Ep}$	2.67	0.22	−0.13	0.03	0.09	0.04	−0.92
$^{3\beta}$**TS**$_{Ep}$	1.00	0.66	−0.04	−0.03	0.00	−0.13	0.54
$^{3\beta}$**IM**$_{Ep}$	0.97	0.15	−0.07	0.01	0.00	−0.05	1.00
$S = 2$							
^{5}**1a**+CHE	3.19	0.56	0.21	0.05	−0.01	0.00	0.00
^{5}**RC**	3.20	0.56	0.21	0.05	−0.01	0.00	0.00
$^{5\alpha}$**TS**$_{H}$	3.91	0.14	0.22	0.08	0.06	0.02	−0.42
$^{5\alpha}$**IM**$_{H}$	4.22	0.28	0.26	0.11	0.11	0.01	−0.99
$^{5\beta}$**TS**$_{H}$	2.99	0.42	0.14	0.05	−0.02	−0.03	0.45
$^{5\beta}$**IM**$_{H}$	2.74	0.26	−0.14	0.05	0.09	0.01	1.00
$^{5\alpha}$**TS**$_{Ep}$	3.87	0.16	0.22	0.07	0.06	0.07	−0.46
$^{5\alpha}$**IM**$_{Ep}$	4.17	0.26	0.25	0.09	0.10	0.04	−0.91
$^{5\alpha}$**TS**$_{Ep}$	2.98	0.48	0.14	0.04	−0.02	−0.10	0.49
$^{5\beta}$**IM**$_{Ep}$	2.88	0.07	0.08	0.06	−0.02	−0.04	0.97

Table S5 Comparison of the reaction energy barriers (in kcal/mol) of hydroxylation ($\mathbf{TS_H}$) and epoxidation ($\mathbf{TS_{Ep}}$) of cyclohexene by **1b** and **2b** calculated at the B3LYP/Def2TZVPP level.

	1b	**2b**
$S = 1/2$		
$\mathbf{TS_H}$	**10.18**	**16.44(13.63)**[a]
$\mathbf{TS_{Ep}}$	**8.39**	**12.88(10.45)**[a]
$S = 3/2$		
$\mathbf{TS_H}$	**12.36**	**19.01**
$\mathbf{TS_{Ep}}$	**10.70**	**18.72**

[a] Values within the parenthesis are taken from reference 11c in the main text, while those out of the parenthesis are obtained from single-point calculations on the previously optimized structures at the B3LYP/Def2-TZVPP level.

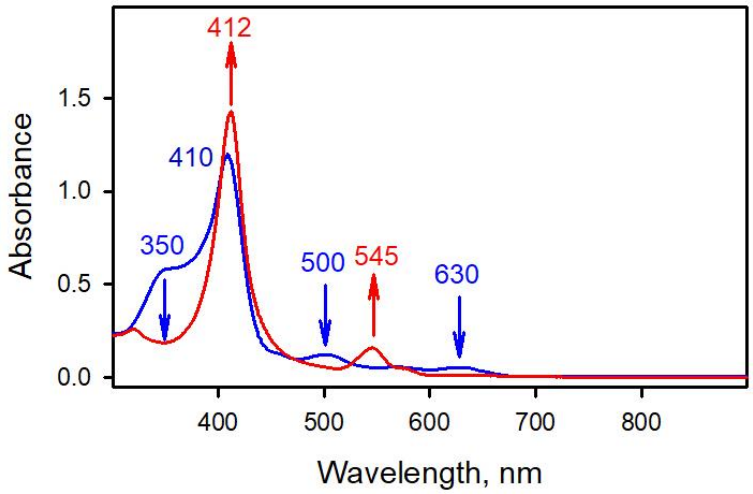

Fig. S1 UV-vis spectral change showing the formation of **1a** (red line) in the reaction of **1** (0.10 mM, blue line) and *m*-CPBA (0.40 mM) in the presence of 15 μL H_2O in MeCN at 283 K. A 0.10 cm quartz cuvette was used.

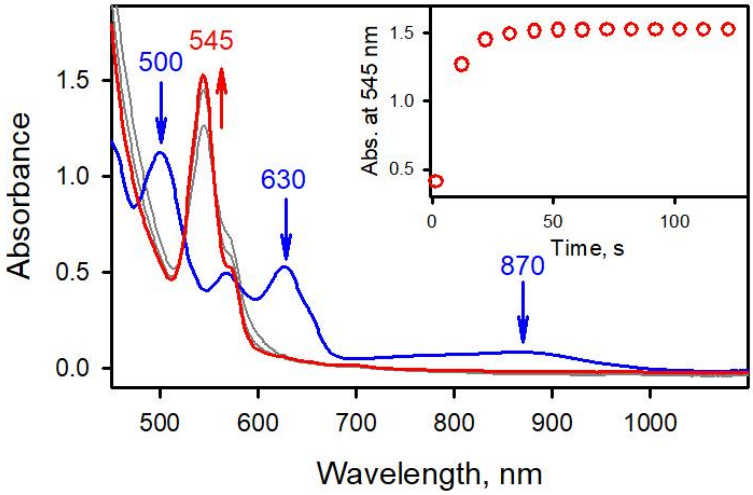

Fig. S2 UV-vis absorption spectral change showing the formation of **1a** (red line) in the reaction of **1** (0.10 mM; blue line) and PhIO (0.40 mM, dissolved in 50 µL MeOH) in the presence of 15 µL H_2O in MeCN at 283 K. Inset shows time profile of absorbance monitored at 545 nm due to the formation of **1a**.

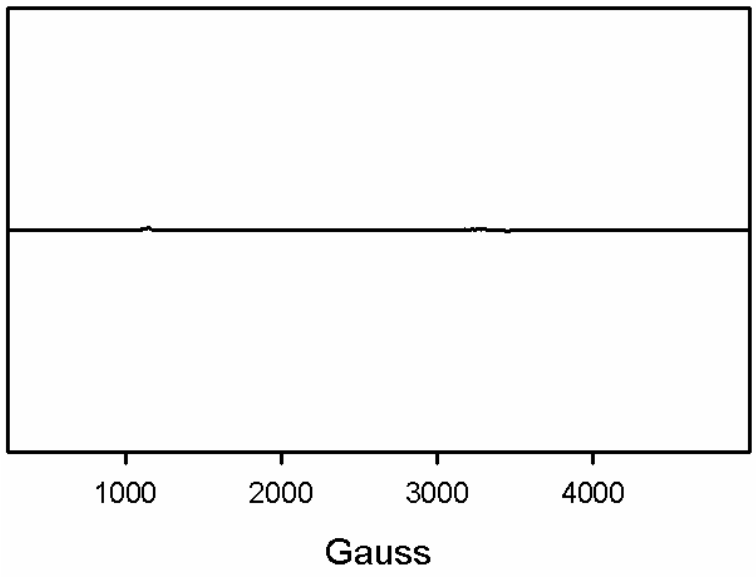

Fig. S3 X-band EPR spectrum of **1a** produced in the reaction of **1** (0.50 mM) with *m*-CPBA (2.0 mM) in MeCN at 283 K. Spectrum was recorded at 5 K.

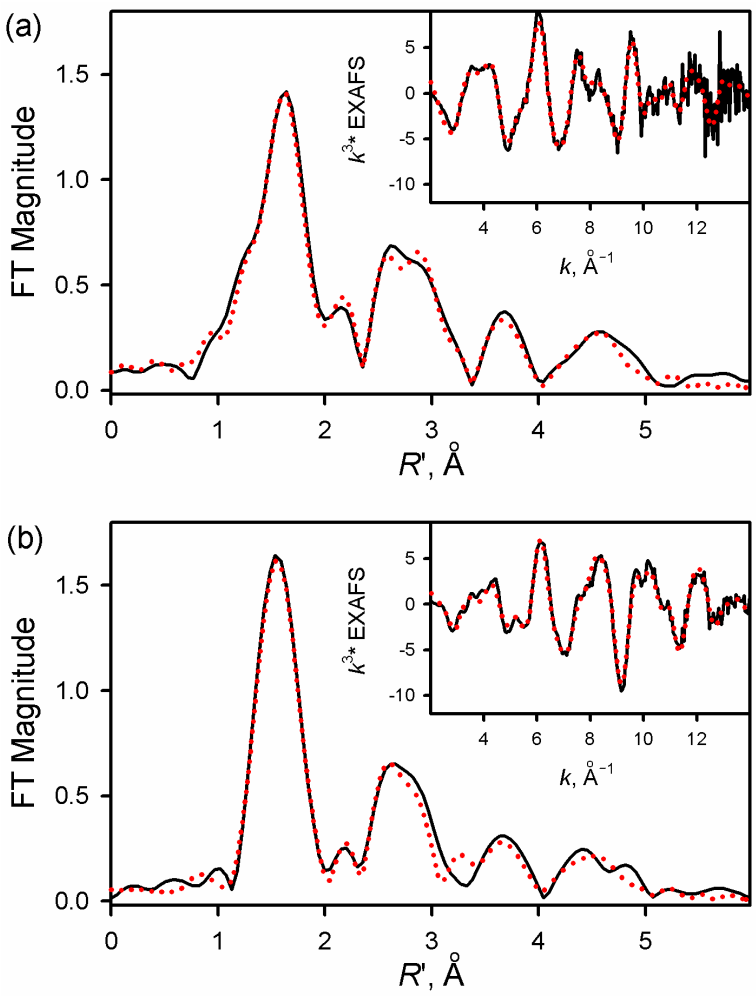

Fig. S4 Nonphase-shift-corrected Fourier transforms (black lines) for (a) **1** and (b) **1a**. Insets show the corresponding EXAFS data. The dotted red lines are FEFF best fits for **1** and **1a**.

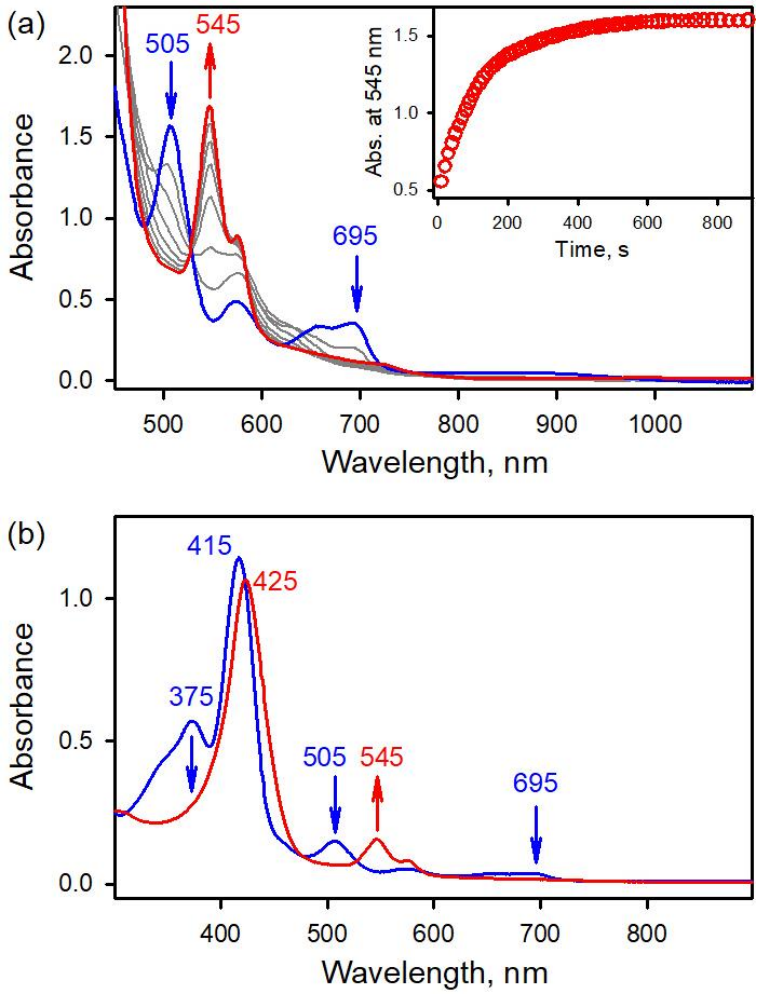

Fig. S5 (a) UV-vis absorption spectral change showing the formation of **2a** (red line) in the reaction of **2** (0.10 mM; blue line) and PhIO (0.30 mM, dissolved in 50 µL MeOH) in butyronitrile at 253 K. Inset shows time profile of absorbance monitored at 545 nm due to the formation of **2a**. (b) UV-vis absorption spectral change, which was measured using a 0.10 cm quartz cuvette, showing the formation of **2a** (red line) in the reaction of **2** (0.10 mM; blue line) and PhIO (0.30 mM, dissolved in 20 µL MeOH) in butyronitrile at 253 K.

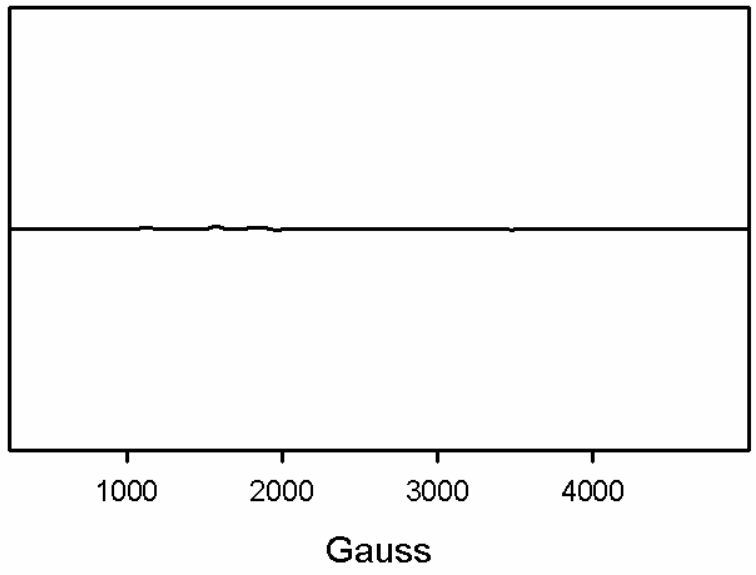

Fig. S6 X-band EPR spectrum of **2a** produced in the reaction of **2** (0.50 mM) with *m*-CPBA (1.5 mM, dissolved in 20 µL MeOH) in butyronitrile at 233 K. Spectrum was recorded at 5 K.

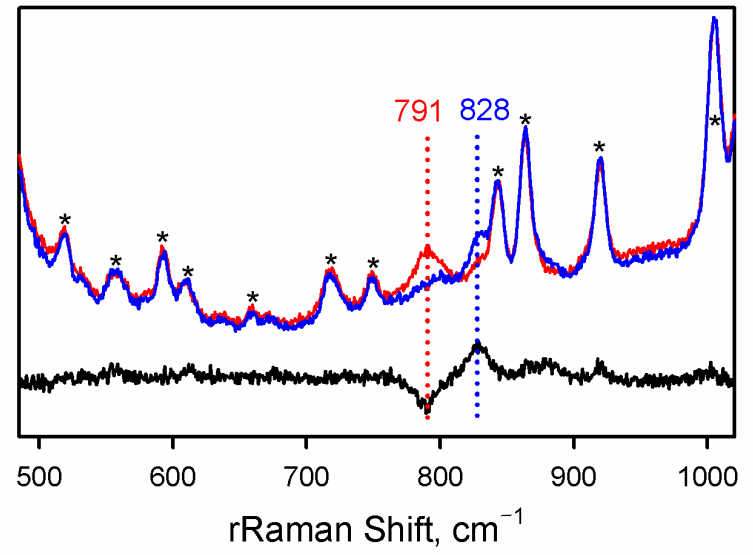

Fig. S7 rRaman spectra of **2a**-^{16}O (blue line) and **2a**-^{18}O (red line) obtained upon excitation at 442 nm in butyronitrile/MeCN (1:1) at 213 K. Black line is the difference spectrum of **2a**-^{16}O and **2a**-^{18}O. The observed isotopic shift of –37 cm^{-1} is in good agreement with the calculated value for a diatomic Fe-O bond oscillator (–37 cm^{-1}). The peaks marked with an asterisk are originated from solvent.

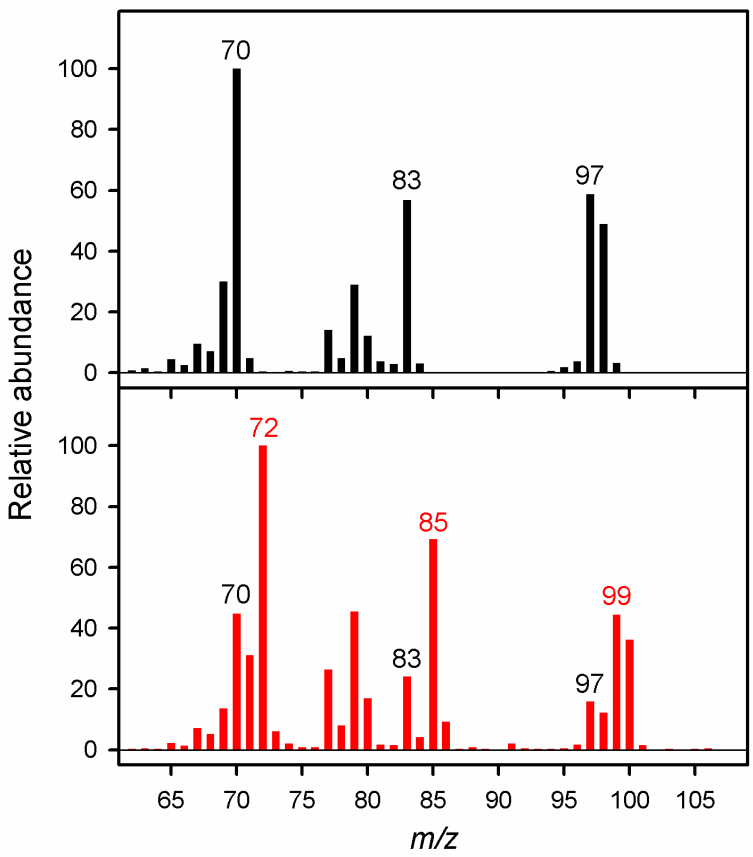

Fig. S8 GC-MS spectra of 2-cyclohexene-1-ol (black, top) as an authentic reference and 2-cyclohexene-1-ol product (red, bottom) obtained in the oxidation of cyclohexene by **1a**-^{18}O in MeCN at 283 K. The percentage of ^{18}O (~75%) in the 2-cyclohexen-1-ol product (red, bottom) was determined by comparison of the relative abundances at *m/z* = 85 for 2-cyclohexen-1-ol-^{18}O and at *m/z* = 83 for 2-cyclohexen-1-ol-^{16}O.

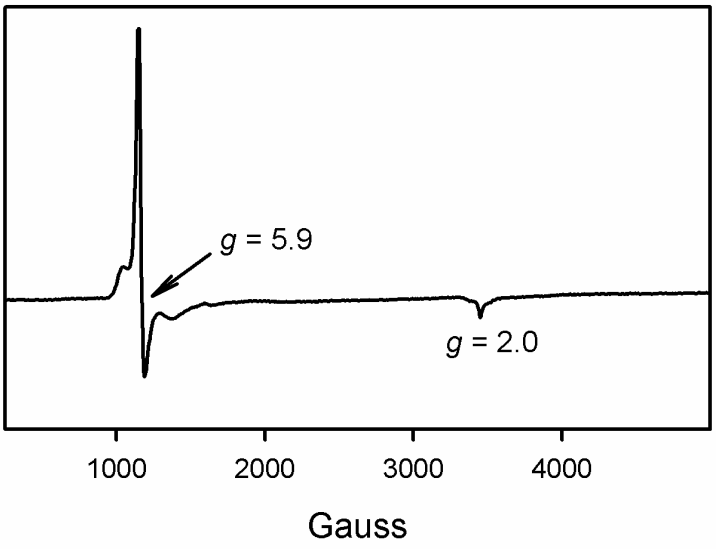

Fig. S9 X-band EPR spectrum of the complete reaction solution obtained in the oxidation of cyclohexene (200 mM) by **1a** (0.50 mM) in MeCN at 283 K. Spectrum was recorded at 5 K.

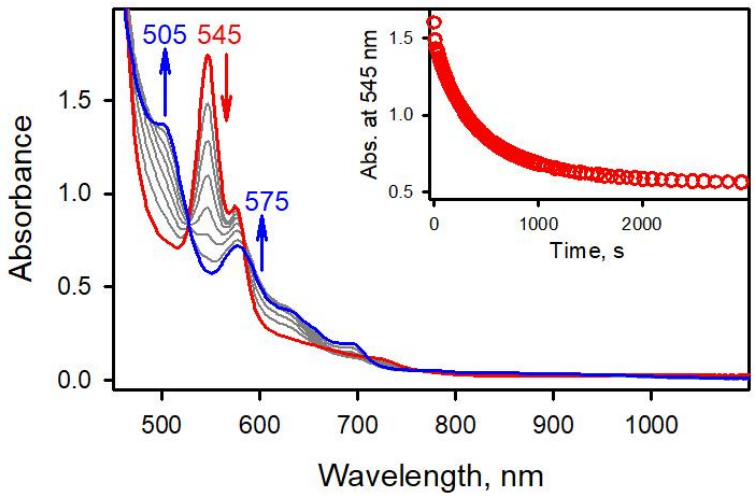

Fig. S10 UV-vis absorption spectral change observed in the reaction of **2a** (0.10 mM, red line) with cyclohexene (100 mM) in butyronitrile at 253 K. Inset shows time profile of absorbance monitored at 545 nm due to the decay of **2a**.

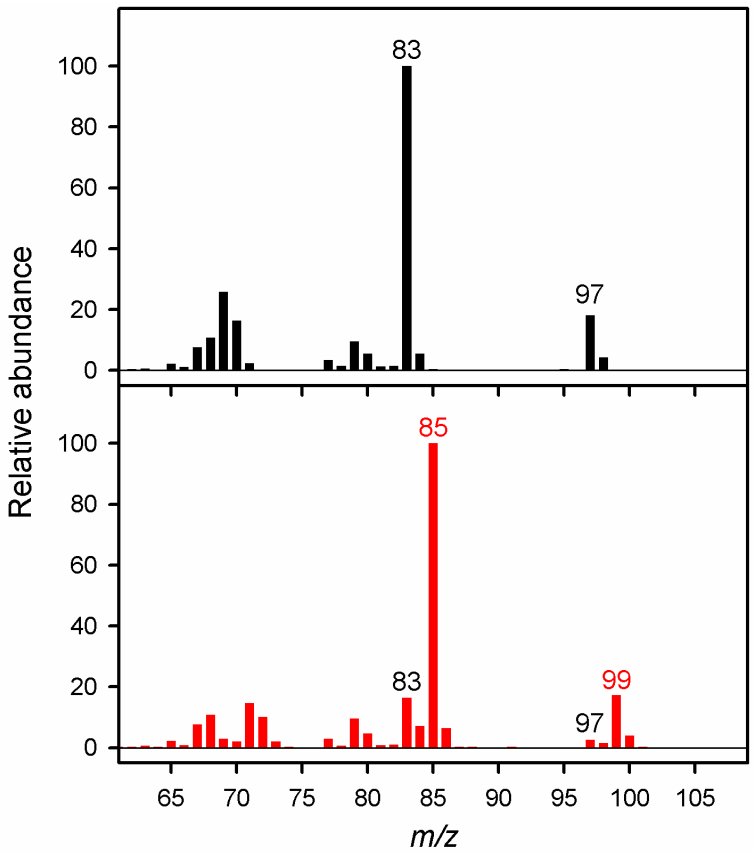

Fig. S11 GC-MS spectra of cyclohexene oxide (black, top) as an authentic reference and cyclohexene oxide product (red, bottom) obtained in the oxidation of cyclohexene by **2a**-^{18}O in butyronitrile at 253 K. The percentage of ^{18}O (~86 %) in the cyclohexene oxide product (red, bottom) was determined by comparison of the relative abundances at *m/z* = 85 for cyclohexene oxide-^{18}O and at *m/z* = 83 for cyclohexene oxide-^{16}O.

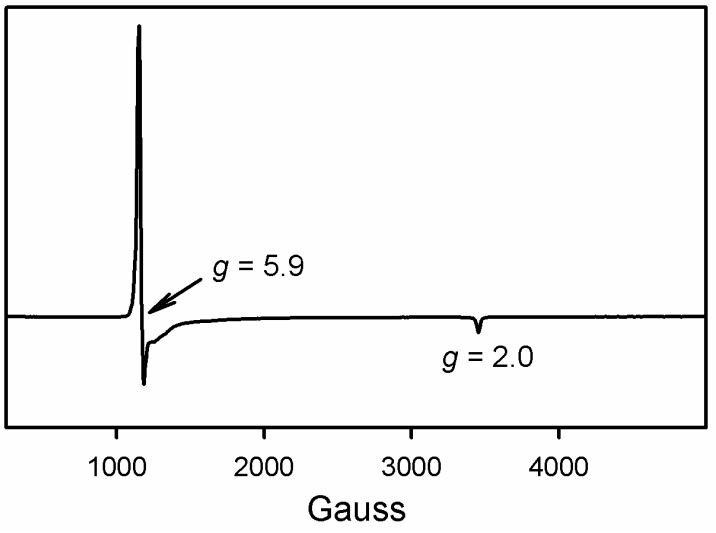

Fig. S12 X-band EPR spectrum of the complete reaction solution obtained in the oxidation of cyclohexene (100 mM) by **2a** (0.50 mM) in butyronitrile at 253 K. Spectrum was recorded at 5 K.

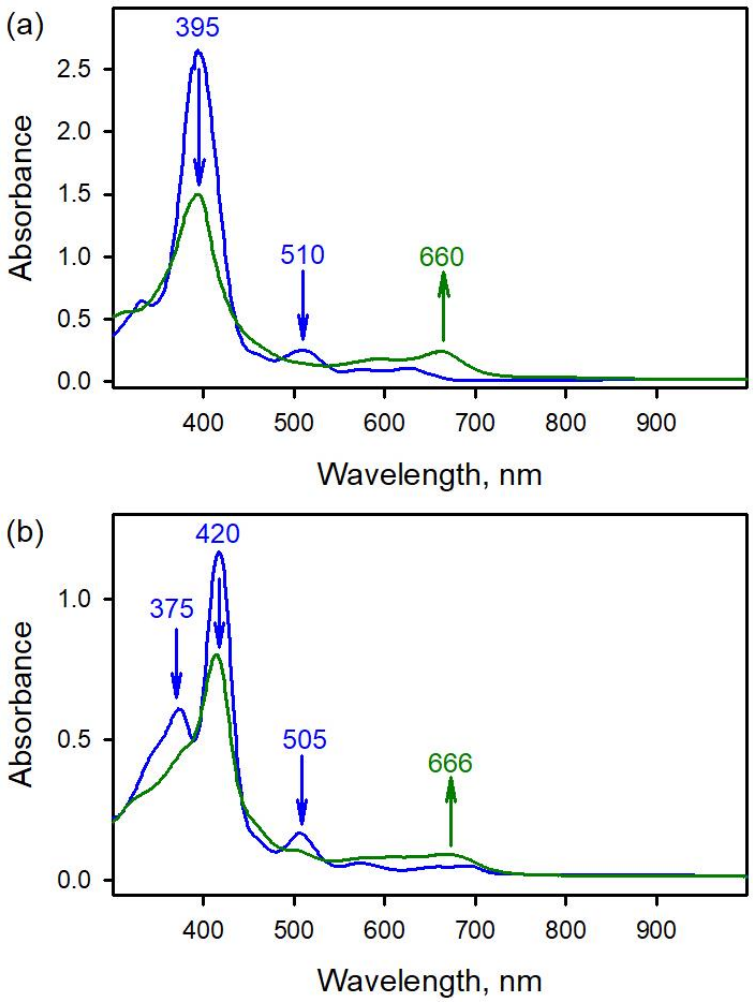

Fig. S13 (a) UV-vis absorption spectral change, measured using a 0.10 cm quartz cuvette, showing the formation of **1b** (green line) in the reaction of $[Fe^{III}(TPFPP)]^+$ (0.020 mM; blue line) and *m*-CPBA (0.080 mM) in CH_2Cl_2 at 213 K. (b) UV-vis absorption spectral change, measured using a 0.10 cm quartz cuvette, showing the formation of **2b** (green line) in the reaction of $[Fe^{III}(TMP)]^+$ (0.10 mM; blue line) and *m*-CPBA (0.40 mM) in butyronitrile at 253 K.

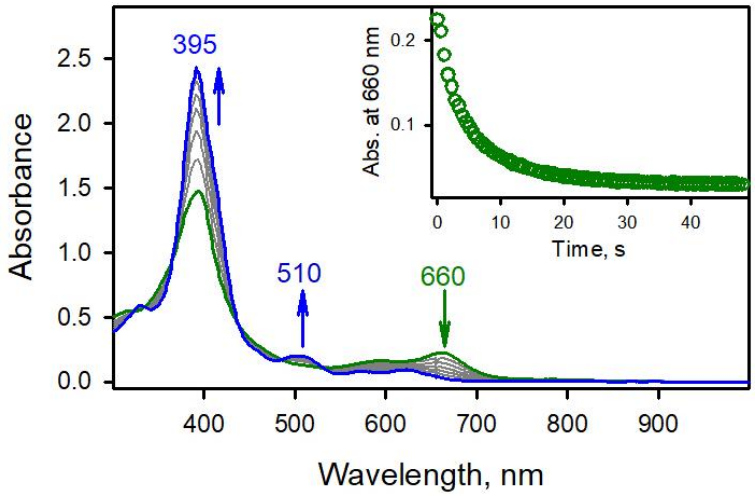

Fig. S14 UV-vis absorption spectral change observed in the reaction of **1b** (0.020 mM; green line) with cyclohexene (0.020 mM) in CH_2Cl_2 at 213 K. Spectra were measured using a 0.10 cm quartz cuvette. Inset shows time profile of absorbance monitored at 660 nm due to the decay of **1b**.

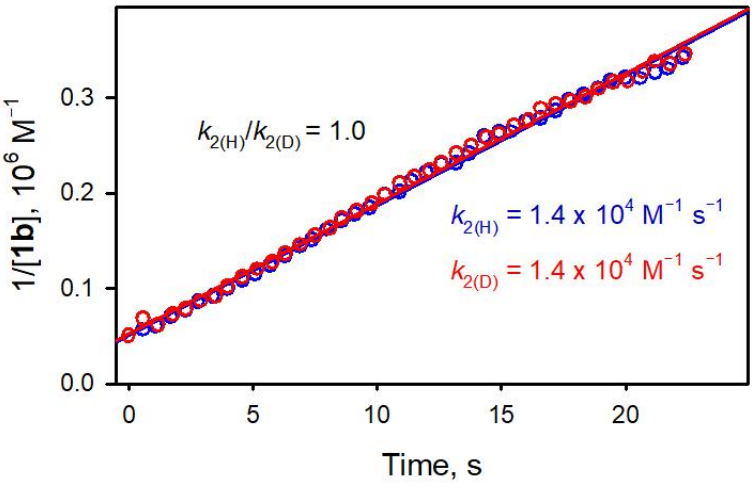

Fig. S15 Second-order plots of 1/[**1b**] *vs.* time for the oxidation of cyclohexene-h_{10} (0.020 mM, blue circles) and cyclohexene-d_{10} (0.020 mM, red circles) by **1b** (0.020 mM) in CH_2Cl_2 at 213 K.

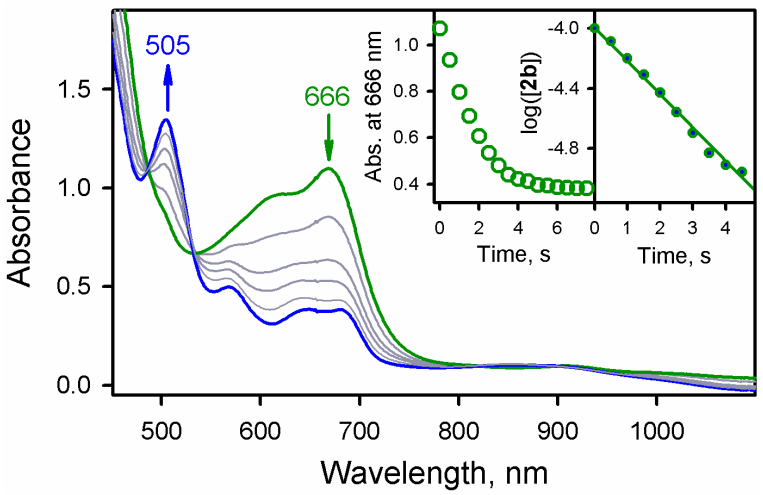

Fig. S16 UV-vis absorption spectral change observed in the oxidation of cyclohexene (5.0 mM) by **2b** (0.10 mM; green line) in butyronitrile at 253 K. Insets show time profile of absorbance monitored at 666 nm due to the decay of **2b** (left panel) and the first-order plot of log([**2b**]) *vs.* time (right panel) in the oxidation of cyclohexene (5.0 mM) by **2b** (0.10 mM; green line) in butyronitrile at 253 K.

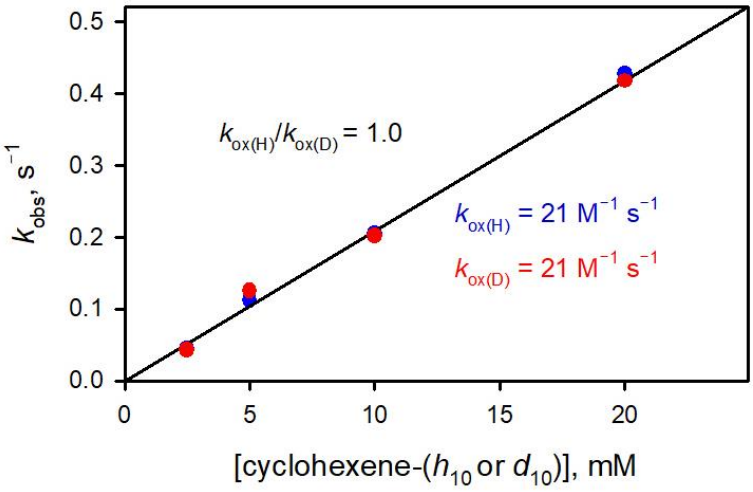

Fig. S17 Plots of pseudo-first-order rate constants (k_{obs}) against the concentration of cyclohexene-h_{10} (blue circles) and cyclohexene-d_{10} (red circles) for the oxidation of cyclohexene-h_{10} and cyclohexene-d_{10} by **2b** in butyronitrile at 253 K to determine KIE value.

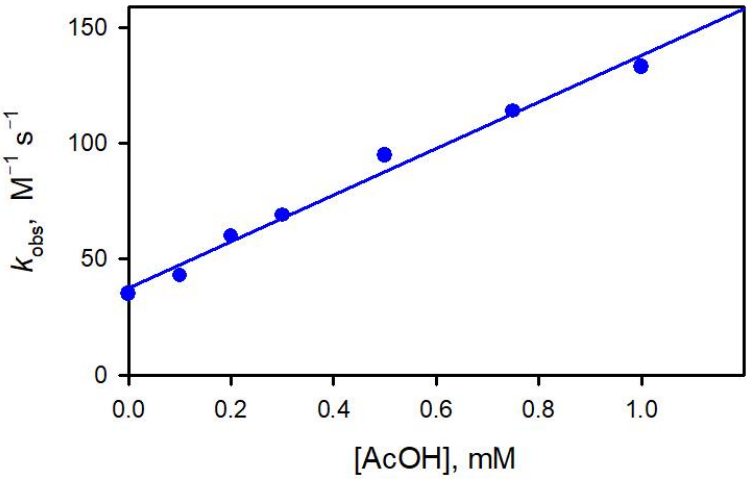

Fig. S18 Plot of the second-order rate constant (k_{obs}) *vs.* concentration of AcOH for the reaction of **2a** (0.10 mM) with cyclohexene-h_{10} (100 mM) in the presence of AcOH in butyronitrile at 253 K.

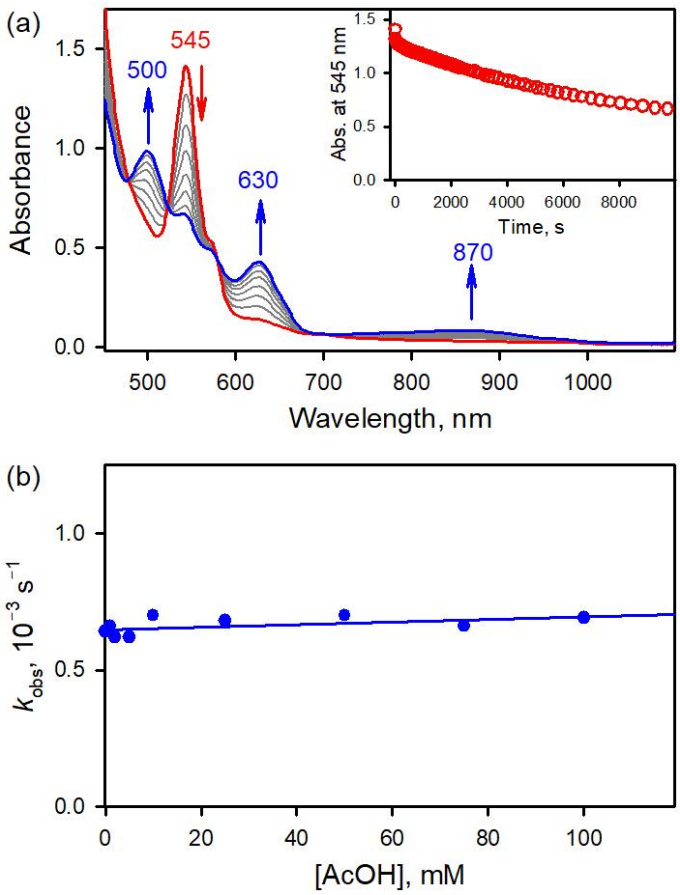

Fig. S19 (a) UV-vis absorption spectral change observed upon addition of AcOH (100 mM) to an MeCN solution of **1a** (0.10 mM; red line) at 283 K. Inset shows time profile of absorbance monitored at 545 nm due to the natural decay of **1a** in the presence of AcOH (100 mM). (b) Plot of the apparent first-order rate constant (k_{obs}) *vs.* the concentration of AcOH for the reaction of **1a** (0.10 mM) with cyclohexene (100 mM) in the presence of AcOH in MeCN at 283 K.

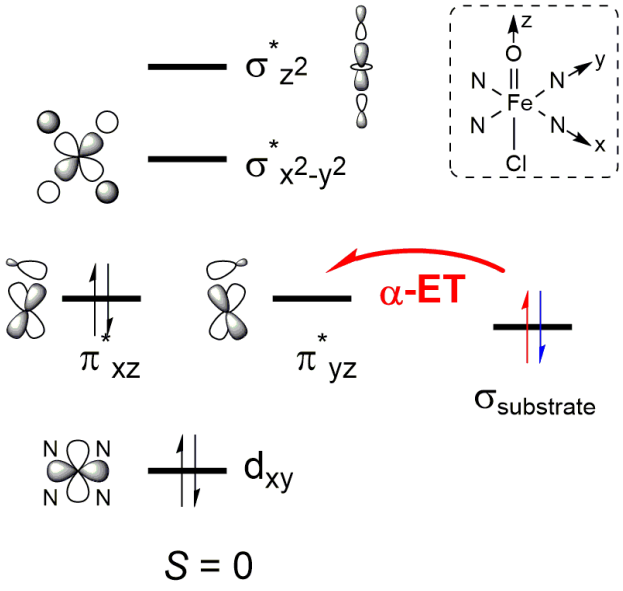

Fig. S20 Electron transfer pathway (α-ET) on the singlet (*S* = 0) spin state surface during the cyclohexene (CHE) oxidation by **1a** and **2a**.

Calculated Cartesian Coordinates

1. $[Fe^{IV}(O)(TPFPP)(Cl)]^-$ (1a)

^{1}1a

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^{3}1a

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^{5}1a

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F 3.04930 -1.89307 -4.19841
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F 6.45433 -0.13362 6.44324
F 6.01269 -2.30207 4.85122
F 4.10597 -2.21578 2.94366
F 3.05425 2.22272 4.21075
F -4.06675 -2.26095 2.97866
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O 0.00389 -1.60173 -0.01357

CHE + 1a

$S = 0$

^{1}RC

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C 2.847442 0.398063 -1.023059
C 1.070999 0.175144 2.902672
C 2.832389 0.330574 1.166967
C -2.859250 0.280715 1.127857
C 1.109715 0.385314 -2.788437
C -2.843062 0.396906 -1.059341
C -1.080830 0.397087 -2.800799
C -0.712226 0.011836 4.271525
C 4.229401 0.483410 -0.595063
C 0.647137 0.036933 4.281787
C 4.219917 0.443304 0.763982
C -4.243582 0.359533 0.705650
C 0.701954 0.397107 -4.179173
C -4.233708 0.426984 -0.652688
C -0.657858 0.412192 -4.186880
H -1.381159 -0.092420 5.122024
H 5.090730 0.577930 -1.251565
H 1.306509 -0.043897 5.142263
H 5.072327 0.498126 1.436369
H -5.107438 0.367435 1.365536
H 1.371587 0.393794 -5.035529
H -5.088092 0.490060 -1.322100
H -1.318314 0.434396 -5.050240
C -2.457672 0.174586 2.467630
C 2.447066 0.405497 -2.366986
C -2.422492 0.418851 -2.396012
C 2.413469 0.243967 2.502704
C -3.523074 0.090347 3.513517
C -3.788999 1.160208 4.377880
C -4.298296 -1.065234 3.674075
C -4.778655 1.089633 5.359569
C -5.533818 -0.076548 5.493457
C 3.463262 0.220502 3.567161
C 3.664618 1.313085 4.420697
C 4.286903 -0.896655 3.757793
C 4.637946 1.301004 5.420926
C 5.267457 -0.932551 4.750292
C 5.442479 0.172304 5.585075
C 3.513921 0.448962 -3.413934
C 4.316409 -0.666669 -3.685260
C 3.759026 1.607408 -4.162334
C 5.319344 -0.638075 -4.655453
C 4.756196 1.661006 -5.137426
C 5.538888 0.531921 -5.384189
C -3.473233 0.458117 -3.460810
C -3.854072 -0.698980 -4.150211
C -4.113940 1.651947 -3.812404
C -4.828278 -0.678096 -5.149374
C -5.091696 1.699601 -4.807661
C -5.447896 0.528697 -5.478905
F -5.682748 2.850748 -5.121258
F -3.795758 2.787092 -3.188522
F 4.966573 2.779006 -5.829464
F 6.491068 0.570942 -6.310249
F 3.029788 2.704380 -3.950841
F 6.063766 -1.716680 -4.891067
F 4.133557 -1.800382 -3.006121
F 4.805995 2.357035 6.214414
F 6.372612 0.149673 6.533765
F 6.031487 -2.011670 4.908136
F 4.144507 -1.970676 2.979117
F 2.913737 2.408108 4.290635
F -4.095659 -2.121758 2.882694
F -3.086053 2.289483 4.276749
F -5.008508 2.125204 6.164229
F -6.479264 -0.154449 6.423860
F -6.376388 0.562313 -6.428913
F -5.169722 -1.796175 -5.786542
F -3.279917 -1.868788 -3.856837
C -5.293620 -1.160677 4.647679
F -6.010425 -2.275256 4.776339
Cl -0.000208 2.658497 0.135713
O -0.005932 -1.407346 -0.006319
C -1.126348 -5.666257 -1.830829
H -0.656773 -6.218851 -2.653441
C -1.823602 -4.551455 -2.097437
H -1.896670 -4.193884 -3.131105
C -2.521623 -3.734734 -1.038354
H -3.508101 -3.409157 -1.411737
C -2.665205 -4.504402 0.282040
H -2.974763 -3.820103 1.088454
H -3.466942 -5.259624 0.184040

C -1.352466 -5.208690 0.646284
H -0.561158 -4.444851 0.750745
H -1.435738 -5.712988 1.623301
C -0.943742 -6.217583 -0.437233
H -1.534680 -7.149182 -0.333493
H 0.106779 -6.528856 -0.295834
H -1.946283 -2.805351 -0.864894

$^{1\alpha}$**TS**$_{H}$

Fe -0.123168 0.155584 0.094801
N -0.107924 0.192315 2.124883
N 1.907190 0.165531 0.108592
N -2.140304 0.244073 0.088088
N -0.133840 0.202252 -1.926381
C -1.201184 0.072739 2.937994
C 2.718773 0.105091 -0.989351
C 0.983852 0.217477 2.946897
C 2.732708 0.263656 1.194230
C -2.955730 0.180981 1.184471
C 0.959303 0.092809 -2.742382
C -2.962748 0.396750 -0.994965
C -1.220099 0.319813 -2.750020
C -0.785853 0.003294 4.325952
C 4.110924 0.180771 -0.587039
C 0.570276 0.106982 4.332224
C 4.118734 0.292629 0.768105
C -4.343783 0.299613 0.782332
C 0.547206 0.116163 -4.132410
C -4.347423 0.441164 -0.570948
C -0.803831 0.277813 -4.137111
H -1.446317 -0.113618 5.181537
H 4.966356 0.172283 -1.258040
H 1.234452 0.088147 5.192817
H 4.982016 0.391525 1.421461
H -5.200615 0.290794 1.451569
H 1.207272 0.028972 -4.991804
H -5.207766 0.556256 -1.225751
H -1.460808 0.357412 -4.999834
C -2.540743 0.057633 2.520276
C 2.298948 0.030675 -2.326695
C -2.553518 0.443310 -2.334992
C 2.323590 0.293758 2.535904
C -3.601396 -0.078108 3.565865
C -3.916994 0.969204 4.440622
C -4.327711 -1.267348 3.708809
C -4.906953 0.844857 5.416764
C -5.612279 -0.353884 5.533494
C 3.375230 0.382415 3.594713
C 3.548590 1.550606 4.348688
C 4.226452 -0.692361 3.882567
C 4.524103 1.653455 5.341517
C 5.209672 -0.614002 4.870080
C 5.357792 0.564870 5.602415
C 3.356415 -0.082132 -3.378919
C 4.054714 -1.279880 -3.578652
C 3.698307 0.998882 -4.201207
C 5.046411 -1.405257 -4.552814
C 4.685599 0.898551 -5.182737
C 5.362131 -0.309648 -5.357873
C -3.608078 0.587789 -3.385961
C -4.053570 -0.509857 -4.132206
C -4.192372 1.829162 -3.664993
C -5.036664 -0.386375 -5.115119
C -5.177169 1.979149 -4.643013
C -5.597765 0.865764 -5.372157
F -5.712756 3.173615 -4.887165
F -3.811825 2.911982 -2.985136
F 4.987990 1.945702 -5.948022
F 6.304783 -0.416329 -6.288711
F 3.073638 2.169416 -4.059106
F 5.689934 -2.559274 -4.719642
F 3.778193 -2.345665 -2.824996
F 4.665964 2.780204 6.037121
F 6.289999 0.650416 6.545804
F 6.001766 -1.654946 5.120354
F 4.110197 -1.836319 3.205355
F 2.768840 2.609913 4.125098
F -4.076738 -2.304431 2.905597
F -3.264292 2.129755 4.355116
F -5.184679 1.860408 6.232132
F -6.557834 -0.482886 6.458450
F -6.533331 0.996546 -6.306991
F -5.442147 -1.450186 -5.805803
F -3.539327 -1.722484 -3.908852
C -5.322019 -1.416855 4.676662
F -5.991666 -2.562405 4.788760
Cl -0.062959 2.561080 0.100476
O -0.078373 -1.602519 0.151488
C -0.541533 -4.959131 -2.154790
H -0.069441 -5.376305 -3.051693
C -1.097517 -3.728684 -2.205010
H -1.045943 -3.153115 -3.135930
C -1.767455 -3.100885 -1.050420
H -2.600557 -2.445706 -1.343587
C -2.103431 -4.064930 0.081876
H -2.357848 -3.504926 0.995988
H -3.005967 -4.649121 -0.186420
C -0.932870 -5.021476 0.344243
H -0.064467 -4.420864 0.665219
H -1.168696 -5.710091 1.172156
C -0.559815 -5.816978 -0.915806
H -1.274880 -6.650658 -1.067344
H 0.421910 -6.306428 -0.785139
H -0.952534 -2.288448 -0.556891

$^{1\alpha}$**TS**$_{Ep}$

Fe -0.116915 0.032533 0.136345
N -0.094535 0.053754 2.158444
N 1.900486 0.012379 0.127465
N -2.146409 0.175309 0.140367
N -0.147852 0.127827 -1.891399
C -1.185536 -0.025010 2.980675
C 2.703482 -0.080310 -0.976177
C 1.002236 0.083803 2.975375
C 2.736856 0.078216 1.208004
C -2.953740 0.114262 1.240981
C 0.932941 -0.006130 -2.716851
C -2.972392 0.344949 -0.935384
C -1.238335 0.270930 -2.702871
C -0.762962 -0.070176 4.367158
C 4.098586 -0.083251 -0.579599
C 0.595227 0.012365 4.364304
C 4.119454 0.039560 0.774873
C -4.343946 0.262623 0.851437
C 0.513096 0.051051 -4.104733
C -4.353940 0.420678 -0.499293
C -0.835256 0.229293 -4.095698
H -1.420313 -0.154429 5.228958
H 4.950174 -0.158523 -1.251085
H 1.263947 0.005955 5.221649
H 4.990232 0.093192 1.423662
H -5.195329 0.268919 1.527755
H 1.167354 -0.021998 -4.970003
H -5.215519 0.578521 -1.143318
H -1.499715 0.314717 -4.952030
C -2.528719 -0.020695 2.572108
C 2.271237 -0.128888 -2.311355
C -2.569130 0.404374 -2.277940
C 2.339240 0.123246 2.552421
C -3.583585 -0.147428 3.624756
C -3.897891 0.905261 4.492905
C -4.306156 -1.337625 3.777857
C -4.884201 0.785468 5.473376
C -5.586342 -0.414070 5.600676
C 3.403869 0.177251 3.600961
C 3.662791 1.353733 4.315405
C 4.182815 -0.943353 3.915045
C 4.654970 1.421136 5.294934
C 5.181278 -0.901398 4.889269
C 5.416580 0.287286 5.582159
C 3.304612 -0.298694 -3.379975
C 3.445043 -1.515047 -4.060281
C 4.164640 0.741369 -3.753635
C 4.397958 -1.698602 -5.063224
C 5.126517 0.583358 -4.752918
C 5.241352 -0.642158 -5.410928
C -3.621627 0.589112 -3.323998
C -4.514003 -0.436574 -3.661059
C -3.753318 1.799822 -4.016376
C -5.495977 -0.271838 -4.639193
C -4.726204 1.989020 -4.999165
C -5.600737 0.946960 -5.311167
F -4.826630 3.153781 -5.637225
F -2.933256 2.816285 -3.742994
F 5.929222 1.592718 -5.085135
F 6.152099 -0.803176 -6.365452
F 4.080670 1.927285 -3.147644
F 4.506859 -2.869240 -5.688624
F 2.651275 -2.545837 -3.756316
F 4.879809 2.556372 5.953829
F 6.364132 0.339294 6.512637
F 5.904764 -1.984993 5.164647
F 3.981937 -2.097775 3.274366
F 2.952402 2.454935 4.065371
F -4.053975 -2.378105 2.979828
F -3.247282 2.066343 4.397163
F -5.161138 1.805870 6.283144
F -6.528364 -0.538786 6.530029
F -6.531128 1.114808 -6.245454
F -6.328131 -1.268082 -4.937475
F -4.440102 -1.616314 -3.041534
C -5.296976 -1.482367 4.750042
F -5.964268 -2.628391 4.872598
Cl -0.037399 2.460768 0.168554
O -0.292186 -1.710301 0.029604
C 0.485056 -3.132099 1.203839
H 0.475942 -2.489652 2.086017
C 1.701225 -3.390041 0.604764
H 2.560780 -2.764385 0.861326
C 1.870124 -4.394293 -0.500008
H 1.874013 -3.859367 -1.472043
H 2.868047 -4.863597 -0.433361
C 0.770342 -5.468373 -0.505628
H 0.794184 -6.029286 -1.454874
H 0.976420 -6.201910 0.295348
C -0.615654 -4.854600 -0.272984
H -0.844062 -4.143167 -1.084622
H -1.392781 -5.636904 -0.299727
C -0.665634 -4.100824 1.060432
H -0.616197 -4.823351 1.899237
H -1.616880 -3.559395 1.174380

$S = 1$

^{3}**RC**

Fe -0.26739 0.22115 -0.27045
N -0.27648 0.00297 1.74808
N 1.76220 0.16869 -0.26336
N -2.28273 0.44924 -0.25347
N -0.24485 0.60932 -2.26364
C -1.37812 -0.07969 2.55446
C 2.58993 0.30840 -1.34361
C 0.80832 -0.21985 2.55115
C 2.57202 -0.02403 0.82200
C -3.10634 0.36203 0.83492
C 0.85252 0.62440 -3.08092
C -3.08780 0.71325 -1.32744
C -1.33277 0.78599 -3.07398
C -0.97845 -0.36977 3.91711
C 3.97470 0.22396 -0.92477
C 0.37866 -0.45575 3.91518
C 3.96354 0.01595 0.41906
C -4.48060 0.59969 0.44099
C 0.44446 0.80010 -4.46033
C -4.46865 0.82098 -0.90067
C -0.91160 0.90065 -4.45597
H -1.65136 -0.49935 4.76104
H 4.84049 0.32440 -1.57459
H 1.03180 -0.66987 4.75731
H 4.81835 -0.08653 1.08289
H -5.33783 0.61151 1.10953
H 1.11050 0.83109 -5.31900
H -5.31442 1.04912 -1.54444
H -1.57094 1.02932 -5.31061
C -2.71025 0.09284 2.15268
C 2.18832 0.50298 -2.67289
C -2.67002 0.85791 -2.65817
C 2.14970 -0.22936 2.14343
C -3.77696 -0.02548 3.19403
C -3.98559 0.97806 4.14832
C -4.61038 -1.14924 3.25822
C -4.97586 0.87358 5.12641
C -5.78974 -0.25977 5.16375
C 3.19639 -0.48642 3.17998
C 3.53454 0.47683 4.13880
C 3.88279 -1.70626 3.23308
C 4.51034 0.24336 5.10924
C 4.86158 -1.96458 4.19359
C 5.17653 -0.98297 5.13480
C 3.25270 0.59145 -3.71965
C 3.96046 -0.54168 -4.14009
C 3.58804 1.81187 -4.31961
C 4.95940 -0.47107 -5.11231
C 4.58265 1.90824 -5.29405
C 5.27145 0.76063 -5.69011
C -3.71494 1.10437 -3.69910
C -4.59340 0.09322 -4.10897
C -3.85652 2.35751 -4.30910
C -5.56996 0.31128 -5.08206
C -4.82468 2.60027 -5.28466
C -5.68446 1.57113 -5.67192
F -4.93500 3.80355 -5.84426
F -3.05132 3.36269 -3.96104
F 4.88026 3.08416 -5.84339
F 6.22145 0.84035 -6.61585
F 2.95065 2.92788 -3.96202
F 5.61218 -1.56755 -5.49288
F 3.68614 -1.73410 -3.60832
F 4.81137 1.18113 6.00523
F 6.10769 -1.21600 6.05363
F 5.49356 -3.13617 4.21878
F 3.60625 -2.66651 2.34652
F 2.91734 1.65948 4.14183
F -4.46153 -2.14238 2.37712
F -3.22470 2.07377 4.13993
F -5.15154 1.84646 6.01828
F -6.73640 -0.36920 6.08979
F -6.61011 1.79057 -6.59969
F -6.38800 -0.67211 -5.45229
F -4.51025 -1.12291 -3.56653
C -5.60644 -1.27850 4.22713
F -6.37938 -2.36195 4.26405
Cl -0.10615 2.62290 0.09391
O -0.38166 -1.38819 -0.51103
C 0.68433 -5.66537 0.27392
H 1.55286 -6.19416 -0.13677
C -0.40576 -5.49669 -0.48988
H -0.40233 -5.87141 -1.52051
C -1.65796 -4.80380 -0.01017
H -2.54788 -5.35233 -0.36683
C -1.68676 -4.66114 1.51839
H -2.49029 -3.96991 1.82037
H -1.92332 -5.64045 1.97406
C -0.33083 -4.17174 2.04184
H -0.11153 -3.19477 1.57762
H -0.36726 -4.00827 3.13154
C 0.79204 -5.15905 1.69178
H 0.77818 -6.02130 2.38793
H 1.77672 -4.68269 1.84413
H -1.71521 -3.80184 -0.47725

$^{3\alpha}$**TS**$_{H}$

Fe -0.36135 0.14364 -0.21900
N -0.38248 -0.01165 1.81546
N 1.67222 0.05467 -0.19793
N -2.37516 0.45037 -0.21159
N -0.32001 0.51799 -2.21911
C -1.49123 -0.06424 2.61379
C 2.50544 0.14591 -1.27849
C 0.69404 -0.24090 2.62681
C 2.47092 -0.13020 0.89707
C -3.20362 0.38943 0.87435
C 0.78074 0.48113 -3.03092
C -3.16692 0.72489 -1.29225
C -1.39996 0.72004 -3.03428
C -1.10462 -0.33960 3.98354
C 3.88585 0.03535 -0.85115
C 0.25180 -0.44654 3.99199
C 3.86432 -0.13700 0.49840
C -4.57044 0.65472 0.47138
C 0.38241 0.64767 -4.41424
C -4.54670 0.86892 -0.87217
C -0.96992 0.79729 -4.41616
H -1.78416 -0.44450 4.82571
H 4.75718 0.09663 -1.49857
H 0.89536 -0.65740 4.84243
H 4.71460 -0.24401 1.16744
H -5.43109 0.68986 1.13490
H 1.05051 0.64053 -5.27194
H -5.38466 1.11294 -1.52044
H -1.62050 0.93504 -5.27613
C -2.81788 0.12247 2.19691
C 2.11122 0.32411 -2.61359
C -2.73646 0.84186 -2.62298
C 2.03668 -0.29048 2.22202
C -3.89612 0.01030 3.22699
C -4.12850 1.02182 4.16661
C -4.71597 -1.12334 3.29196
C -5.13243 0.91704 5.13080
C -5.93353 -0.22540 5.16913
C 3.07213 -0.55513 3.26798
C 3.44217 0.42038 4.20200
C 3.71552 -1.79635 3.35352
C 4.40957 0.17863 5.17897
C 4.68475 -2.06339 4.32111
C 5.03420 -1.06837 5.23585
C 3.18152 0.35961 -3.65738
C 3.85778 -0.80202 -4.05101
C 3.55608 1.55742 -4.27949
C 4.86386 -0.78029 -5.01822
C 4.55830 1.60492 -5.24969
C 5.21488 0.42979 -5.61890
C -3.76821 1.10682 -3.67251
C -4.67830 0.11943 -4.07137
C -3.86332 2.35347 -4.30454
C -5.64074 0.35389 -5.05465
C -4.81624 2.61212 -5.29096
C -5.70811 1.60641 -5.66695
F -4.88164 3.80863 -5.87168
F -3.02673 3.33668 -3.96810
F 4.89343 2.76039 -5.82038
F 6.17164 0.46297 -6.54046
F 2.95092 2.69887 -3.94725
F 5.48662 -1.90280 -5.37228
F 3.54598 -1.97497 -3.49696
F 4.74229 1.12810 6.05112
F 5.95702 -1.30932 6.16100
F 5.27554 -3.25521 4.37792
F 3.40138 -2.76998 2.49421
F 2.86449 1.62245 4.17471
F -4.53976 -2.12421 2.42547

F -3.37907 2.12535 4.15670
F -5.33235 1.89746 6.00929
F -6.89261 -0.33521 6.08234
F -6.61960 1.84131 -6.60487
F -6.48944 -0.60743 -5.41369
F -4.63971 -1.08977 -3.50867
C -5.72531 -1.25259 4.24695
F -6.48603 -2.34471 4.28595
Cl -0.11905 2.66778 0.11790
O -0.53171 -1.58833 -0.44502
C 1.19483 -5.27765 0.05604
H 2.09486 -5.76672 -0.33312
C 0.29300 -4.74958 -0.80778
H 0.49550 -4.79723 -1.88415
C -0.93479 -4.08787 -0.37225
H -1.76844 -4.15089 -1.08773
C -1.31302 -4.30966 1.08244
H -2.06615 -3.57046 1.40241
H -1.79124 -5.30417 1.19446
C -0.06986 -4.23354 1.97933
H 0.34603 -3.21501 1.90164
H -0.34008 -4.38960 3.03647
C 1.00712 -5.24231 1.55101
H 0.74648 -6.25915 1.90873
H 1.96599 -5.00171 2.04255
H -0.68924 -2.75911 -0.45601

$^{3\alpha}$**IM**$_{H}$

Fe -0.24640 0.23029 0.07275
N -0.25923 0.10996 2.08557
N 1.81062 -0.03119 0.07405
N -2.26629 0.62530 0.08473
N -0.19909 0.51516 -1.92482
C -1.35936 0.17393 2.90027
C 2.63604 -0.00391 -1.01275
C 0.81446 -0.16384 2.89395
C 2.60541 -0.21269 1.16853
C -3.07627 0.69622 1.18137
C 0.89466 0.39330 -2.74318
C -3.04289 0.92194 -0.99873
C -1.27612 0.75121 -2.73906
C -0.97155 -0.08738 4.27086
C 4.01397 -0.16969 -0.59318
C 0.37348 -0.29406 4.26731
C 3.99501 -0.29815 0.76328
C -4.42137 1.06023 0.78130
C 0.49110 0.54176 -4.12615
C -4.40051 1.20069 -0.57333
C -0.85151 0.76360 -4.12355
H -1.64450 -0.11993 5.12404
H 4.88220 -0.17171 -1.24808
H 1.01032 -0.52768 5.11682
H 4.84505 -0.42597 1.42930
H -5.26662 1.20539 1.44987
H 1.14973 0.47372 -4.98841
H -5.22538 1.48216 -1.22341
H -1.50009 0.91046 -4.98346
C -2.67746 0.46146 2.50720
C 2.22236 0.16654 -2.34401
C -2.60458 0.96238 -2.33204
C 2.15567 -0.29490 2.49654
C -3.72498 0.53903 3.57150
C -3.78357 1.61765 4.46346
C -4.69644 -0.45991 3.71374
C -4.76229 1.70517 5.45460
C -5.71604 0.69259 5.57100
C 3.17908 -0.52394 3.56363
C 3.58563 0.51015 4.41671
C 3.77647 -1.77625 3.75147
C 4.54448 0.31389 5.41178
C 4.73691 -1.99866 4.73937
C 5.12207 -0.94677 5.57207
C 3.27211 0.11033 -3.40823
C 3.84143 -1.10468 -3.80874
C 3.73066 1.26989 -4.04627
C 4.82628 -1.17236 -4.79522
C 4.71400 1.22912 -5.03611
C 5.26272 0.00164 -5.41138
C -3.62100 1.25791 -3.38848
C -4.59042 0.31471 -3.75295
C -3.64865 2.49029 -4.05403
C -5.54548 0.57747 -4.73626
C -4.59366 2.77688 -5.04030
C -5.54572 1.81497 -5.38191
F -4.59521 3.95915 -5.65288
F -2.75413 3.43212 -3.75030
F 5.13149 2.34949 -5.62169
F 6.19854 -0.04907 -6.35306
F 3.22579 2.45813 -3.71168
F 5.34584 -2.34436 -5.15403
F 3.44215 -2.24786 -3.24443
F 4.91251 1.31817 6.20470
F 6.03575 -1.14516 6.51611
F 5.28366 -3.20283 4.89342
F 3.42851 -2.80428 2.97336
F 3.05273 1.72631 4.29026
F -4.69432 -1.51280 2.89437
F -2.88804 2.60259 4.37793
F -4.79351 2.74545 6.28515
F -6.65204 0.76450 6.51138
F -6.45014 2.07708 -6.31938
F -6.45121 -0.34234 -5.06285
F -4.61724 -0.87812 -3.15601
C -5.68457 -0.39552 4.69736
F -6.59225 -1.36332 4.80932
Cl 0.17199 2.74886 0.33464
O -0.53268 -1.67038 -0.13648
C 2.80855 -4.79621 0.55394
H 3.82266 -4.74108 0.95949
C 2.55386 -4.36106 -0.74412
H 3.37564 -3.94653 -1.33632
C 1.28859 -4.44832 -1.32444
H 1.14439 -4.12933 -2.36103
C 0.12490 -5.01487 -0.55894
H -0.80666 -4.50967 -0.86262
H -0.00937 -6.08444 -0.82566
C 0.32431 -4.86894 0.95867
H 0.21343 -3.79864 1.20027
H -0.46802 -5.40733 1.50381
C 1.71000 -5.35334 1.41469
H 1.74795 -6.46296 1.39011
H 1.88371 -5.08070 2.46975
H 0.27049 -2.10033 -0.46603

$^{3\beta}$**TS**$_{H}$

Fe -0.12762 0.14730 0.09144
N -0.11558 0.18571 2.12117
N 1.90194 0.15600 0.10222
N -2.14552 0.25081 0.08566
N -0.13738 0.20913 -1.93025
C -1.20890 0.07340 2.93500
C 2.71436 0.10107 -0.99520
C 0.97708 0.20519 2.94217
C 2.72653 0.24761 1.18921
C -2.96219 0.18779 1.18163
C 0.95546 0.10107 -2.74762
C -2.96741 0.40072 -0.99813
C -1.22428 0.32631 -2.75315
C -0.79311 0.00284 4.32266
C 4.10623 0.17203 -0.59140
C 0.56363 0.09790 4.32784
C 4.11304 0.27593 0.76433
C -4.34986 0.30513 0.77827
C 0.54241 0.12704 -4.13715
C -4.35252 0.44444 -0.57517
C -0.80871 0.28725 -4.14060
H -1.45385 -0.10908 5.17870
H 4.96208 0.16611 -1.26188
H 1.22830 0.07590 5.18796
H 4.97588 0.36988 1.41900
H -5.20715 0.29673 1.44691
H 1.20207 0.04210 -4.99708
H -5.21243 0.55777 -1.23084
H -1.46643 0.36758 -5.00268
C -2.54850 0.06416 2.51745
C 2.29491 0.03513 -2.33307
C -2.55785 0.44707 -2.33805
C 2.31692 0.27538 2.53069
C -3.60954 -0.06734 3.56315
C -3.92258 0.98230 4.43599
C -4.33825 -1.25480 3.70848
C -4.91258 0.86191 5.41259
C -5.62042 -0.33511 5.53172
C 3.36914 0.35779 3.58953
C 3.54921 1.52472 4.34385
C 4.21469 -0.72168 3.87635
C 4.52583 1.62187 5.33616
C 5.19882 -0.64910 4.86342
C 5.35374 0.52865 5.59615
C 3.35203 -0.07446 -3.38585
C 4.04976 -1.27184 -3.58990
C 3.69405 1.00920 -4.20459
C 5.04106 -1.39432 -4.56482
C 4.68097 0.91178 -5.18679
C 5.35694 -0.29610 -5.36626
C -3.61263 0.58734 -3.38938
C -4.05450 -0.51290 -4.13397
C -4.20062 1.82645 -3.67056
C -5.03765 -0.39404 -5.11738
C -5.18557 1.97182 -4.64913
C -5.60252 0.85596 -5.37660
F -5.72478 3.16423 -4.89537
F -3.82363 2.91153 -2.99232
F 4.98353 1.96139 -5.94861
F 6.29920 -0.40002 -6.29780
F 3.06986 2.17947 -4.05833
F 5.68400 -2.54804 -4.73583
F 3.77289 -2.34012 -2.83990
F 4.67417 2.74752 6.03216
F 6.28694 0.60879 6.53902
F 5.98546 -1.69439 5.11274
F 4.09210 -1.86448 3.19832
F 2.77507 2.58830 4.12112
F -4.08958 -2.29383 2.90707
F -3.26713 2.14113 4.34823
F -5.18789 1.87954 6.22616
F -6.56603 -0.46035 6.45713
F -6.53819 0.98236 -6.31194
F -5.43964 -1.46020 -5.80649
F -3.53642 -1.72346 -3.90847
C -5.33265 -1.40034 4.67683
F -6.00474 -2.54422 4.79127
Cl -0.05010 2.55570 0.11270
O -0.10021 -1.59257 0.14025
C -0.49788 -4.94694 -2.12893
H -0.00807 -5.35598 -3.01989
C -1.07789 -3.72524 -2.18598
H -1.02758 -3.15081 -3.11778
C -1.76509 -3.11065 -1.04371
H -2.59072 -2.44548 -1.33325
C -2.08839 -4.06614 0.09686
H -2.34948 -3.50224 1.00701
H -2.98495 -4.66371 -0.16407
C -0.90688 -5.00757 0.36730
H -0.04752 -4.39533 0.69045
H -1.13826 -5.69636 1.19632
C -0.51637 -5.80237 -0.88825
H -1.22179 -6.64399 -1.04201
H 0.46920 -6.28143 -0.74802
H -0.92876 -2.25766 -0.52750

$^{3\beta}$**IM**$_{H}$

Fe 0.21628 0.24807 0.01838
N 0.23176 0.20776 2.04376
N 2.24196 0.29838 0.03589
N -1.80629 0.24583 -0.00105
N 0.19948 0.31442 -2.00671
C -0.86189 0.05834 2.85099
C 3.05482 0.30042 -1.06328
C 1.31858 0.24620 2.87159
C 3.06614 0.38418 1.12417
C -2.61893 0.13947 1.09510
C 1.29881 0.27156 -2.82180
C -2.63504 0.37353 -1.08278
C -0.88817 0.40348 -2.83401
C -0.45140 -0.01940 4.24052
C 4.44433 0.40325 -0.65830
C 0.90252 0.10826 4.25392
C 4.45021 0.46658 0.70009
C -4.01050 0.20486 0.69329
C 0.89075 0.30982 -4.21270
C -4.02013 0.35549 -0.65929
C -0.46591 0.41110 -4.21975
H -1.11341 -0.15868 5.09164
H 5.29921 0.44207 -1.32897
H 1.56360 0.09081 5.11693
H 5.31094 0.56571 1.35675
H -4.86648 0.15315 1.36170
H 1.55707 0.27092 -5.07085
H -4.88423 0.43712 -1.31418
H -1.12302 0.48025 -5.08328
C -2.19994 0.01701 2.42951
C 2.63860 0.25310 -2.40335
C -2.22701 0.46256 -2.42144
C 2.65675 0.36402 2.46581
C -3.25785 -0.14759 3.47469
C -3.61802 0.90065 4.33060
C -3.93311 -1.36356 3.63850
C -4.60616 0.75319 5.30548
C -5.26209 -0.47135 5.44146
C 3.70593 0.45044 3.52726
C 3.85310 1.60245 4.31101
C 4.58217 -0.61139 3.78665
C 4.82680 1.70197 5.30598
C 5.56432 -0.53594 4.77542
C 5.68585 0.62669 5.53801
C 3.70074 0.21544 -3.45658
C 4.43682 -0.95031 -3.70331
C 4.00825 1.33927 -4.23364
C 5.43329 -1.00398 -4.67921
C 5.00004 1.31105 -5.21535
C 5.71486 0.13308 -5.43809
C -3.28452 0.60955 -3.46920
C -3.69510 -0.46826 -4.26232
C -3.90940 1.84217 -3.69717
C -4.68095 -0.33522 -5.24128
C -4.89749 2.00209 -4.67008
C -5.28259 0.90751 -5.44590
F -5.47105 3.18800 -4.86438
F -3.56446 2.90718 -2.97176
F 5.26967 2.39772 -5.93649
F 6.66149 0.09447 -6.37019
F 3.34517 2.48187 -4.04579
F 6.11325 -2.12928 -4.89145
F 4.19366 -2.05436 -2.99458
F 4.94349 2.81347 6.03024
F 6.61679 0.70927 6.48294
F 6.38054 -1.56438 4.99845
F 4.49171 -1.73958 3.07966
F 3.04932 2.64920 4.11490
F -3.63346 -2.40420 2.85581
F -3.01133 2.08439 4.22737
F -4.92758 1.77029 6.10265
F -6.20498 -0.62275 6.36573
F -6.22175 1.04756 -6.37567
F -5.05075 -1.38160 -5.97703
F -3.14307 -1.67324 -4.09137
C -4.92594 -1.53630 4.60399
F -5.54857 -2.70614 4.73432
Cl 0.19867 2.62556 0.09154
O 0.25556 -1.58410 -0.00000
C -0.56330 -4.72471 -1.52615
H 0.34693 -4.91516 -2.10260
C -1.61715 -4.01842 -2.10321
H -1.50721 -3.63903 -3.12445
C -2.81768 -3.79141 -1.43153
H -3.62963 -3.26304 -1.93833
C -3.02063 -4.28928 -0.02803
H -3.68033 -3.60651 0.53273
H -3.55933 -5.26031 -0.05478
C -1.68237 -4.45810 0.70984
H -1.25519 -3.45878 0.89676
H -1.84161 -4.93682 1.68943
C -0.66707 -5.25684 -0.12370
H -0.96227 -6.32700 -0.15534
H 0.32337 -5.24330 0.36318
H -0.37816 -1.89089 -0.66628

$^{3\alpha}$**TS**$_{Ep}$

Fe 0.09306 -0.03352 0.32317
N 0.09087 0.14875 2.35653
N 2.12161 0.13848 0.32070
N -1.93988 0.04246 0.32224
N 0.09066 0.01904 -1.71025
C -1.00258 0.09149 3.17599
C 2.93846 0.12673 -0.77540
C 1.18669 0.19737 3.17250
C 2.93630 0.26288 1.41259
C -2.75655 0.07367 1.41899
C 1.18706 -0.04633 -2.52568
C -2.75872 0.05143 -0.77302
C -1.00557 -0.04115 -2.52675
C -0.58416 0.08530 4.56420
C 4.32169 0.27086 -0.36683
C 0.77449 0.15570 4.56203
C 4.31966 0.36207 0.99072
C -4.14431 0.12642 1.00381
C 0.77124 -0.16587 -3.90930
C -4.14541 0.11597 -0.35684
C -0.58914 -0.15846 -3.91021
H -1.24440 0.02705 5.42604
H 5.17865 0.31531 -1.03455
H 1.43996 0.16516 5.42170
H 5.17536 0.49458 1.64811
H -5.00272 0.18191 1.66878
H 1.43476 -0.25156 -4.76619
H -5.00504 0.16021 -1.02103
H -1.25276 -0.23835 -4.76764
C -2.34278 0.06275 2.76037
C 2.52700 0.00536 -2.11203
C -2.34600 -0.01057 -2.11320
C 2.52441 0.27686 2.75439
C -3.40214 0.01526 3.81450
C -3.71125 1.13215 4.60069
C -4.12912 -1.15720 4.05758
C -4.69816 1.09125 5.58694
C -5.40480 -0.09249 5.80522
C 3.58036 0.37608 3.80840
C 3.76068 1.54902 4.55284
C 4.43358 -0.69746 4.09440
C 4.74467 1.65709 5.53674
C 5.42495 -0.61404 5.07327
C 5.57966 0.56931 5.79714
C 3.58821 -0.08691 -3.16114
C 4.35534 -1.24947 -3.31113
C 3.85799 0.97239 -4.03652
C 5.34739 -1.36120 -4.28622
C 4.84513 0.88549 -5.01958
C 5.59259 -0.28679 -5.14307
C -3.40447 -0.07727 -3.16715
C -4.16183 -1.23956 -3.36196
C -3.67869 1.01001 -4.00626

C -5.14902 -1.32437 -4.34459
C -4.66133 0.95041 -4.99594
C -5.39925 -0.22235 -5.16409
F -4.90034 2.00249 -5.77630
F -2.99083 2.14521 -3.87290
F 5.07986 1.91128 -5.83545
F 6.53550 -0.38000 -6.07484
F 3.16181 2.10677 -3.94521
F 6.05682 -2.48163 -4.40606
F 4.14505 -2.29643 -2.50888
F 4.89328 2.78781 6.22424
F 6.51977 0.65999 6.73204
F 6.21917 -1.65344 5.32263
F 4.31175 -1.84380 3.42204
F 2.98001 2.60739 4.32861
F -3.87941 -2.25608 3.34242
F -3.05484 2.27903 4.41737
F -4.97086 2.17132 6.31649
F -6.34644 -0.14285 6.74159
F -6.33741 -0.29004 -6.10280
F -5.84894 -2.44545 -4.50693
F -3.94585 -2.31297 -2.59728
C -5.11999 -1.22343 5.03809
F -5.79119 -2.35432 5.24763
Cl 0.03684 2.56373 0.26343
O 0.13045 -1.77374 0.38091
C -0.27578 -3.55828 0.78009
H -0.57101 -3.34141 1.81093
C 0.95596 -4.17543 0.58572
H 1.70590 -4.11890 1.38228
C 1.38700 -4.70933 -0.75087
H 1.98123 -3.93401 -1.27971
H 2.08280 -5.55642 -0.61491
C 0.19796 -5.12698 -1.63160
H 0.53881 -5.31159 -2.66418
H -0.20775 -6.08582 -1.25997
C -0.91490 -4.07214 -1.60926
H -0.52885 -3.12160 -2.01421
H -1.75404 -4.37731 -2.25620
C -1.41359 -3.82707 -0.18149
H -1.96074 -4.72064 0.17870
H -2.12958 -2.99274 -0.15318

$^{3\alpha}$**IM**$_{Ep}$

Fe 0.03138 0.22478 -0.08630
N 0.03148 0.28811 1.95175
N 2.05980 0.35838 -0.09123
N -2.00182 0.26025 -0.07944
N 0.02769 0.31307 -2.12153
C -1.06376 0.26896 2.77236
C 2.87364 0.46618 -1.18645
C 1.13014 0.25335 2.76680
C 2.87715 0.37548 1.00656
C -2.81880 0.31454 1.01753
C 1.12184 0.35196 -2.94107
C -2.82000 0.26069 -1.17603
C -1.06893 0.22082 -2.93607
C -0.64427 0.20585 4.15712
C 4.25563 0.57744 -0.76616
C 0.71717 0.19214 4.15365
C 4.25869 0.51289 0.59342
C -4.20449 0.37232 0.60026
C 0.70599 0.26331 -4.32614
C -4.20556 0.33539 -0.76050
C -0.65228 0.17468 -4.32281
H -1.30597 0.16428 5.01880
H 5.11117 0.69854 -1.42590
H 1.38246 0.13887 5.01189
H 5.11609 0.57045 1.25955
H -5.06301 0.44387 1.26355
H 1.36871 0.25413 -5.18795
H -5.06521 0.37210 -1.42504
H -1.31257 0.08054 -5.18129
C -2.40492 0.29558 2.35851
C 2.46052 0.45065 -2.52821
C -2.40826 0.19973 -2.51728
C 2.46887 0.29144 2.34668
C -3.46226 0.27503 3.41537
C -3.74057 1.40023 4.20104
C -4.21529 -0.87981 3.66316
C -4.72419 1.38406 5.19138
C -5.45788 0.21769 5.41411
C 3.53250 0.24038 3.39644
C 3.82845 1.34606 4.20281
C 4.27522 -0.92691 3.61375
C 4.82029 1.29955 5.18393
C 5.27087 -0.99888 4.58896
C 5.54395 0.12147 5.37585
C 3.51269 0.53945 -3.58663
C 4.38327 -0.52668 -3.84762
C 3.67097 1.69572 -4.36185
C 5.37009 -0.45183 -4.83173
C 4.64979 1.79460 -5.35180
C 5.50244 0.71474 -5.58661
C -3.47067 0.10230 -3.56480
C -4.19912 -1.08065 -3.74659
C -3.78177 1.17837 -4.40549
C -5.19384 -1.19528 -4.71862
C -4.77214 1.08847 -5.38502
C -5.48031 -0.10417 -5.54089
F -5.04654 2.13038 -6.16722
F -3.12436 2.33260 -4.28241
F 4.77728 2.90947 -6.06859
F 6.43783 0.79687 -6.52682
F 2.87344 2.74633 -4.16224
F 6.18078 -1.48384 -5.05708
F 4.28260 -1.65716 -3.14596
F 5.08115 2.36845 5.93371
F 6.49043 0.06607 6.30685
F 5.95796 -2.12419 4.77441
F 4.03545 -2.01526 2.87871
F 3.15371 2.48586 4.04483
F -3.99314 -1.98587 2.94973
F -3.05608 2.52973 4.01385
F -4.96806 2.47106 5.92056
F -6.39633 0.19097 6.35442
F -6.42556 -0.20062 -6.46975
F -5.86644 -2.33454 -4.86856
F -3.94935 -2.14369 -2.97821
C -5.20277 -0.92132 4.64833
F -5.89896 -2.03575 4.86324
Cl -0.03173 2.80995 -0.07038
O 0.08681 -1.70898 -0.13441
C -0.50607 -2.73055 0.62602
H -1.01077 -2.30919 1.52173
C 0.60962 -3.64399 1.06340
H 1.25996 -3.29369 1.87477
C 1.16435 -4.65023 0.10273
H 1.85500 -4.13909 -0.60481
H 1.79122 -5.38894 0.63310
C 0.06793 -5.35496 -0.71601
H 0.52560 -5.96230 -1.51544
H -0.47701 -6.05804 -0.05948
C -0.92954 -4.34788 -1.30163
H -0.40703 -3.68107 -2.01009
H -1.71038 -4.87284 -1.87838
C -1.56347 -3.49545 -0.19665
H -2.13704 -4.14987 0.48702
H -2.27518 -2.77061 -0.62378

$^{3\beta}$**TS**$_{Ep}$

Fe -0.11491 0.02141 0.14117
N -0.09253 0.05592 2.16219
N 1.90603 0.01039 0.13197
N -2.14273 0.16152 0.14714
N -0.14085 0.12115 -1.88705
C -1.18342 -0.01946 2.98619
C 2.71024 -0.08142 -0.97111
C 1.00538 0.08352 2.97882
C 2.74154 0.07328 1.21256
C -2.95139 0.10874 1.24702
C 0.94095 -0.00493 -2.71246
C -2.96785 0.32469 -0.93071
C -1.23236 0.25772 -2.69802
C -0.75969 -0.06280 4.37189
C 4.10534 -0.08697 -0.57349
C 0.59873 0.01574 4.36778
C 4.12503 0.03321 0.78099
C -4.34136 0.25365 0.85533
C 0.52086 0.05254 -4.10004
C -4.35008 0.40166 -0.49638
C -0.82883 0.22079 -4.09076
H -1.41655 -0.14395 5.23434
H 4.95732 -0.16182 -1.24454
H 1.26799 0.00841 5.22468
H 4.99512 0.08441 1.43091
H -5.19323 0.26467 1.53098
H 1.17573 -0.01440 -4.96533
H -5.21106 0.55502 -1.14228
H -1.49381 0.30290 -4.94700
C -2.52674 -0.01688 2.57912
C 2.27939 -0.12509 -2.30658
C -2.56406 0.38235 -2.27295
C 2.34263 0.11854 2.55668
C -3.58115 -0.13636 3.63289
C -3.89080 0.92041 4.49785
C -4.30802 -1.32336 3.79079
C -4.87645 0.80747 5.47980
C -5.58280 -0.38906 5.61194
C 3.40683 0.16832 3.60590
C 3.67079 1.34366 4.32032
C 4.18086 -0.95566 3.92009
C 4.66298 1.40670 5.30013
C 5.17925 -0.91810 4.89457
C 5.41958 0.26955 5.58751
C 3.31400 -0.28675 -3.37527
C 3.45812 -1.49865 -4.06268
C 4.17198 0.75760 -3.74171
C 4.41275 -1.67393 -5.06549
C 5.13539 0.60788 -4.74076
C 5.25401 -0.61343 -5.40588
C -3.61772 0.55798 -3.31951
C -4.50301 -0.47468 -3.65393
C -3.75840 1.76633 -4.01419
C -5.48674 -0.31887 -4.63175
C -4.73329 1.94669 -4.99667
C -5.60059 0.89782 -5.30605
F -4.84242 3.10945 -5.63696
F -2.94546 2.78917 -3.74329
F 5.93603 1.62114 -5.06601
F 6.16626 -0.76651 -6.36028
F 4.08443 1.93968 -3.12880
F 4.52525 -2.84058 -5.69768
F 2.66645 -2.53312 -3.76600
F 4.89263 2.54095 5.95909
F 6.36714 0.31743 6.51823
F 5.89798 -2.00484 5.17009
F 3.97511 -2.10914 3.27924
F 2.96532 2.44800 4.07010
F -4.06050 -2.36753 2.99616
F -3.23621 2.07886 4.39752
F -5.14881 1.83162 6.28638
F -6.52420 -0.50726 6.54276
F -6.53276 1.05719 -6.24006
F -6.31205 -1.32155 -4.92745
F -4.42057 -1.65247 -3.03179
C -5.29828 -1.46122 4.76453
F -5.96952 -2.60443 4.89171
Cl -0.04470 2.45289 0.15507
O -0.26882 -1.70653 0.02803
C 0.46215 -3.08433 1.15556
H 0.46791 -2.46634 2.05574
C 1.69164 -3.38869 0.58634
H 2.56191 -2.78262 0.85389
C 1.84770 -4.39284 -0.51990
H 1.85536 -3.85850 -1.49300
H 2.83980 -4.87462 -0.45627
C 0.73485 -5.45367 -0.52652
H 0.75579 -6.01852 -1.47357
H 0.92852 -6.18630 0.27835
C -0.64455 -4.82221 -0.30245
H -0.86347 -4.11528 -1.12081
H -1.43047 -5.59587 -0.32499
C -0.68961 -4.05807 1.02508
H -0.63253 -4.77452 1.86813
H -1.64202 -3.51900 1.14065

$^{3\beta}$**IM**$_{Ep}$

Fe 0.01682 0.22536 0.02268
N 0.02272 0.21460 2.04344
N 2.03875 0.20169 0.03896
N -2.01118 0.33154 0.00282
N 0.00842 0.30904 -2.00806
C -1.07869 0.15231 2.85420
C 2.85403 0.18921 -1.05953
C 1.11097 0.22177 2.87466
C 2.86429 0.27176 1.12853
C -2.82881 0.29776 1.09756
C 1.10290 0.20075 -2.82118
C -2.83020 0.46028 -1.08437
C -1.07890 0.37520 -2.83332
C -0.67262 0.08957 4.24426
C 4.24376 0.25848 -0.65201
C 0.68691 0.14160 4.25710
C 4.24963 0.31779 0.70712
C -4.21611 0.42837 0.69258
C 0.69248 0.17853 -4.21262
C -4.21589 0.53982 -0.66267
C -0.66241 0.29545 -4.22024
H -1.34182 0.01264 5.09764
H 5.09998 0.28078 -1.32172
H 1.34567 0.11352 5.12158
H 5.11078 0.39644 1.36617
H -5.07284 0.44959 1.36182
H 1.35490 0.07869 -5.06895
H -5.07291 0.66973 -1.31892
H -1.32346 0.30910 -5.08331
C -2.41736 0.17884 2.43393
C 2.44055 0.14394 -2.40044
C -2.41751 0.47862 -2.42497
C 2.45275 0.27258 2.46930
C -3.48079 0.08073 3.48130
C -3.80173 1.15863 4.31507
C -4.20126 -1.10588 3.66617
C -4.79396 1.06652 5.29266
C -5.49464 -0.13011 5.45181
C 3.50601 0.29709 3.52945
C 3.74439 1.44233 4.29959
C 4.29708 -0.82747 3.79690
C 4.72586 1.47494 5.29157
C 5.28389 -0.82014 4.78370
C 5.49855 0.33789 5.53303
C 3.50169 0.04072 -3.44941
C 4.20435 -1.15376 -3.65529
C 3.83746 1.12568 -4.26898
C 5.19740 -1.27061 -4.62901
C 4.82599 1.03394 -5.25016
C 5.50797 -0.17045 -5.43000
C -3.46613 0.59140 -3.48463
C -4.33436 -0.46886 -3.77555
C -3.62106 1.76446 -4.23468
C -5.31567 -0.37238 -4.76332
C -4.59422 1.88541 -5.22785
C -5.44463 0.81075 -5.49244
F -4.71811 3.01633 -5.92026
F -2.82511 2.81098 -4.00734
F 5.12350 2.08531 -6.01153
F 6.45142 -0.26924 -6.36092
F 3.20662 2.29236 -4.12302
F 5.84536 -2.42131 -4.80115
F 3.93158 -2.22728 -2.90921
F 4.93121 2.58086 6.00451
F 6.43574 0.35725 6.47515
F 6.01742 -1.90700 5.01641
F 4.11461 -1.95169 3.10057
F 3.02315 2.54580 4.09426
F -3.93914 -2.17016 2.90342
F -3.15051 2.31634 4.18903
F -5.07771 2.11021 6.06969
F -6.44204 -0.22866 6.37877
F -6.37472 0.91353 -6.43631
F -6.12420 -1.39987 -5.01687
F -4.23665 -1.61610 -3.10075
C -5.19732 -1.22363 4.63659
F -5.86257 -2.36700 4.79045
Cl 0.09072 2.60092 0.06754
O -0.13875 -1.60782 -0.10813
C 0.60491 -2.57102 0.61594
H 1.14397 -2.10581 1.46122
C 1.60602 -3.23472 -0.29575
H 2.58197 -2.76093 -0.44081
C 1.12399 -4.22571 -1.30804
H 0.62685 -3.68177 -2.14255
H 1.97160 -4.76009 -1.77068
C 0.11015 -5.22174 -0.71310
H -0.33656 -5.83295 -1.51592
H 0.64475 -5.92129 -0.04449
C -0.98090 -4.50115 0.08922
H -1.57438 -3.86213 -0.58767
H -1.67927 -5.23517 0.52699
C -0.37317 -3.62162 1.18891
H 0.17372 -4.25914 1.90861
H -1.16500 -3.10145 1.75318

$S = 2$

^{5}**RC**

Fe -0.27182 0.19096 -0.28031
N -0.28556 -0.00320 1.80306
N 1.81873 0.15462 -0.26391
N -2.34525 0.45240 -0.26504
N -0.23912 0.64125 -2.32438
C -1.39830 -0.08350 2.58639
C 2.63080 0.30372 -1.34892
C 0.80514 -0.22959 2.58916
C 2.60501 -0.04437 0.83193
C -3.15320 0.35554 0.82869
C 0.86966 0.66145 -3.11797
C -3.12803 0.71430 -1.35020
C -1.33320 0.81987 -3.11825
C -0.99629 -0.37673 3.95350
C 4.01749 0.20971 -0.91961
C 0.36417 -0.46592 3.95535
C 4.00150 -0.00677 0.42636
C -4.53094 0.58545 0.42259
C 0.46014 0.85445 -4.50045
C -4.51512 0.80949 -0.92216
C -0.89962 0.95197 -4.50062
H -1.66538 -0.50760 4.80077
H 4.89125 0.31060 -1.55924
H 1.00765 -0.68333 4.80457
H 4.85971 -0.11442 1.08560
H -5.39642 0.59203 1.08113
H 1.12290 0.89778 -5.36160
H -5.36565 1.03230 -1.56223
H -1.54896 1.08917 -5.36208
C -2.73233 0.08820 2.15142
C 2.20627 0.52250 -2.67954
C -2.67647 0.87256 -2.68052
C 2.15060 -0.24355 2.15597
C -3.80344 -0.03689 3.18952

C -4.01236 0.95794 4.15297
C -4.63962 -1.15943 3.24196
C -5.00529 0.84675 5.12767
C -5.82189 -0.28495 5.15273
C 3.19475 -0.50292 3.19657
C 3.52324 0.45572 4.16363
C 3.88835 -1.71899 3.24561
C 4.49559 0.22155 5.13737
C 4.86374 -1.97815 4.20940
C 5.16862 -1.00108 5.15855
C 3.27540 0.62090 -3.72258
C 3.99340 -0.50595 -4.14314
C 3.60478 1.84484 -4.31914
C 4.99566 -0.42612 -5.11125
C 4.60255 1.95048 -5.28941
C 5.30127 0.80889 -5.68529
C -3.71939 1.11968 -3.72533
C -4.59654 0.10869 -4.13884
C -3.86030 2.37312 -4.33518
C -5.57060 0.32701 -5.11442
C -4.82591 2.61622 -5.31323
C -5.68426 1.58715 -5.70371
F -4.93551 3.82015 -5.87187
F -3.05763 3.37940 -3.98380
F 4.89425 3.12995 -5.83462
F 6.25450 0.89746 -6.60712
F 2.95932 2.95638 -3.96141
F 5.65738 -1.51733 -5.49199
F 3.72514 -1.70225 -3.61658
F 4.78735 1.15559 6.04047
F 6.09658 -1.23485 6.08062
F 5.50171 -3.14670 4.23047
F 3.62111 -2.67644 2.35284
F 2.90089 1.63583 4.17101
F -4.49017 -2.14615 2.35353
F -3.24978 2.05270 4.15665
F -5.18120 1.81207 6.02787
F -6.77122 -0.40075 6.07546
F -6.60757 1.80690 -6.63393
F -6.38682 -0.65680 -5.48801
F -4.51395 -1.10863 -3.59861
C -5.63843 -1.29531 4.20716
F -6.41361 -2.37766 4.23247
Cl -0.09693 2.57350 0.09297
O -0.39009 -1.41559 -0.52905
C 0.72139 -5.67720 0.33925
H 1.60569 -6.20358 -0.03964
C -0.34978 -5.53284 -0.45571
H -0.31543 -5.92461 -1.47939
C -1.62128 -4.84543 -0.02071
H -2.49579 -5.40938 -0.39113
C -1.69188 -4.67745 1.50392
H -2.50952 -3.98930 1.77349
H -1.93108 -5.65137 1.96961
C -0.35522 -4.16590 2.05479
H -0.13351 -3.19383 1.58154
H -0.42226 -3.98538 3.14030
C 0.78677 -5.14637 1.75060
H 0.76377 -5.99706 2.46054
H 1.76208 -4.65678 1.91989
H -1.67763 -3.85231 -0.50665

$^{5\alpha}$**TS**$_{H}$

Fe -0.36020 0.10688 -0.23505
N -0.37863 -0.01176 1.86392
N 1.73571 0.04061 -0.21000
N -2.43005 0.45629 -0.22198
N -0.31287 0.54526 -2.28469
C -1.49427 -0.05232 2.64519
C 2.55185 0.15194 -1.29571
C 0.70539 -0.24890 2.65525
C 2.51418 -0.15067 0.89243
C -3.23972 0.39593 0.87252
C 0.79761 0.52316 -3.07593
C -3.20427 0.72018 -1.31197
C -1.40125 0.74454 -3.08164
C -1.10161 -0.32901 4.01915
C 3.93588 0.03708 -0.86125
C 0.25713 -0.44902 4.02552
C 3.91246 -0.15215 0.48945
C -4.61205 0.65193 0.46147
C 0.39481 0.70690 -4.46192
C -4.58960 0.85614 -0.88707
C -0.96221 0.84330 -4.46545
H -1.77429 -0.42782 4.86809
H 4.81368 0.10713 -1.49964
H 0.89341 -0.66470 4.88075
H 4.76751 -0.26422 1.15223
H -5.47823 0.68883 1.11836
H 1.05844 0.71882 -5.32352
H -5.43470 1.08997 -1.53055
H -1.60517 0.98634 -5.33078
C -2.82390 0.13792 2.20019
C 2.13069 0.35693 -2.63124
C -2.74406 0.84204 -2.64482
C 2.05057 -0.30870 2.22028
C -3.90187 0.03314 3.23352
C -4.12439 1.04571 4.17455
C -4.73041 -1.09413 3.30104
C -5.12672 0.94851 5.14126
C -5.93669 -0.18753 5.18141
C 3.08594 -0.58493 3.26538
C 3.45819 0.38071 4.20892
C 3.72791 -1.82775 3.33958
C 4.42540 0.12831 5.18344
C 4.69676 -2.10563 4.30454
C 5.04813 -1.12007 5.22867
C 3.20325 0.41301 -3.67391
C 3.89791 -0.73628 -4.07243
C 3.56154 1.61874 -4.29075
C 4.90493 -0.69537 -5.03805
C 4.56431 1.68554 -5.25929
C 5.23912 0.52227 -5.63284
C -3.77871 1.09518 -3.69654
C -4.68221 0.09930 -4.08978
C -3.88436 2.33750 -4.33559
C -5.64730 0.32116 -5.07343
C -4.83999 2.58378 -5.32264
C -5.72470 1.56963 -5.69262
F -4.91509 3.77701 -5.90943
F -3.05628 3.33011 -4.00469
F 4.88340 2.84875 -5.82393
F 6.19689 0.57383 -6.55287
F 2.94059 2.75071 -3.95422
F 5.54416 -1.80735 -5.39683
F 3.60228 -1.91733 -3.52615
F 4.76028 1.06946 6.06405
F 5.97080 -1.37132 6.15155
F 5.28515 -3.29934 4.35041
F 3.41141 -2.79422 2.47255
F 2.88410 1.58493 4.19287
F -4.56328 -2.09773 2.43548
F -3.36721 2.14420 4.16339
F -5.31706 1.93054 6.02039
F -6.89450 -0.29023 6.09712
F -6.63880 1.79258 -6.63128
F -6.48888 -0.64875 -5.42689
F -4.63411 -1.10749 -3.52207
C -5.73838 -1.21596 4.25849
F -6.50703 -2.30271 4.29955
Cl -0.10505 2.60473 0.10651
O -0.53353 -1.60398 -0.46513
C 1.14892 -5.35346 0.11561
H 2.02782 -5.88755 -0.26291
C 0.26363 -4.82539 -0.75992
H 0.45690 -4.91162 -1.83516
C -0.95250 -4.11338 -0.33476
H -1.79512 -4.22616 -1.03564
C -1.32647 -4.30830 1.12841
H -2.07246 -3.55756 1.43643
H -1.81134 -5.29686 1.25313
C -0.07906 -4.22835 2.01731
H 0.35323 -3.21885 1.91350
H -0.34640 -4.35377 3.07899
C 0.97760 -5.26573 1.60929
H 0.70741 -6.26805 1.99859
H 1.94676 -5.02601 2.08038
H -0.71433 -2.88154 -0.45946

$^{5\alpha}$**IM**$_{H}$

Fe -0.14587 0.21905 0.09600
N -0.10136 0.14425 2.19710
N 1.94743 -0.00001 0.05749
N -2.19775 0.60447 0.15037
N -0.13929 0.54829 -1.98110
C -1.19110 0.19884 3.01330
C 2.73397 0.05584 -1.05549
C 0.99543 -0.11715 2.96343
C 2.75571 -0.14345 1.14714
C -2.96588 0.67869 1.27620
C 0.94172 0.42506 -2.80278
C -2.98621 0.89023 -0.92629
C -1.24343 0.75264 -2.75326
C -0.76935 -0.05474 4.38312
C 4.12669 -0.05654 -0.65465
C 0.58031 -0.25002 4.35225
C 4.14017 -0.17769 0.70518
C -4.32361 1.03230 0.89702
C 0.50104 0.54894 -4.18454
C -4.33619 1.16236 -0.46192
C -0.84737 0.75233 -4.15385
H -1.41864 -0.09290 5.25489
H 4.98709 -0.02586 -1.31931
H 1.23027 -0.47603 5.19451
H 5.01378 -0.26345 1.34721
H -5.15853 1.18127 1.57797
H 1.13349 0.47669 -5.06643
H -5.18300 1.43625 -1.08697
H -1.51188 0.87576 -5.00592
C -2.52025 0.46440 2.60346
C 2.27902 0.21562 -2.38772
C -2.56510 0.93279 -2.27793
C 2.32655 -0.23185 2.49459
C -3.55589 0.54105 3.68117
C -3.60022 1.61622 4.57844
C -4.52667 -0.45706 3.83571
C -4.56346 1.70141 5.58488
C -5.51652 0.68971 5.71266
C 3.38936 -0.45553 3.52455
C 3.75928 0.55209 4.42557
C 4.06351 -1.67915 3.63130
C 4.75194 0.35851 5.38752
C 5.05960 -1.89792 4.58392
C 5.40494 -0.87254 5.46558
C 3.31825 0.16196 -3.46337
C 3.95815 -1.03703 -3.80358
C 3.69509 1.30685 -4.17788
C 4.92375 -1.10394 -4.80894
C 4.65827 1.26665 -5.18724
C 5.27448 0.05484 -5.50345
C -3.62064 1.20005 -3.30465
C -4.59635 0.24377 -3.61579
C -3.67651 2.41497 -4.00039
C -5.58332 0.47749 -4.57457
C -4.65355 2.67253 -4.96332
C -5.61075 1.69821 -5.25076
F -4.68102 3.83965 -5.60417
F -2.77978 3.37020 -3.74807
F 4.99547 2.37430 -5.84481
F 6.19238 0.00438 -6.46298
F 3.13027 2.48286 -3.89908
F 5.50817 -2.26175 -5.11027
F 3.64774 -2.16771 -3.16293
F 5.08205 1.33922 6.22555
F 6.35229 -1.06798 6.37669
F 5.67761 -3.07496 4.65900
F 3.75853 -2.68587 2.80712
F 3.16024 1.74319 4.37744
F -4.53824 -1.50880 3.01454
F -2.70684 2.60251 4.48248
F -4.58096 2.73940 6.41905
F -6.43790 0.75922 6.66787
F -6.54573 1.93222 -6.16579
F -6.49332 -0.45499 -4.85038
F -4.59717 -0.93581 -2.99198
C -5.49946 -0.39514 4.83464
F -6.40594 -1.36305 4.95769
Cl 0.25023 2.70029 0.34121
O -0.40329 -1.65369 -0.08294
C 1.59876 -4.84778 1.31812
H 2.11029 -4.79886 2.28338
C 2.14932 -4.20275 0.21159
H 3.08032 -3.64134 0.34026
C 1.56404 -4.25993 -1.05255
H 2.05265 -3.77361 -1.90128
C 0.28416 -5.01704 -1.27594
H -0.31544 -4.52511 -2.06095
H 0.51820 -6.02651 -1.67500
C -0.53568 -5.14007 0.01905
H -0.93129 -4.13961 0.26115
H -1.39780 -5.80917 -0.13344
C 0.32081 -5.62991 1.19827
H 0.55858 -6.70701 1.06886
H -0.25265 -5.57318 2.13974
H 0.41654 -2.16734 -0.14655

$^{5\beta}$**TS**$_{H}$

Fe -0.10474 0.15963 -0.06069
N -0.12946 0.16103 2.05403
N 1.96330 0.16461 -0.03734
N -2.16475 0.26436 -0.08179
N -0.07910 0.33808 -2.16905
C -1.24030 0.08995 2.83546
C 2.77693 0.25137 -1.13000
C 0.96289 0.05171 2.85773
C 2.75110 0.13676 1.07721
C -2.98104 0.24062 1.01436
C 1.03282 0.34819 -2.95298
C -2.95468 0.34776 -1.19452
C -1.17010 0.38376 -2.97924
C -0.83787 -0.07076 4.22558
C 4.16285 0.28697 -0.68733
C 0.52597 -0.09380 4.23924
C 4.14687 0.21620 0.67304
C -4.36513 0.32076 0.57696
C 0.63016 0.40341 -4.35144
C -4.34932 0.37783 -0.78474
C -0.73352 0.43247 -4.36760
H -1.50609 -0.16893 5.07820
H 5.03479 0.37365 -1.33138
H 1.17257 -0.21525 5.10538
H 5.00355 0.23535 1.34252
H -5.23785 0.33767 1.22541
H 1.29819 0.41522 -5.20976
H -5.20762 0.43653 -1.44976
H -1.38026 0.48508 -5.24059
C -2.57290 0.14370 2.36561
C 2.36587 0.31638 -2.48263
C -2.51328 0.39243 -2.53800
C 2.30749 0.06158 2.41915
C -3.65456 0.06907 3.39714
C -3.91244 1.13513 4.26861
C -4.44870 -1.07605 3.54135
C -4.91387 1.07236 5.23899
C -5.68862 -0.08267 5.35537
C 3.36162 -0.01693 3.47851
C 3.59823 1.04920 4.35657
C 4.15123 -1.16266 3.64391
C 4.57251 0.98542 5.35394
C 5.13177 -1.25065 4.63321
C 5.34217 -0.17063 5.49189
C 3.44860 0.36326 -3.51530
C 4.23098 -0.76178 -3.80635
C 3.72694 1.53378 -4.23275
C 5.24625 -0.73053 -4.76353
C 4.73674 1.59049 -5.19472
C 5.49885 0.45188 -5.46076
C -3.56919 0.45097 -3.59807
C -3.86193 -0.65953 -4.39952
C -4.30180 1.61988 -3.84051
C -4.83876 -0.61905 -5.39556
C -5.28322 1.68692 -4.83081
C -5.55111 0.56157 -5.61189
F -5.96043 2.81480 -5.03733
F -4.07051 2.71410 -3.11277
F 4.97882 2.72093 -5.85609
F 6.46314 0.49370 -6.37457
F 3.02027 2.64192 -4.00168
F 5.97052 -1.81899 -5.01768
F 4.01594 -1.90917 -3.15974
F 4.77460 2.01863 6.16970
F 6.27304 -0.24255 6.43786
F 5.86164 -2.35678 4.76642
F 3.97399 -2.21643 2.84445
F 2.88365 2.17135 4.25202
F -4.25076 -2.13105 2.74635
F -3.19219 2.25519 4.18395
F -5.13668 2.10535 6.04946
F -6.64543 -0.15330 6.27515
F -6.48283 0.61357 -6.55824
F -5.09415 -1.69463 -6.13786
F -3.19800 -1.80590 -4.22302
C -5.45603 -1.16349 4.50319
F -6.19060 -2.26857 4.61647
Cl -0.01988 2.55377 0.02955
O -0.05528 -1.57800 -0.12848
C -1.44346 -5.11430 -1.48806
H -1.45985 -5.61195 -2.46423
C -2.01050 -3.89177 -1.35188
H -2.45038 -3.40396 -2.22862
C -2.04352 -3.16629 -0.07824
H -2.91734 -2.51118 0.04477
C -1.70328 -3.99913 1.14817
H -1.47987 -3.34396 2.00549
H -2.58863 -4.59735 1.44293
C -0.52106 -4.93344 0.86027
H 0.36235 -4.30995 0.63920
H -0.27320 -5.53584 1.74947
C -0.80335 -5.85038 -0.33969
H -1.46510 -6.68631 -0.03480
H 0.12845 -6.33666 -0.67959
H -1.08892 -2.27316 -0.15555

$^{5\beta}$**IM**$_{H}$

Fe 0.18010 0.22727 0.02429
N 0.15307 0.24355 2.04521
N 2.22895 0.29753 0.05426
N -1.88025 0.31764 -0.00091
N 0.20057 0.37465 -1.99362
C -0.95770 0.15286 2.84383
C 3.05546 0.37847 -1.03142
C 1.24033 0.19266 2.87695
C 3.02994 0.33028 1.16070
C -2.70774 0.29402 1.08514
C 1.30892 0.37780 -2.79874
C -2.68117 0.41957 -1.10289
C -0.88886 0.42040 -2.82429
C -0.55713 0.02329 4.22961
C 4.43458 0.47653 -0.59763
C 0.80287 0.05021 4.25039
C 4.41842 0.44986 0.76374
C -4.08927 0.39482 0.65843

C 0.90682 0.40808 -4.18974
C -4.07303 0.46756 -0.70181
C -0.45329 0.44578 -4.20543
H -1.23052 -0.08601 5.07596
H 5.29995 0.57221 -1.24886
H 1.45351 -0.03451 5.11709
H 5.26845 0.51931 1.43805
H -4.95702 0.41348 1.31326
H 1.57949 0.40313 -5.04365
H -4.92573 0.54554 -1.37197
H -1.10501 0.48973 -5.07447
C -2.29726 0.19163 2.42449
C 2.64829 0.38701 -2.37510
C -2.23747 0.45541 -2.43413
C 2.59024 0.25675 2.49239
C -3.36086 0.11761 3.47345
C -3.61937 1.19328 4.33289
C -4.14471 -1.03139 3.63957
C -4.60950 1.13423 5.31494
C -5.37300 -0.02586 5.45430
C 3.62603 0.24181 3.57026
C 3.80837 1.33498 4.42763
C 4.45738 -0.86859 3.76894
C 4.76930 1.32918 5.43978
C 5.42570 -0.89793 4.77351
C 5.58115 0.20694 5.61209
C 3.71493 0.43410 -3.42231
C 4.51721 -0.68082 -3.69709
C 3.96414 1.59696 -4.16267
C 5.52341 -0.64761 -4.66378
C 4.96474 1.65517 -5.13390
C 5.74689 0.52653 -5.38463
C -3.27444 0.53922 -3.50969
C -3.62514 -0.57707 -4.27802
C -3.93599 1.74088 -3.79111
C -4.59107 -0.51055 -5.28317
C -4.90484 1.83424 -4.79164
C -5.23134 0.70278 -5.54105
F -5.51500 2.99179 -5.03698
F -3.64681 2.83935 -3.09207
F 5.17909 2.77705 -5.81825
F 6.70228 0.56997 -6.30703
F 3.23590 2.69358 -3.94657
F 6.26745 -1.72554 -4.90319
F 4.33089 -1.81793 -3.02475
F 4.91922 2.38539 6.23651
F 6.49955 0.19046 6.57213
F 6.19648 -1.97094 4.93930
F 4.33284 -1.94318 2.98813
F 3.05108 2.42447 4.28935
F -3.94812 -2.09478 2.85477
F -2.90853 2.31689 4.22641
F -4.83186 2.17503 6.11463
F -6.31856 -0.09289 6.38518
F -6.15113 0.77998 -6.49679
F -4.90340 -1.59129 -5.99499
F -3.02875 -1.75232 -4.05847
C -5.14035 -1.11568 4.61372
F -5.86428 -2.22478 4.74784
Cl 0.18352 2.81131 0.08136
O 0.15832 -1.70409 -0.03539
C -1.44978 -4.93381 -1.62365
H -1.20432 -5.10731 -2.67573
C -2.44489 -4.01815 -1.28410
H -2.94403 -3.46027 -2.08309
C -2.83190 -3.79835 0.03682
H -3.64031 -3.09770 0.26357
C -2.17482 -4.54081 1.16685
H -2.15636 -3.91045 2.07151
H -2.79352 -5.42256 1.43765
C -0.75327 -4.99155 0.79402
H -0.12177 -4.08985 0.72865
H -0.33359 -5.63735 1.58229
C -0.72123 -5.71272 -0.56368
H -1.17905 -6.71996 -0.46591
H 0.32106 -5.90000 -0.87558
H -0.68945 -2.04343 -0.35745

$^{5\alpha}\mathbf{TS}_{Ep}$

Fe 0.06870 -0.09813 0.35477
N 0.06427 0.16797 2.44166
N 2.15966 0.10998 0.35101
N -2.02476 0.03054 0.34990
N 0.06967 -0.00071 -1.74190
C -1.03984 0.15349 3.24060
C 2.95805 0.11363 -0.75296
C 1.16778 0.19872 3.24074
C 2.95468 0.21846 1.45250
C -2.82432 0.10674 1.45104
C 1.17510 -0.04693 -2.53794
C -2.82145 0.01524 -0.75552
C -1.03330 -0.07869 -2.53934
C -0.61806 0.16375 4.63381
C 4.34579 0.24848 -0.33506
C 0.74540 0.19184 4.63389
C 4.34347 0.31527 1.02723
C -4.21488 0.15857 1.02430
C 0.75512 -0.16928 -3.92637
C -4.21315 0.10066 -0.33850
C -0.60853 -0.18835 -3.92719
H -1.27498 0.14172 5.50038
H 5.20894 0.30334 -0.99464
H 1.40227 0.19675 5.50070
H 5.20467 0.43435 1.68077
H -5.08014 0.24475 1.67767
H 1.41332 -0.24143 -4.78915
H -5.07669 0.13097 -0.99914
H -1.26366 -0.27909 -4.79057
C -2.38362 0.13927 2.79592
C 2.51814 0.01310 -2.09485
C -2.37749 -0.06442 -2.09737
C 2.51149 0.23705 2.79684
C -3.44516 0.16359 3.85072
C -3.70149 1.31370 4.60837
C -4.23011 -0.96457 4.12239
C -4.69185 1.34741 5.59139
C -5.45666 0.20614 5.83765
C 3.57016 0.30390 3.85267
C 3.77526 1.46164 4.61443
C 4.40380 -0.78967 4.12137
C 4.76265 1.53575 5.59818
C 5.39796 -0.74050 5.09970
C 5.57692 0.42846 5.84106
C 3.57969 -0.04901 -3.14794
C 4.37753 -1.18952 -3.30729
C 3.81929 1.02106 -4.01956
C 5.36847 -1.27070 -4.28655
C 4.80467 0.96506 -5.00666
C 5.58255 -0.18623 -5.13891
C -3.43622 -0.15785 -3.15102
C -4.18896 -1.32730 -3.31990
C -3.71757 0.90968 -4.01298
C -5.17767 -1.43771 -4.29851
C -4.70167 0.82450 -4.99934
C -5.43477 -0.35470 -5.14086
F -4.94745 1.85899 -5.80121
F -3.03670 2.05207 -3.90473
F 5.01000 2.00129 -5.81755
F 6.52417 -0.25013 -6.07471
F 3.09557 2.13760 -3.91999
F 6.10594 -2.37215 -4.41489
F 4.19733 -2.24765 -2.51174
F 4.93470 2.65344 6.30172
F 6.52018 0.48698 6.77564
F 6.17182 -1.79922 5.33241
F 4.25880 -1.92431 3.43332
F 3.01695 2.53982 4.40698
F -4.03463 -2.09366 3.43801
F -2.99123 2.42347 4.39771
F -4.91327 2.45873 6.29119
F -6.40229 0.22623 6.77143
F -6.37475 -0.44653 -6.07606
F -5.87245 -2.56558 -4.43598
F -3.96556 -2.38432 -2.53419
C -5.22576 -0.95630 5.10041
F -5.95209 -2.04749 5.33631
Cl 0.02110 2.48331 0.26829
O 0.09063 -1.82473 0.42771
C -0.17189 -3.78106 0.71388
H -0.42834 -3.60865 1.76171
C 1.10896 -4.20062 0.41598
H 1.88606 -4.10983 1.18235
C 1.52656 -4.62784 -0.96051
H 2.05571 -3.78319 -1.44809
H 2.28264 -5.42992 -0.88990
C 0.34180 -5.07446 -1.83233
H 0.65799 -5.14980 -2.88575
H 0.03006 -6.08964 -1.52605
C -0.85109 -4.12160 -1.69038
H -0.55702 -3.11174 -2.02170
H -1.68468 -4.44076 -2.33703
C -1.31717 -4.04005 -0.23310
H -1.79357 -4.99577 0.06270
H -2.08546 -3.26310 -0.10655

$^{5\alpha}\mathbf{IM}_{Ep}$

Fe 0.00596 0.17293 -0.11671
N 0.02440 0.26655 1.98065
N 2.09777 0.30391 -0.14527
N -2.09334 0.25436 -0.08065
N -0.01775 0.31937 -2.20796
C -1.06941 0.25524 2.79580
C 2.88278 0.39675 -1.25623
C 1.14075 0.24321 2.76400
C 2.90573 0.33384 0.95321
C -2.87912 0.30898 1.03169
C 1.07521 0.33314 -3.02214
C -2.90156 0.29127 -1.17763
C -1.13445 0.26403 -2.99012
C -0.62677 0.20509 4.18029
C 4.27399 0.50211 -0.84406
C 0.73772 0.19605 4.16076
C 4.28862 0.45870 0.51974
C -4.27237 0.39587 0.62308
C 0.63345 0.26999 -4.40703
C -4.28654 0.38317 -0.74149
C -0.72989 0.22386 -4.38719
H -1.27112 0.17018 5.05576
H 5.12998 0.60978 -1.50629
H 1.40640 0.15363 5.01748
H 5.15781 0.52339 1.17041
H -5.12922 0.47231 1.28870
H 1.27810 0.24844 -5.28272
H -5.15702 0.44881 -1.39026
H -1.39647 0.15905 -5.24406
C -2.41968 0.28345 2.37066
C 2.42513 0.38980 -2.59646
C -2.47266 0.25879 -2.52768
C 2.47874 0.27374 2.30168
C -3.46509 0.27219 3.44134
C -3.70577 1.39040 4.24974
C -4.24549 -0.86652 3.68010
C -4.67692 1.38260 5.25238
C -5.43765 0.23189 5.46539
C 3.55324 0.24135 3.34339
C 3.83937 1.35320 4.14520
C 4.31942 -0.91190 3.55544
C 4.84262 1.32619 5.11547
C 5.32683 -0.96457 4.51976
C 5.58906 0.16159 5.30185
C 3.46898 0.45046 -3.66682
C 4.32578 -0.62963 -3.91763
C 3.63550 1.59144 -4.46315
C 5.30504 -0.58326 -4.91102
C 4.60693 1.66198 -5.46280
C 5.44489 0.56850 -5.68684
C -3.54745 0.20820 -3.56787
C -4.31885 -0.94633 -3.75579
C -3.83011 1.30350 -4.39406
C -5.32547 -1.01622 -4.71980
C -4.83208 1.25880 -5.36487
C -5.58245 0.09317 -5.52710
F -5.07857 2.31892 -6.13216
F -3.13439 2.43458 -4.26406
F 4.74209 2.76375 -6.19864
F 6.37329 0.62377 -6.63623
F 2.85468 2.65682 -4.27411
F 6.10104 -1.62912 -5.12609
F 4.21772 -1.74844 -3.19807
F 5.09345 2.40157 5.85985
F 6.54674 0.12456 6.22263
F 6.03509 -2.07788 4.69997
F 4.09098 -2.00650 2.82607
F 3.14519 2.48230 3.99219
F -4.06102 -1.96699 2.94706
F -2.99681 2.50671 4.07260
F -4.88408 2.46341 6.00226
F -6.36465 0.21309 6.41753
F -6.53922 0.03952 -6.44794
F -6.03759 -2.13058 -4.87623
F -4.09910 -2.02700 -3.00249
C -5.22158 -0.89960 4.67697
F -5.94316 -1.99985 4.88248
Cl -0.03854 2.71009 -0.08393
O 0.01423 -1.71880 -0.17908
C -0.58866 -2.77651 0.53238
H -1.28264 -2.37524 1.29870
C 0.52916 -3.52814 1.20337
H 0.96858 -3.08678 2.10562
C 1.35263 -4.49425 0.41130
H 2.09159 -3.92614 -0.19686
H 1.95756 -5.12845 1.08270
C 0.50260 -5.35727 -0.53786
H 1.15841 -5.93662 -1.20941
H -0.06775 -6.09323 0.05805
C -0.48119 -4.50182 -1.34552
H 0.08017 -3.81060 -1.99851
H -1.08770 -5.14127 -2.00926
C -1.39011 -3.68449 -0.41991
H -2.00522 -4.37181 0.19054
H -2.08750 -3.06165 -1.00406

$^{5\beta}\mathbf{TS}_{Ep}$

Fe -0.05096 0.06065 0.37319
N -0.04452 0.22918 2.47811
N 2.01930 0.06702 0.37346
N -2.11719 0.18692 0.36426
N -0.04352 0.10592 -1.74367
C -1.14819 0.22800 3.27431
C 2.82081 0.04987 -0.73211
C 1.05598 0.22950 3.27782
C 2.82208 0.17216 1.47386
C -2.91589 0.24572 1.46846
C 1.05507 -0.01306 -2.53652
C -2.91627 0.21899 -0.74109
C -1.14679 0.07646 -2.53876
C -0.73024 0.22073 4.66919
C 4.21087 0.14889 -0.31437
C 0.63426 0.22433 4.67140
C 4.21153 0.22665 1.04633
C -4.30572 0.33689 1.04437
C 0.63209 -0.12776 -3.92572
C -4.30562 0.32530 -0.31820
C -0.73067 -0.06925 -3.92738
H -1.38921 0.20558 5.53456
H 5.07407 0.17864 -0.97528
H 1.29091 0.21037 5.53851
H 5.07503 0.33070 1.69926
H -5.16794 0.41826 1.70233
H 1.28591 -0.25040 -4.78634
H -5.16853 0.39654 -0.97619
H -1.39022 -0.13498 -4.78986
C -2.48647 0.23868 2.81705
C 2.39369 -0.02829 -2.07956
C -2.48587 0.15476 -2.08820
C 2.39545 0.22146 2.82246
C -3.55660 0.23111 3.86358
C -3.84751 1.36555 4.63104
C -4.30974 -0.92190 4.11958
C -4.84401 1.36141 5.60864
C -5.57777 0.19667 5.83889
C 3.46368 0.25384 3.86973
C 3.72312 1.40800 4.61986
C 4.24830 -0.87351 4.14538
C 4.71738 1.44647 5.59888
C 5.24742 -0.86087 5.11960
C 5.48246 0.30612 5.84853
C 3.46327 -0.14148 -3.11996
C 4.21941 -1.31266 -3.26312
C 3.75103 0.91073 -3.99911
C 5.21833 -1.43736 -4.22969
C 4.74450 0.81068 -4.97448
C 5.48043 -0.36956 -5.08955
C -3.55033 0.15835 -3.14031
C -4.40067 -0.93913 -3.32953
C -3.73812 1.25970 -3.98602
C -5.39459 -0.94652 -4.30933
C -4.72419 1.27628 -4.97370
C -5.55586 0.16715 -5.13499
F -4.87908 2.34175 -5.75783
F -2.96367 2.33894 -3.85822
F 4.99615 1.83197 -5.79142
F 6.42923 -0.47587 -6.01432
F 3.07035 2.05549 -3.91561
F 5.91608 -2.56634 -4.34101
F 3.99370 -2.35826 -2.46240
F 4.94252 2.56161 6.29146
F 6.43177 0.33091 6.77856
F 5.97310 -1.95148 5.36012
F 4.04676 -2.00780 3.47028
F 3.01243 2.51683 4.40554
F -4.07604 -2.03813 3.42536
F -3.16548 2.49581 4.43610
F -5.09989 2.45856 6.31913
F -6.52878 0.18098 6.76746
F -6.49862 0.17141 -6.07199
F -6.18401 -2.00803 -4.46493
F -4.27200 -2.02354 -2.56215
C -5.31052 -0.95182 5.09179
F -6.00717 -2.06520 5.31344
Cl 0.00473 2.47862 0.29892
O -0.23814 -1.66709 0.39667
C 0.89908 -2.99348 1.17484
H 1.36562 -2.32286 1.89945
C 1.66831 -3.39587 0.09117
H 2.55718 -2.81631 -0.17300
C 1.22718 -4.47092 -0.85864
H 0.72678 -3.99498 -1.72859
H 2.10737 -4.98413 -1.28441
C 0.26788 -5.48085 -0.20972
H -0.19176 -6.11813 -0.98340
H 0.84459 -6.15481 0.44976
C -0.81037 -4.77272 0.61944
H -1.41549 -4.12694 -0.03966
H -1.49838 -5.50964 1.06662
C -0.18327 -3.90330 1.71562
H 0.27124 -4.55086 2.49061
H -0.95063 -3.30096 2.22551

$^{5\beta}\mathbf{IM}_{Ep}$

Fe -0.01593 0.21895 0.01661
N -0.01851 0.36923 2.13634

N 2.02461 0.19317 0.01819
N -2.06114 0.32585 0.00208
N -0.00840 0.20914 -2.11593
C -1.12149 0.37703 2.93007
C 2.83116 0.18295 -1.08824
C 1.07890 0.37724 2.93755
C 2.82768 0.31189 1.12180
C -2.86553 0.38200 1.10601
C 1.08909 0.09942 -2.90832
C -2.86244 0.33892 -1.10496
C -1.10901 0.17919 -2.91214
C -0.70791 0.38279 4.32645
C 4.21656 0.29512 -0.66595
C 0.65697 0.38515 4.33101
C 4.21443 0.37535 0.69410
C -4.25375 0.45569 0.67812
C 0.66996 -0.01661 -4.29883
C -4.25161 0.43433 -0.68370
C -0.69323 0.03492 -4.30135
H -1.36881 0.37695 5.19056
H 5.08015 0.33003 -1.32576
H 1.31260 0.37902 5.19905
H 5.07557 0.48812 1.34837
H -5.11734 0.53125 1.33475
H 1.32560 -0.13511 -5.15872
H -5.11398 0.49006 -1.34361
H -1.35252 -0.03276 -5.16394
C -2.45363 0.38197 2.45983
C 2.42224 0.09735 -2.44039
C -2.44393 0.25953 -2.45487
C 2.41395 0.36516 2.47374
C -3.53365 0.37103 3.49618
C -3.84776 1.50996 4.24728
C -4.26802 -0.79155 3.76262
C -4.85016 1.50140 5.21886
C -5.56538 0.32730 5.45965
C 3.49036 0.39692 3.51233
C 3.75897 1.55103 4.25908
C 4.27137 -0.73383 3.78498
C 4.76018 1.58696 5.23113
C 5.27731 -0.72349 4.75212
C 5.52183 0.44367 5.47774
C 3.50203 -0.00147 -3.47150
C 4.27445 -1.16231 -3.61224
C 3.77926 1.05519 -4.34889
C 5.27876 -1.27265 -4.57501
C 4.77786 0.96929 -5.32030
C 5.52978 -0.20099 -5.43336
C -3.51569 0.24679 -3.49954
C -4.35298 -0.86217 -3.67908
C -3.72092 1.34173 -4.34921
C -5.35218 -0.88627 -4.65318
C -4.71268 1.34167 -5.33138
C -5.53145 0.22164 -5.48299
F -4.88471 2.40129 -6.11977
F -2.95837 2.43044 -4.23067
F 5.01900 1.99446 -6.13548
F 6.48336 -0.29407 -6.35455
F 3.08300 2.19069 -4.26731
F 5.99191 -2.39211 -4.68438
F 4.06025 -2.21108 -2.81304
F 4.99465 2.70222 5.92033
F 6.47756 0.46603 6.40114
F 6.00017 -1.81659 4.98952
F 4.06085 -1.86775 3.11247
F 3.05162 2.66247 4.04729
F -4.01046 -1.91226 3.08423
F -3.18279 2.64852 4.04213
F -5.12856 2.60279 5.91404
F -6.52162 0.30727 6.38269
F -6.47943 0.21015 -6.41457
F -6.12951 -1.95789 -4.79947
F -4.20699 -1.94058 -2.90640
C -5.27437 -0.82600 4.72889
F -5.95356 -1.94800 4.96067
Cl 0.06107 2.59126 -0.08211
O -0.22891 -1.62306 0.07327
C 0.65002 -2.56311 0.67331
H 1.24446 -2.08448 1.47337
C 1.58039 -3.16179 -0.34618
H 2.53576 -2.67025 -0.55109
C 1.04401 -4.15119 -1.33211
H 0.44035 -3.61608 -2.09900
H 1.86508 -4.63381 -1.88930
C 0.14192 -5.20700 -0.66382
H -0.35628 -5.82177 -1.43281
H 0.77309 -5.89408 -0.07080
C -0.89353 -4.55531 0.26132
H -1.58247 -3.93398 -0.33724
H -1.50864 -5.33030 0.75020
C -0.21981 -3.66885 1.31601
H 0.42352 -4.29166 1.96503
H -0.97379 -3.19242 1.96473

2. [Fe^{IV}(O)(TMP)(Cl)]$^{-}$ (2a)

^{1}2a

Fe 0.000347 -0.000246 -0.318998
N 2.023301 0.014754 -0.217746
N -0.014675 2.023878 -0.223321
N 0.015221 -2.024301 -0.218705
N -2.022847 -0.015516 -0.223022
C 2.851028 -1.077773 -0.190937
C -1.119201 2.835755 -0.209704
C 2.834684 1.119563 -0.191267
C 1.077462 2.852219 -0.207501
C 1.119694 -2.836295 -0.204689
C -2.850582 1.077082 -0.198452
C -1.077037 -2.852663 -0.205311
C -2.834334 -1.120136 -0.196549
C 4.233649 -0.649605 -0.147475
C -0.712151 4.225374 -0.195670
C 4.223500 0.711991 -0.147530
C 0.649637 4.235586 -0.194925
C 0.712513 -4.225927 -0.192673
C -4.233285 0.649135 -0.157225
C -0.649249 -4.236067 -0.192828
C -4.223248 -0.712470 -0.156297
H 5.092285 -1.315855 -0.118041
H -1.392287 5.073745 -0.186916
H 5.072177 1.390902 -0.118305
H 1.317067 5.093982 -0.185631
H 1.392598 -5.074350 -0.184648
H -5.091757 1.315665 -0.129743
H -1.316735 -5.094433 -0.184945
H -5.071989 -1.391354 -0.128161
C 2.459359 -2.424685 -0.175858
C -2.458740 2.423763 -0.181371
C -2.422758 -2.460998 -0.178477
C 2.423125 2.460411 -0.176740
C 3.529762 -3.473938 -0.061246
C 3.904982 -3.952520 1.213293
C 4.168683 -3.977844 -1.220128
C 4.923491 -4.916000 1.307411
C 5.173673 -4.942703 -1.079920
C 5.571064 -5.424784 0.176793
H 5.215750 -5.277915 2.298085
H 5.663777 -5.328242 -1.979546
C 3.477167 3.525775 -0.059163
C 3.840939 4.010161 1.216917
C 4.108561 4.042628 -1.215974
C 4.841170 4.991740 1.314013
C 5.095453 5.026144 -1.072792
C 5.482577 5.512794 0.184979
H 5.122999 5.359610 2.305560
H 5.577962 5.423606 -1.971279
C -3.529091 3.472718 -0.063103
C -4.160314 3.987144 -1.222105
C -3.910738 3.942625 1.212515
C -5.162935 4.953929 -1.080784
C -4.926954 4.908829 1.307498
C -5.566855 5.427392 0.177409
H -5.645477 5.348831 -1.980402
H -5.222660 5.265272 2.299259
C -3.477026 -3.526201 -0.061577
C -4.106279 -4.044699 -1.218785
C -3.843167 -4.008756 1.214539
C -5.093355 -5.028126 -1.076003
C -4.843421 -4.990314 1.311220
C -5.482697 -5.513060 0.181727
H -5.574191 -5.426897 -1.974805
H -5.127034 -5.356789 2.302772
C -3.723604 -3.554598 -2.596026
H -3.935601 -2.479672 -2.715577
H -2.645561 -3.682856 -2.784392
H -4.274406 -4.097944 -3.377491
C -6.571335 -6.552350 0.304444
H -7.565027 -6.112411 0.110339
H -6.435266 -7.365855 -0.426127
H -6.596615 -6.995767 1.310919
C -3.158811 -3.522873 2.472909
H -2.234655 -4.097430 2.661007
H -2.858833 -2.466881 2.411788
H -3.807920 -3.653206 3.351693
C 3.779072 -3.488855 -2.595822
H 2.702767 -3.630732 -2.784166
H 3.976864 -2.410873 -2.712483
H 4.336763 -4.022649 -3.378989
C 3.214553 -3.480311 2.473566
H 2.894191 -2.430247 2.413664
H 2.302264 -4.072828 2.663861
H 3.868330 -3.598444 3.350630
C 6.664843 -6.459488 0.292560
H 6.402718 -7.381210 -0.253501
H 7.610407 -6.092408 -0.140606
H 6.856533 -6.730876 1.341100
C 3.728415 3.550573 -2.593225
H 3.941584 2.475693 -2.711191
H 2.650559 3.677633 -2.783423
H 4.279961 4.093475 -3.374475
C 3.154080 3.526657 2.474866
H 2.232786 4.105733 2.663223
H 2.848917 2.472224 2.413081
H 3.803669 3.653344 3.353846
C 6.571023 6.552235 0.308126
H 7.564833 6.112503 0.114196
H 6.435000 7.365801 -0.422400
H 6.595931 6.995576 1.314639
C -3.763227 3.507953 -2.599097
H -2.687036 3.656558 -2.782996
H -3.954761 2.429586 -2.722202
H -4.320975 4.043145 -3.381267
C -3.233442 3.463523 2.477940
H -2.795894 2.460980 2.373926
H -2.407138 4.141293 2.756495
H -3.938820 3.452619 3.322897
C -6.669193 6.452558 0.296517
H -6.503192 7.302031 -0.385736
H -7.648063 6.017577 0.030472
H -6.747410 6.846505 1.320607
Cl -0.003653 0.005556 2.201250
O 0.002487 -0.002357 -1.945553

^{3}2a

Fe 0.00304 0.00197 -0.31329
N -1.00505 -1.75308 -0.23790
N 1.75768 -1.00298 -0.17940
N -1.75249 1.01003 -0.24040
N 1.01062 1.75742 -0.19718
C -2.36524 -1.91838 -0.26596
C 3.01534 -0.45751 -0.16847
C -0.45977 -3.00942 -0.18478
C 1.92110 -2.36292 -0.11826
C -3.00999 0.46421 -0.25505
C 2.37154 1.92358 -0.20927
C -1.91733 2.36950 -0.18604
C 0.46445 3.01451 -0.16997
C -2.69218 -3.32901 -0.24235
C 4.00892 -1.50853 -0.09701
C -1.51100 -4.00510 -0.19200
C 3.33059 -2.68885 -0.05840
C -4.00522 1.51545 -0.21862
C 2.69753 3.33460 -0.19887
C -3.32817 2.69597 -0.16931
C 1.51559 4.01052 -0.16819
H -3.70020 -3.73603 -0.25733
H 5.08429 -1.34941 -0.07296
H -1.35132 -5.08017 -0.15990
H 3.73580 -3.69594 0.00151
H -5.08081 1.35609 -0.22531
H 3.70596 3.74128 -0.20791
H -3.73449 3.70347 -0.12678
H 1.35489 5.08579 -0.14965
C -3.33025 -0.90050 -0.26188
C 3.33752 0.90772 -0.18990
C -0.90003 3.33370 -0.13510
C 0.90324 -3.32737 -0.10524
C -4.77769 -1.29681 -0.17389
C -5.40153 -1.37891 1.09019
C -5.51575 -1.59448 -1.34554
C -6.74955 -1.77017 1.16157
C -6.85818 -1.97418 -1.22767
C -7.49622 -2.07311 0.01871
H -7.22635 -1.83791 2.14451
H -7.42386 -2.20153 -2.13681
C 1.29409 -4.77037 0.05210
C 1.32356 -5.34978 1.33935
C 1.63661 -5.54981 -1.08027
C 1.70987 -6.69456 1.47337
C 2.00818 -6.88754 -0.90044
C 2.05673 -7.48117 0.37061
H 1.73726 -7.13680 2.47424
H 2.26948 -7.48515 -1.77951
C 4.78843 1.30016 -0.14280
C 5.52846 1.44885 -1.33714
C 5.41419 1.52535 1.10598
C 6.88087 1.81559 -1.26160
C 6.76778 1.88921 1.13531
C 7.52257 2.03814 -0.03658
H 7.44753 1.93148 -2.19062
H 7.24564 2.06292 2.10456
C -1.29510 4.77605 0.01746
C -1.60824 5.56209 -1.11844
C -1.35804 5.34784 1.30726
C -1.98487 6.89890 -0.94004
C -1.74809 6.69143 1.43951
C -2.06695 7.48462 0.33273
H -2.22300 7.50195 -1.82195
H -1.80145 7.12762 2.44197
C -1.53713 4.97897 -2.51076
H -0.54256 4.55364 -2.72031
H -2.26172 4.15902 -2.64281
H -1.74926 5.74389 -3.27183
C -2.50246 8.92166 0.49260
H -1.95967 9.58560 -0.19951
H -3.57696 9.03922 0.26914
H -2.33438 9.28439 1.51742
C -0.98142 4.56666 2.54720
H -1.14216 3.48519 2.43610
H 0.08959 4.70190 2.78058
H -1.54884 4.91794 3.42242
C -4.87443 -1.50450 -2.71087
H -4.44769 -0.50474 -2.89111
H -4.04417 -2.22182 -2.81560
H -5.60474 -1.71322 -3.50612
C -4.67188 -1.02243 2.36696
H -3.58487 -1.16486 2.29129
H -4.83214 0.04023 2.62158
H -5.04609 -1.61691 3.21433
C -8.94022 -2.50494 0.11169
H -9.58346 -1.89954 -0.54781
H -9.06334 -3.55570 -0.20215
H -9.32429 -2.41544 1.13849
C 1.60296 -4.95778 -2.47027
H 0.61416 -4.53182 -2.70440
H 2.33009 -4.13637 -2.57707
H 1.83652 -5.71756 -3.23021
C 0.91501 -4.57745 2.57477
H 1.04268 -3.49195 2.46210
H -0.15254 -4.74662 2.80171
H 1.48724 -4.90902 3.45470
C 2.48453 -8.92038 0.53173
H 1.93313 -9.58251 -0.15555
H 3.55663 -9.04555 0.30160
H 2.31959 -9.27974 1.55820
C 4.88350 1.22476 -2.68516
H 4.49301 0.19869 -2.78033
H 4.02649 1.90017 -2.83911
H 5.60110 1.39318 -3.50117
C 4.64117 1.39312 2.39797
H 3.84398 2.15176 2.46720
H 4.14093 0.41504 2.47627
H 5.30069 1.51406 3.26952
C 8.98687 2.40177 0.02479
H 9.60982 1.50981 0.21407
H 9.33315 2.84750 -0.91985
H 9.19239 3.11472 0.83849
Cl -0.06814 -0.01758 2.20227
O 0.03337 0.00549 -1.93895

^{5}2a

Fe -0.00553 0.00327 -0.38221
N 0.01851 -2.08140 -0.28115
N 2.07870 0.02864 -0.29666
N -2.08659 -0.02076 -0.19625
N -0.03120 2.08550 -0.21055
C -1.07807 -2.89449 -0.24021
C 2.86508 1.14463 -0.25231
C 1.13595 -2.86792 -0.28580
C 2.89136 -1.06970 -0.29253
C -2.87351 -1.13824 -0.17903
C 1.06724 2.89884 -0.19800
C -2.90102 1.07638 -0.17586
C -1.14724 2.87335 -0.18694
C -0.63634 -4.27938 -0.22786
C 4.25964 0.73594 -0.22844
C 0.72867 -4.26282 -0.25750
C 4.27585 -0.62916 -0.25360
C -4.26834 -0.73078 -0.14161
C 0.62686 4.28358 -0.16342
C -4.28543 0.63440 -0.14198
C -0.73842 4.26803 -0.15926
H -1.29148 -5.14702 -0.19687
H 5.11138 1.41134 -0.19196
H 1.40555 -5.11435 -0.25755
H 5.14336 -1.28505 -0.24169
H -5.11937 -1.40796 -0.12066
H 1.28382 5.15040 -0.14673
H -5.15265 1.29057 -0.11896
H -1.41488 5.11954 -0.13607
C -2.42898 -2.47944 -0.18257
C 2.41837 2.48547 -0.19929
C -2.48910 2.42868 -0.16566
C 2.47667 -2.42176 -0.28084
C -3.47299 -3.55686 -0.06542
C -3.93129 -3.94981 1.21195
C -3.99420 -4.18205 -1.22350
C -4.89145 -4.97032 1.30874

C -4.95564 -5.19097 -1.08064
C -5.41615 -5.60595 0.17780
H -5.23893 -5.27381 2.30126
H -5.35665 -5.66815 -1.98041
C 3.55475 -3.46734 -0.18465
C 3.94718 -3.95143 1.08308
C 4.18207 -3.96320 -1.35299
C 4.97013 -4.91130 1.16044
C 5.19252 -4.92521 -1.22950
C 5.60749 -5.41106 0.01974
H 5.27386 -5.27835 2.14583
H 5.67173 -5.30598 -2.13698
C 3.47021 3.55510 -0.08014
C 4.08634 4.09000 -1.23679
C 3.84639 4.02558 1.19790
C 5.06963 5.07741 -1.09196
C 4.84184 5.01147 1.29666
C 5.46803 5.55046 0.16715
H 5.53949 5.48916 -1.99072
H 5.13244 5.36837 2.28970
C -3.56541 3.47879 -0.09852
C -4.11692 4.01499 -1.28551
C -4.02526 3.93401 1.15804
C -5.11694 4.99319 -1.19297
C -5.02793 4.91487 1.20466
C -5.59045 5.45710 0.04234
H -5.53728 5.40555 -2.11565
H -5.37727 5.26487 2.18092
C -3.64147 3.55010 -2.64242
H -2.56262 3.73099 -2.77570
H -3.79430 2.46667 -2.77367
H -4.17678 4.07017 -3.45007
C -6.68911 6.49076 0.11182
H -6.55666 7.27298 -0.65229
H -7.67758 6.03243 -0.06729
H -6.72655 6.97625 1.09849
C -3.45177 3.38183 2.44274
H -3.60033 2.29231 2.51603
H -2.36414 3.54783 2.50486
H -3.92021 3.85040 3.32042
C -3.53122 -3.77259 -2.60249
H -3.68220 -2.69484 -2.77503
H -2.45435 -3.96269 -2.73992
H -4.07533 -4.32366 -3.38327
C -3.43747 -3.27332 2.47126
H -2.37423 -2.99842 2.41281
H -3.99007 -2.33503 2.65425
H -3.58554 -3.91745 3.35078
C -6.43037 -6.71805 0.30044
H -7.24362 -6.60415 -0.43404
H -5.96637 -7.70208 0.11270
H -6.87712 -6.75009 1.30530
C 3.77318 -3.47130 -2.72209
H 2.69571 -3.61967 -2.89859
H 3.96240 -2.39156 -2.83658
H 4.32533 -3.99818 -3.51387
C 3.26919 -3.48983 2.35413
H 2.93690 -2.44318 2.30139
H 2.36585 -4.09239 2.55528
H 3.93622 -3.60349 3.22181
C 6.71931 -6.42795 0.12078
H 6.57220 -7.25674 -0.59045
H 7.69696 -5.97408 -0.11715
H 6.78861 -6.85346 1.13288
C 3.69331 3.61499 -2.61647
H 3.90822 2.54244 -2.75082
H 2.61314 3.74138 -2.79378
H 4.23512 4.16992 -3.39612
C 3.17724 3.51894 2.45611
H 2.23359 4.06123 2.64272
H 2.91331 2.45325 2.39426
H 3.82092 3.67082 3.33535
C 6.55380 6.59241 0.29289
H 7.55167 6.14841 0.13135
H 6.43496 7.39072 -0.45692
H 6.55692 7.05584 1.29072
Cl 0.07969 -0.05514 2.10226
O -0.05025 0.03357 -2.00749

CHE + 2a

$S = 0$

^{1}RC

Fe -0.034934 0.143250 0.414298
N -0.014393 0.373610 2.424528
N 1.988819 0.127374 0.404508
N -2.048122 0.348866 0.412671
N -0.045834 0.108883 -1.608233
C -1.094787 0.609644 3.234087
C 2.802748 0.113034 -0.698071
C 1.081214 0.295392 3.244569
C 2.810915 0.069484 1.499795
C -2.850108 0.575454 1.500223
C 1.048112 0.107883 -2.434040
C -2.879790 0.232413 -0.670830
C -1.149315 0.038750 -2.418231
C -0.666942 0.690834 4.615325
C 4.189585 0.044666 -0.286506
C 0.678676 0.478885 4.623588
C 4.194124 0.003008 1.075009
C -4.239176 0.603858 1.091490
C 0.621511 0.045832 -3.816679
C -4.258687 0.375156 -0.251412
C -0.739232 -0.013893 -3.806207
H -1.323373 0.878339 5.461541
H 5.040149 0.022511 -0.963778
H 1.351609 0.461151 5.477526
H 5.049751 -0.054355 1.743535
H -5.081925 0.769039 1.758544
H 1.288310 0.040087 -4.675507
H -5.120596 0.319883 -0.912088
H -1.416558 -0.074068 -4.654700
C -2.431583 0.739913 2.828520
C 2.394438 0.138384 -2.039508
C -2.490970 0.067605 -2.008729
C 2.415937 0.129283 2.844633
C -3.460402 1.096814 3.865358
C -3.805350 2.451983 4.063491
C -4.083493 0.090220 4.643182
C -4.755049 2.778135 5.046441
C -5.029688 0.460524 5.606634
C -5.378488 1.801562 5.829698
H -5.013374 3.830661 5.199313
H -5.508685 -0.322366 6.203081
C 3.480002 0.071126 3.905712
C 4.104381 1.258813 4.347548
C 3.859984 -1.173188 4.462267
C 5.097560 1.181254 5.337024
C 4.857190 -1.204676 5.446099
C 5.490656 -0.038578 5.899949
H 5.577101 2.104991 5.674879
H 5.147260 -2.170746 5.871220
C 3.447855 0.219184 -3.109236
C 3.945377 -0.956615 -3.722230
C 3.939462 1.481550 -3.508471
C 4.915169 -0.844731 -4.726184
C 4.907352 1.547022 -4.524979
C 5.409036 0.399338 -5.147604
H 5.295296 -1.757466 -5.195848
H 5.278744 2.528560 -4.835520
C -3.562493 -0.030161 -3.059347
C -4.075396 -1.292606 -3.431652
C -4.062402 1.142071 -3.674763
C -5.075543 -1.361469 -4.414178
C -5.062273 1.027347 -4.650213
C -5.582619 -0.215464 -5.038631
H -5.469729 -2.342570 -4.696244
H -5.446224 1.938126 -5.120412
C -3.567611 -2.560929 -2.785699
H -2.482907 -2.684798 -2.935630
H -3.732617 -2.552292 -1.696087
H -4.072089 -3.446167 -3.199289
C -6.640823 -0.309489 -6.111735
H -6.203775 -0.161575 -7.114742
H -7.134143 -1.292865 -6.108930
H -7.414685 0.464130 -5.983992
C -3.535696 2.505968 -3.292623
H -3.682147 2.709525 -2.219679
H -2.452287 2.586962 -3.477130
H -4.039331 3.299738 -3.863111
C -3.742935 -1.368442 4.443945
H -3.885909 -1.676453 3.395821
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C -3.209381 3.557119 3.219676
H -2.187473 3.332613 2.883433
H -3.809263 3.714879 2.305824
H -3.198011 4.510820 3.768604
C -6.389225 2.167972 6.890027
H -6.011924 1.931756 7.899691
H -6.631018 3.240749 6.865555
H -7.327569 1.603659 6.761957
C 3.205721 -2.457964 4.010492
H 2.119047 -2.442039 4.193071
H 3.335853 -2.622531 2.928857
H 3.626947 -3.325147 4.539461
C 3.722616 2.602173 3.769922
H 3.934372 2.651413 2.689328
H 2.644791 2.800376 3.882336
H 4.274186 3.416456 4.261795
C 6.557434 -0.106756 6.966580
H 7.375812 -0.784554 6.672146
H 6.992705 0.883117 7.167940
H 6.149731 -0.494901 7.915373
C 3.446122 -2.321027 -3.307207
H 3.577013 -2.486866 -2.225895
H 2.369548 -2.437806 -3.512193
H 3.981393 -3.118392 -3.842894
C 3.475921 2.758954 -2.844580
H 2.417188 2.724143 -2.550480
H 4.047612 2.947565 -1.918752
H 3.628802 3.625817 -3.504614
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H 6.725559 1.526339 -6.455514
H 7.367734 -0.058656 -5.958801
H 6.085078 0.028462 -7.175107
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O -0.122327 -1.482076 0.518028
C 2.351525 -5.072879 0.396834
H 3.379343 -4.792217 0.137295
C 2.133058 -5.839580 1.476543
H 2.985544 -6.191296 2.069741
C 0.755934 -6.255971 1.932987
H 0.618328 -7.337714 1.736307
H 0.681793 -6.153540 3.030356
C -0.353570 -5.447584 1.244851
H -1.333202 -5.923506 1.416689
H -0.406947 -4.441690 1.698092
C -0.078703 -5.293228 -0.256033
H -0.040597 -6.294834 -0.722660
H -0.903192 -4.749064 -0.745519
C 1.249701 -4.561868 -0.498046
H 1.556805 -4.658508 -1.554753
H 1.109337 -3.477437 -0.326376

$^{1\alpha}$TS$_{H}$

Fe -0.028045 0.010206 0.472332
N -0.014834 0.286787 2.477444
N 1.984825 -0.130746 0.452713
N -2.040098 0.243784 0.477435
N -0.031984 -0.149273 -1.540496
C -1.080451 0.595086 3.280809
C 2.806417 -0.166662 -0.644119
C 1.081297 0.202398 3.293726
C 2.800996 -0.177306 1.554222
C -2.839664 0.530810 1.551737
C 1.055285 -0.150410 -2.376747
C -2.871724 0.086913 -0.599656
C -1.142474 -0.213267 -2.343241
C -0.642623 0.721965 4.656091
C 4.188778 -0.264792 -0.224867
C 0.695475 0.465244 4.666309
C 4.184440 -0.290505 1.137655
C -4.229146 0.558904 1.141812
C 0.619453 -0.219732 -3.755442
C -4.250512 0.267915 -0.189134
C -0.741676 -0.281116 -3.734068
H -1.286892 0.968053 5.496794
H 5.042655 -0.315709 -0.896596
H 1.372279 0.462186 5.517405
H 5.035436 -0.361451 1.810986
H -5.070380 0.764715 1.799650
H 1.279840 -0.230723 -4.619402
H -5.113706 0.191882 -0.846184
H -1.424053 -0.346840 -4.578183
C -2.415384 0.743007 2.872198
C 2.403709 -0.121686 -1.988006
C -2.483054 -0.140848 -1.930114
C 2.407090 -0.037613 2.894726
C -3.434774 1.159258 3.895844
C -3.755893 2.526203 4.045436
C -4.073943 0.192923 4.711641
C -4.697643 2.904870 5.017647
C -5.011531 0.614510 5.662071
C -5.336524 1.968772 5.836640
H -4.936717 3.966742 5.132916
H -5.503071 -0.137501 6.287417
C 3.472557 -0.049602 3.956359
C 4.173158 1.138520 4.263067
C 3.771469 -1.243024 4.656424
C 5.158951 1.112116 5.263085
C 4.765653 -1.224955 5.643377
C 5.473397 -0.057167 5.964722
H 5.694861 2.036794 5.498472
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C 3.997527 -1.086765 -3.727278
C 3.901952 1.333312 -3.385231
C 4.966395 -0.883222 -4.721737
C 4.869449 1.490486 -4.388110
C 5.418360 0.396087 -5.069392
H 5.377153 -1.754342 -5.241530
H 5.202481 2.501134 -4.644283
C -3.557601 -0.238022 -2.978863
C -4.091746 -1.495886 -3.335415
C -4.039202 0.933985 -3.610426
C -5.093867 -1.561321 -4.316662
C -5.040201 0.822991 -4.584880
C -5.582000 -0.415967 -4.956439
H -5.504367 -2.539498 -4.585328
H -5.408023 1.733638 -5.068173
C -3.603245 -2.765158 -2.677012
H -2.530997 -2.932064 -2.869645
H -3.721119 -2.723931 -1.582337
H -4.154451 -3.641690 -3.047341
C -6.645011 -0.504816 -6.025288
H -6.220565 -0.311452 -7.025765
H -7.111974 -1.500584 -6.050262
H -7.439096 0.242616 -5.866903
C -3.493482 2.294973 -3.244641
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H -2.401099 2.343092 -3.379009
H -3.949972 3.083742 -3.860045
C -3.760490 -1.278249 4.565965
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H -2.138949 3.319852 2.805591
H -3.761111 3.754085 2.262974
H -3.079424 4.554220 3.691212
C -6.340043 2.390077 6.883459
H -5.974565 2.165951 7.900132
H -6.549931 3.468642 6.832892
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C 3.030182 -2.525424 4.358145
H 1.955686 -2.429316 4.584567
H 3.098208 -2.799457 3.293394
H 3.428050 -3.360673 4.952779
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H 4.337078 2.405415 2.511084
H 2.818560 2.602639 3.384922
H 4.325339 3.289243 4.053861
C 6.535371 -0.070967 7.038237
H 7.328832 -0.801306 6.807261
H 7.007445 0.915823 7.153626
H 6.113158 -0.360071 8.015416
C 3.547763 -2.491439 -3.401733
H 3.675395 -2.719124 -2.332047
H 2.479144 -2.635639 -3.629201
H 4.118366 -3.233387 -3.978818
C 3.361371 2.550677 -2.670529
H 2.261071 2.566758 -2.650067
H 3.680274 2.568553 -1.614992
H 3.714569 3.477343 -3.145887
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H 6.352810 1.541468 -6.659338
H 7.489994 0.605629 -5.672015
H 6.471945 -0.227288 -6.862344
Cl 0.196182 2.441014 0.236733
O -0.270490 -1.709901 0.742947
C 2.159687 -3.984425 0.241503
H 3.068583 -3.373784 0.196757
C 2.152623 -5.099953 1.005285
H 3.062497 -5.394050 1.540769
C 0.943145 -5.988830 1.144111
H 1.113595 -6.923682 0.572738
H 0.835892 -6.313862 2.194377
C -0.343023 -5.301225 0.663168
H -1.156807 -6.038815 0.567837
H -0.664851 -4.566798 1.421691
C -0.123155 -4.558532 -0.661423
H 0.139731 -5.287091 -1.453722
H -1.054974 -4.067669 -0.986108
C 0.988458 -3.524902 -0.526836
H 1.258089 -3.034299 -1.472941
H 0.473791 -2.564821 0.098902

$^{1\alpha}$TS$_{Ep}$

Fe -0.36135 0.14364 -0.21900
N -0.382

$S = 1$

^{3}RC

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N 0.22464 0.60111 -1.99487
C -0.91614 0.02806 2.82447
C 3.05980 0.55388 -1.04316
C 1.28051 -0.03324 2.83852
C 3.04202 0.18921 1.12363
C -2.64429 0.21565 1.07332
C 1.32932 0.77946 -2.78715
C -2.62491 0.40656 -1.11604
C -0.86515 0.66235 -2.82499
C -0.51029 -0.09376 4.20915

C 4.44220 0.52951 -0.61207
C 0.85076 -0.13778 4.21742
C 4.43137 0.29521 0.72955
C -4.02684 0.24649 0.64452
C 0.92485 0.96202 -4.16546
C -4.01497 0.35789 -0.71290
C -0.43443 0.88162 -4.19018
H -1.19008 -0.13771 5.05655
H 5.30113 0.67424 -1.26273
H 1.51601 -0.22280 5.07316
H 5.27922 0.20833 1.40477
H -4.88597 0.18559 1.30835
H 1.60535 1.12286 -4.99821
H -4.86276 0.40995 -1.39176
H -1.09826 0.96677 -5.04714
C -2.25553 0.11407 2.41606
C 2.66702 0.78777 -2.36935
C -2.21246 0.57215 -2.44630
C 2.62769 0.02010 2.45195
C -3.32083 0.15364 3.47595
C -3.79139 1.40530 3.94042
C -3.84805 -1.04062 4.01638
C -4.76725 1.43544 4.94648
C -4.82896 -0.96317 5.01711
C -5.30086 0.26361 5.50044
H -5.12177 2.40638 5.30732
H -5.23367 -1.89179 5.43098
C 3.67617 -0.01835 3.52808
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C 4.16565 -1.25793 4.00858
C 5.13687 1.13683 5.08563
C 5.13339 -1.26289 5.01974
C 5.63291 -0.07472 5.57651
H 5.51107 2.07621 5.50480
H 5.50868 -2.22368 5.38608
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C 4.41528 0.07860 -4.06601
C 4.05360 2.46218 -3.64157
C 5.41045 0.41599 -4.99095
C 5.06397 2.75432 -4.57385
C 5.75478 1.75018 -5.25924
H 5.93489 -0.38741 -5.51787
H 5.31446 3.80216 -4.76698
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C -3.76707 1.99587 -3.83521
C -4.72889 -0.26078 -5.18552
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C -5.24183 0.99881 -5.52197
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H -3.72987 -2.57070 -4.48309
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H -2.17654 3.36047 -3.26069
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C -3.37632 -2.39115 3.52999
H -3.51977 -2.50017 2.44279
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H -3.92194 -3.20494 4.02929
C -3.29321 2.70587 3.35007
H -2.23681 2.65897 3.04901
H -3.86259 2.96271 2.43941
H -3.42042 3.53702 4.05966
C -6.34971 0.33176 6.58481
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H -6.68031 -0.67127 6.89211
H -5.96648 0.85020 7.47983
C 3.65768 -2.56422 3.44354
H 2.57794 -2.69025 3.62534
H 3.79776 -2.61352 2.35170
H 4.17963 -3.42080 3.89430
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H 4.41624 2.92798 2.80189
H 2.72401 2.50275 3.08021
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C 6.67047 -0.11703 6.67283
H 6.97433 0.89370 6.98248
H 6.28942 -0.64353 7.56410
H 7.57453 -0.65841 6.34744
C 4.07985 -1.37318 -3.81497
H 4.26908 -1.65715 -2.76709
H 3.01441 -1.57885 -4.00679
H 4.67673 -2.03501 -4.45919
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H 2.91637 3.33356 -1.98754
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O 0.22318 -1.38531 -0.21751
C -0.04843 -5.49560 0.28824
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C -0.18368 -6.42785 -0.66711
H 0.65854 -7.09190 -0.89534
C -1.45117 -6.62294 -1.46342
H -1.29082 -6.26394 -2.49926
H -1.66453 -7.70206 -1.56415
C -2.64859 -5.89707 -0.83344
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H -2.99947 -6.47048 0.04396
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H -1.92741 -3.90251 -1.26206
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$^{3\alpha}TS_{H}$

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C -2.60984 0.14650 1.48255
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C -2.65788 -0.05670 -0.70664
C -0.94983 -0.15728 -2.48866
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C 0.98349 0.35868 4.53152
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C -4.00371 0.15411 1.09227
C 0.79770 -0.13227 -3.91560
C -4.03357 0.02434 -0.26371
C -0.56265 -0.20033 -3.88284
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H 5.32365 0.29294 1.55702
H -4.84296 0.25102 1.77664
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H -4.90225 -0.00614 -0.91669
H -1.25294 -0.26509 -4.72055
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C -3.56770 1.80557 4.25993
C -3.84231 -0.61602 4.49500
C -4.55266 1.98554 5.24645
C -4.81318 -0.38963 5.47759
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C 4.96952 1.53960 -4.74923
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C -5.44876 -0.06402 -5.02100
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H -5.13886 2.06893 -5.03057
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H -2.48667 -2.83314 -3.08605
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H -6.35130 -0.71765 -6.88249
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H -2.39761 -2.22066 4.25597
H -4.03378 -2.76287 4.70809
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H -2.03476 3.33323 4.28624
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H -3.58676 3.87677 3.62515
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H -5.96005 0.63084 7.87610
H -6.40993 2.18318 7.12778
H -7.20804 0.67377 6.62179
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H 3.99691 -2.35242 2.81213
H 4.38833 -2.98413 4.43154
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H 3.86311 2.92850 2.47043
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C 6.91246 0.63207 6.75866
H 6.48107 0.52099 7.76905
H 7.66677 -0.16211 6.64362
H 7.42764 1.60386 6.72774
C 3.76451 -2.36820 -3.38633
H 3.94511 -2.49861 -2.30713
H 2.68862 -2.54508 -3.54644
H 4.32071 -3.15058 -3.92276
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H 2.50390 2.59886 -2.63771
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H 3.45946 3.53685 -3.81993
C 6.53693 0.51764 -6.46462
H 6.75889 1.56745 -6.70638
H 7.48567 0.02332 -6.19653
H 6.17321 0.02825 -7.38375
O 0.27524 -1.81702 0.46572
C 0.72169 -4.68902 2.04615
H 1.69417 -4.55326 2.53357
C -0.31747 -5.17019 2.77217
H -0.16478 -5.44184 3.82262
C -1.69062 -5.37746 2.18650
H -1.86524 -6.46343 2.04544
H -2.45991 -5.05840 2.91222
C -1.87446 -4.63255 0.85529
H -2.79393 -4.97169 0.35091
H -1.99610 -3.55508 1.05992
C -0.65488 -4.79772 -0.06149
H -0.54243 -5.86434 -0.34346
H -0.80488 -4.24205 -1.00184
C 0.60388 -4.31421 0.63826
H 1.53213 -4.42146 0.05710
H 0.49712 -2.96992 0.61211
Cl 0.04235 2.60513 0.05987

$^{3\alpha}IM_{H}$

Fe -0.05993 0.06105 -0.21423
N -0.02471 0.21972 1.81330
N 1.97286 0.13900 -0.23922
N -2.08165 0.20226 -0.19092
N -0.08565 0.15593 -2.24228
C -1.11328 0.28224 2.64597
C 2.77696 0.12448 -1.35198
C 1.08636 0.26971 2.61641
C 2.80926 0.19829 0.84776
C -2.88336 0.27361 0.92136
C 1.00504 0.14267 -3.07523
C -2.91524 0.26552 -1.27948
C -1.19365 0.21898 -3.04882
C -0.67609 0.35656 4.02301
C 4.16679 0.15116 -0.95405
C 0.68652 0.35230 4.00457
C 4.18673 0.19967 0.40836
C -4.27016 0.36243 0.52198
C 0.57071 0.18610 -4.45469
C -4.28977 0.35871 -0.84101
C -0.79116 0.23383 -4.43810
H -1.33661 0.40944 4.88500
H 5.01162 0.13986 -1.63847
H 1.36977 0.40181 4.84880
H 5.05123 0.23532 1.06688
H -5.11339 0.42841 1.20498
H 1.23236 0.18422 -5.31730
H -5.15214 0.42030 -1.50014
H -1.47249 0.27696 -5.28440
C -2.46081 0.31883 2.25889
C 2.35431 0.13579 -2.68945
C -2.53003 0.28347 -2.62894
C 2.42462 0.27820 2.19442
C -3.50338 0.50780 3.32523
C -3.82600 1.81042 3.76307
C -4.16621 -0.61116 3.88742
C -4.81531 1.97189 4.74879
C -5.13949 -0.40338 4.87130
C -5.48323 0.88310 5.31671
H -5.06678 2.98430 5.08039
H -5.64771 -1.27166 5.30244
C 3.49620 0.45330 3.23385
C 3.96299 1.74924 3.54318
C 4.03624 -0.67114 3.90543
C 4.95397 1.89895 4.52881
C 5.02650 -0.47518 4.87500
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H 5.30924 2.90620 4.76841
H 5.44174 -1.34796 5.38870
C 3.39737 0.23202 -3.76721
C 3.89237 -0.93849 -4.39310
C 3.87715 1.49922 -4.16285
C 4.85137 -0.81629 -5.40498
C 4.83572 1.57464 -5.18835
C 5.33636 0.43360 -5.82230
H 5.23028 -1.72397 -5.88523
H 5.19955 2.55987 -5.49655
C -3.60059 0.45803 -3.66950
C -4.28573 -0.66844 -4.18860
C -3.92959 1.75326 -4.12413
C -5.28943 -0.47474 -5.14438
C -4.94912 1.90054 -5.08089
C -5.64206 0.80460 -5.60316
H -5.81452 -1.34868 -5.54261
H -5.20467 2.90738 -5.42606
C -3.94470 -2.06560 -3.72472
H -2.87670 -2.29135 -3.87470
H -4.14290 -2.19372 -2.64809
H -4.53297 -2.81840 -4.26916
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H -6.82321 2.02395 -6.95659
H -6.57310 0.34773 -7.50853
H -7.72176 0.68469 -6.20472
C -3.19916 2.98770 -3.64098
H -2.67967 2.83521 -2.68524
H -2.43237 3.29424 -4.37418
H -3.89194 3.83630 -3.53025
C -3.83562 -2.01497 3.43670
H -4.07500 -2.16331 2.37110
H -2.76133 -2.23345 3.54772
H -4.39816 -2.76057 4.01701
C -3.11973 3.03836 3.23011
H -2.32293 3.35795 3.92476
H -2.64072 2.87141 2.25570
H -3.81879 3.88371 3.13543
C -6.54197 1.07182 6.37664
H -6.26263 0.56392 7.31505
H -6.70268 2.13597 6.60363
H -7.50713 0.64297 6.05907
C 3.55838 -2.06836 3.58638
H 2.49021 -2.19650 3.82552
H 3.66585 -2.29859 2.51435
H 4.12398 -2.82047 4.15529
C 3.45754 2.98083 2.82327
H 4.15634 3.27295 2.01958
H 2.47706 2.83157 2.35070
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C 6.55249 0.98285 6.27382
H 6.14818 0.75396 7.27493
H 7.40556 0.30386 6.11291
H 6.93547 2.01376 6.29681
C 3.39734 -2.30576 -3.98212
H 3.54327 -2.48066 -2.90409
H 2.31763 -2.41865 -4.17289
H 3.92345 -3.09966 -4.53183
C 3.41717 2.77730 -3.49520
H 2.44241 2.67571 -2.99832
H 4.13793 3.08891 -2.71868
H 3.35481 3.60119 -4.22275
C 6.36585 0.52917 -6.92282
H 6.63561 1.57398 -7.13586
H 7.28912 -0.01117 -6.65425
H 5.99478 0.07736 -7.85799
O -0.06637 -1.87996 -0.17567
C 1.60072 -5.41255 2.47210
H 2.63933 -5.48329 2.81346
C 0.57959 -5.42328 3.42070
H 0.82171 -5.52591 4.48282
C -0.86164 -5.34532 3.00275
H -1.28928 -6.37000 2.97374

H -1.45445 -4.80956 3.76456
C -1.02751 -4.67657 1.62888
H -2.06755 -4.78102 1.27893
H -0.83464 -3.59400 1.71070
C -0.05667 -5.23508 0.57573
H -0.39471 -6.23464 0.22965
H -0.07625 -4.58088 -0.31147
C 1.34663 -5.33757 1.10391
H 2.17808 -5.37836 0.39340
H 0.73762 -2.20469 0.25465
Cl -0.04643 2.82462 -0.24604

$^{3}\beta$**TS**$_{H}$

Fe -0.02275 0.00171 0.46883
N -0.00682 0.27855 2.47334
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N -2.03412 0.23580 0.47007
N -0.02579 -0.14354 -1.54638
C -1.07495 0.57868 3.27647
C 2.81310 -0.16309 -0.64837
C 1.08960 0.20182 3.28978
C 2.80959 -0.16853 1.55007
C -2.83382 0.51437 1.54649
C 1.06230 -0.14711 -2.38147
C -2.86553 0.08602 -0.60809
C -1.13559 -0.20506 -2.35097
C -0.63832 0.70706 4.65204
C 4.19569 -0.26113 -0.22979
C 0.70172 0.46099 4.66233
C 4.19246 -0.28302 1.13271
C -4.22333 0.54327 1.13665
C 0.62784 -0.21414 -3.76081
C -4.24435 0.26268 -0.19649
C -0.73332 -0.27200 -3.74122
H -1.28467 0.94772 5.49270
H 5.04889 -0.31472 -0.90216
H 1.37858 0.46258 5.51337
H 5.04380 -0.35277 1.80573
H -5.06477 0.74340 1.79594
H 1.28925 -0.22587 -4.62394
H -5.10725 0.19070 -0.85437
H -1.41498 -0.33508 -4.58610
C -2.41042 0.72081 2.86802
C 2.41042 -0.12050 -1.99211
C -2.47630 -0.13356 -1.93959
C 2.41663 -0.02989 2.89050
C -3.43217 1.12679 3.89354
C -3.76054 2.49131 4.04948
C -4.06654 0.15320 4.70432
C -4.70491 2.86031 5.02279
C -5.00701 0.56524 5.65612
C -5.33941 1.91687 5.83685
H -4.94975 3.92032 5.14290
H -5.49487 -0.19238 6.27756
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C 3.78558 -1.22464 4.65583
C 5.16233 1.13849 5.25613
C 4.77887 -1.19904 5.64384
C 5.48221 -0.02766 5.96096
H 5.69233 2.06680 5.49071
H 5.00791 -2.12286 6.18445
C 3.46367 0.02661 -3.05668
C 3.99578 -1.09490 -3.73289
C 3.91775 1.32570 -3.38936
C 4.96426 -0.89785 -4.72879
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C -5.08633 -1.53838 -4.33622
C -5.02951 0.84733 -4.59151
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H -7.10394 -1.46515 -6.07024
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C -3.48169 2.30999 -3.24220
H -3.66885 2.54205 -2.18121
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C -3.74479 -1.31549 4.55196
H -3.89504 -1.65575 3.51492
H -2.69214 -1.52646 4.80138
H -4.37775 -1.92963 5.20895
C -3.15151 3.56281 3.17217
H -2.14344 3.30209 2.82122
H -3.76591 3.72069 2.26802
H -3.10196 4.52631 3.70173
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H -5.97950 2.10208 7.90082
H -6.56234 3.40538 6.83840
H -7.29695 1.78371 6.76260
C 3.04800 -2.51055 4.36343
H 1.97441 -2.41867 4.59595
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H 2.81750 2.60999 3.36560
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H 7.44553 -0.59746 6.68338
H 6.88462 0.98297 7.27448
H 6.20693 -0.52312 7.94608
C 3.53689 -2.49635 -3.40605
H 3.66026 -2.72262 -2.33556
H 2.46798 -2.63488 -3.63579
H 4.10461 -3.24273 -3.98028
C 3.39124 2.54676 -2.67023
H 2.29224 2.55740 -2.61462
H 3.74473 2.57636 -1.62578
H 3.72465 3.47092 -3.16445
C 6.48752 0.56347 -6.13315
H 6.37647 1.52663 -6.65451
H 7.49727 0.55175 -5.68599
H 6.45655 -0.24116 -6.88360
Cl 0.18333 2.43988 0.24794
O -0.24734 -1.70241 0.72498
C 2.12183 -3.99521 0.23494
H 3.03891 -3.39993 0.15899
C 2.10786 -5.08136 1.04425
H 3.01823 -5.36617 1.58360
C 0.88737 -5.94760 1.22408
H 1.03685 -6.90266 0.68061
H 0.78580 -6.23824 2.28500
C -0.39448 -5.25647 0.73546
H -1.21983 -5.98472 0.67308
H -0.69681 -4.49361 1.47358
C -0.18205 -4.55882 -0.61509
H 0.04763 -5.31764 -1.38997
H -1.10966 -4.05805 -0.93754
C 0.95391 -3.54969 -0.53185
H 1.20497 -3.06328 -1.48460
H 0.44051 -2.52779 0.10559

$^{3}\beta$**IM**$_{H}$

Fe -0.12879 0.31974 -0.04179
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C 0.96127 0.37768 2.79191
C 2.70033 0.13247 1.04666
C -2.95642 0.70408 1.04819
C 0.97224 0.19806 -2.89143
C -2.96699 0.35733 -1.12007
C -1.22555 0.14228 -2.86664
C -0.78127 0.77679 4.17104
C 4.09968 0.10644 -0.72570
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C 4.08815 0.05820 0.63603
C -4.34290 0.73918 0.62879
C 0.54198 0.13561 -4.27224
C -4.35081 0.50858 -0.71399
C -0.81966 0.08490 -4.25635
H -1.43502 0.95864 5.02074
H 4.95789 0.08049 -1.39332
H 1.23362 0.50769 5.02942
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H -5.19130 0.90841 1.28779
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H -5.20771 0.45498 -1.38143
H -1.49909 0.02668 -5.10339
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C 2.31870 0.22018 -2.49518
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C 2.29532 0.19631 2.38987
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C -3.90632 2.57386 3.63268
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C -5.16491 0.57259 5.13479
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C 3.74344 -1.13183 3.98490
C 4.95769 1.21088 4.92042
C 4.73510 -1.17826 4.97395
C 5.35770 -0.01836 5.45742
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H 5.02904 -2.15147 5.37977
C 3.37657 0.29895 -3.56007
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C 4.84908 -0.76653 -5.17174
C 4.84829 1.62483 -4.96578
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H 5.22463 2.60573 -5.27239
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C -4.12428 1.28479 -4.12323
C -5.15524 -1.20501 -4.88270
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H -5.49476 2.10173 -5.57006
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H -2.58013 -2.56109 -3.40922
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H -6.26725 0.04257 -7.57831
H -7.19336 -1.11474 -6.59808
H -7.48404 0.63751 -6.43761
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H -3.74246 2.84275 -2.65864
H -2.50168 2.71235 -3.90422
H -4.07771 3.44298 -4.30319
C -3.89187 -1.25211 3.95165
H -4.05069 -1.54547 2.90151
H -2.83640 -1.47063 4.18133
H -4.51747 -1.89733 4.58550
C -3.29186 3.68914 2.81557
H -2.30576 3.42603 2.40941
H -3.93296 3.93516 1.95047
H -3.19236 4.60800 3.41348
C -6.51549 2.27465 6.43494
H -6.14773 2.02002 7.44368
H -6.74680 3.34999 6.42465
H -7.45832 1.72143 6.29210
C 3.10472 -2.41216 3.49931
H 2.01166 -2.39590 3.63683
H 3.27974 -2.57005 2.42269
H 3.50361 -3.28356 4.03869
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H 3.73231 2.71514 2.29337
H 2.50857 2.86703 3.55336
H 4.16197 3.45953 3.85492
C 6.42765 -0.10373 6.51971
H 7.30659 -0.66365 6.15765
H 6.77000 0.89424 6.83076
H 6.06212 -0.63237 7.41571
C 3.36623 -2.24034 -3.76412
H 3.49004 -2.40975 -2.68255
H 2.29018 -2.35134 -3.97548
H 3.90071 -3.03878 -4.29910
C 3.40796 2.83686 -3.29185
H 2.33800 2.81430 -3.03913
H 3.94567 3.00409 -2.34200
H 3.59878 3.70940 -3.93419
C 6.39715 0.55997 -6.67241
H 6.67335 1.60227 -6.88965
H 7.31475 0.01978 -6.38458
H 6.04028 0.10147 -7.60984
Cl 0.00984 2.72250 -0.18879
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C 2.26918 -5.10189 -0.59513
H 3.12957 -5.03216 -1.26979
C 2.47634 -5.51971 0.71833
H 3.48132 -5.79527 1.05189
C 1.32689 -5.64101 1.67923
H 0.99140 -6.69910 1.71785
H 1.65909 -5.40766 2.70571
C 0.14950 -4.73785 1.27906
H -0.72909 -4.95501 1.90823
H 0.41637 -3.68293 1.45765
C -0.21410 -4.87297 -0.20844
H -0.73761 -5.83536 -0.38988
H -0.92916 -4.08068 -0.48415
C 1.00240 -4.79242 -1.08757
H 0.88078 -4.51353 -2.13876
H 0.42306 -1.88109 -0.48371

$^{3}\alpha$**TS**$_{Ep}$

Fe 0.04226 -0.42092 -0.19921
N 0.02790 -0.42806 1.83423
N 2.07612 -0.30327 -0.16511
N -1.97121 -0.18923 -0.19810
N 0.07162 -0.05066 -2.19550
C -1.07634 -0.40216 2.64906
C 2.90936 -0.19638 -1.24899
C 1.12082 -0.48332 2.66344
C 2.88548 -0.41457 0.93662
C -2.80313 -0.22975 0.89348
C 1.18187 0.06107 -2.99418
C -2.77995 -0.03182 -1.29595
C -1.01534 0.11722 -3.01490
C -0.66901 -0.44992 4.03644
C 4.29077 -0.26386 -0.82141
C 0.69239 -0.50197 4.04532
C 4.27598 -0.39990 0.53415
C -4.18216 -0.12145 0.46895
C 0.78223 0.29849 -4.36496
C -4.16791 0.00123 -0.88780
C -0.57941 0.33196 -4.37796
H -1.34658 -0.43825 4.88666
H 5.15224 -0.20962 -1.48268
H 1.35785 -0.54162 4.90417
H 5.12243 -0.47888 1.21221
H -5.04157 -0.13360 1.13501
H 1.46498 0.42736 -5.20117
H -5.01374 0.11095 -1.56213
H -1.23961 0.49395 -5.22640
C -2.41451 -0.30563 2.23848
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C -4.04221 -1.34203 3.88641
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C -5.01710 -1.19450 4.88028
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C 3.98980 -1.66648 3.91788
C 4.99137 0.78478 4.82590
C 4.95612 -1.61325 4.92892
C 5.47031 -0.39546 5.40220
H 5.37767 1.74634 5.17844
H 5.31787 -2.55077 5.36291
C 3.59143 0.24517 -3.60867
C 4.07946 -0.81603 -4.40996
C 4.10632 1.54911 -3.77782
C 5.06498 -0.54977 -5.36776
C 5.09034 1.77132 -4.75651
C 5.58361 0.74023 -5.56191
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H 5.48114 2.78518 -4.88859
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C -3.94808 -0.61430 -4.45558
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C -4.90625 -0.30496 -5.42764
C -4.78857 2.02465 -4.86125
C -5.34007 1.01165 -5.65111
H -5.32637 -1.11577 -6.03113
H -5.11274 3.05861 -5.01638
C -3.50954 -2.04668 -4.25710
H -2.44051 -2.17731 -4.49212
H -3.64051 -2.36882 -3.21162
H -4.08317 -2.72968 -4.90029
C -6.36564 1.31250 -6.71774
H -5.98201 1.06465 -7.72204
H -7.28167 0.71630 -6.57222
H -6.64865 2.37539 -6.71904
C -3.31323 2.90803 -3.02785
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H -2.35713 2.68710 -2.53406
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C -3.36933 2.36471 3.08394
H -2.37430 2.23936 2.63546
H -4.03872 2.70469 2.27395
H -3.32050 3.17943 3.82261
C -6.48280 0.19240 6.41001
H -7.33923 -0.47760 6.23131
H -6.06034 -0.08563 7.39117
H -6.86370 1.22113 6.49216
C 3.46700 -3.00245 3.44314
H 2.38404 -3.10037 3.62326
H 3.61629 -3.13100 2.35891
H 3.97285 -3.83196 3.95822

C 3.59287 2.09741 3.20006
H 4.31265 2.42572 2.42944
H 2.61077 2.04419 2.71062
H 3.56033 2.88838 3.96513
C 6.50768 -0.37416 6.49927
H 6.13460 -0.86699 7.41266
H 7.42002 -0.91547 6.19716
H 6.79691 0.65359 6.76360
C 3.55352 -2.22244 -4.23976
H 3.66332 -2.57107 -3.20027
H 2.47916 -2.28435 -4.47789
H 4.08648 -2.92679 -4.89481
C 3.65894 2.70751 -2.91275
H 3.68616 3.65285 -3.47599
H 2.64900 2.57394 -2.50085
H 4.33600 2.82745 -2.04844
C 6.63722 0.99557 -6.61301
H 7.51794 0.34944 -6.46232
H 6.25377 0.77850 -7.62440
H 6.97730 2.04151 -6.59959
Cl 0.12409 2.44923 0.02685
O -0.00208 -2.15247 -0.36385
C 0.24028 -3.97473 0.09928
H 0.92723 -3.74098 0.91708
C 0.78813 -4.47538 -1.07434
H 1.85597 -4.32347 -1.26514
C -0.05176 -5.03319 -2.18774
H -0.23814 -4.23415 -2.93618
H 0.51177 -5.80963 -2.73499
C -1.39627 -5.58924 -1.69305
H -2.06088 -5.79079 -2.54956
H -1.22468 -6.56033 -1.19365
C -2.06491 -4.62921 -0.70199
H -2.26819 -3.66820 -1.20467
H -3.03706 -5.03114 -0.37083
C -1.16176 -4.36762 0.50805
H -1.58860 -3.58893 1.15667
H -1.09403 -5.28452 1.12617

$^{3\alpha}$IM$_{Ep}$

Fe -0.06057 -0.05645 -0.03469
N -0.07214 -0.12596 1.99872
N 1.96745 -0.04736 -0.00885
N -2.07420 0.19622 -0.03192
N -0.03368 0.30099 -2.03668
C -1.17691 -0.08078 2.81340
C 2.79901 0.03690 -1.09821
C 1.02120 -0.18707 2.82708
C 2.77869 -0.16836 1.09269
C -2.90412 0.14205 1.06077
C 1.07797 0.38059 -2.83718
C -2.87975 0.40462 -1.12313
C -1.11603 0.53976 -2.84526
C -0.76851 -0.12841 4.19945
C 4.17791 -0.06837 -0.67467
C 0.59328 -0.19343 4.20777
C 4.16529 -0.19412 0.68258
C -4.28106 0.28565 0.64135
C 0.68398 0.66517 -4.19976
C -4.26568 0.45121 -0.71138
C -0.67531 0.76500 -4.20427
H -1.44474 -0.10640 5.05048
H 5.03813 -0.04204 -1.33917
H 1.25840 -0.23616 5.06675
H 5.01269 -0.29087 1.35712
H -5.14046 0.26761 1.30720
H 1.36806 0.77964 -5.03695
H -5.11019 0.59638 -1.38071
H -1.33050 0.97668 -5.04569
C -2.51425 0.03564 2.40377
C 2.41494 0.25684 -2.42905
C -2.46035 0.59558 -2.44774
C 2.36811 -0.21299 2.43298
C -3.57235 0.15183 3.46553
C -3.98818 1.43040 3.89815
C -4.14877 -1.00860 4.03767
C -4.96356 1.52491 4.90557
C -5.12213 -0.86659 5.03378
C -5.54277 0.39316 5.48787
H -5.27802 2.51821 5.24109
H -5.56599 -1.76720 5.46956
C 3.42186 -0.20091 3.50538
C 3.95793 1.02999 3.94301
C 3.87390 -1.41276 4.08376
C 4.92672 1.02808 4.96151
C 4.84607 -1.36720 5.08971
C 5.38572 -0.15500 5.54810
H 5.33299 1.98567 5.30209
H 5.19167 -2.30700 5.53180
C 3.49097 0.47127 -3.45674
C 3.93249 -0.59862 -4.27336
C 4.05671 1.75569 -3.61267
C 4.92537 -0.36053 -5.23089
C 5.04656 1.94988 -4.59147
C 5.49617 0.90942 -5.41019
H 5.26359 -1.19161 -5.85778
H 5.47687 2.94890 -4.71329
C -3.49147 0.96364 -3.47743
C -4.07930 -0.03302 -4.29547
C -3.87156 2.31456 -3.63069
C -5.02996 0.34294 -5.25108
C -4.82527 2.64674 -4.60883
C -5.41667 1.68113 -5.42844
H -5.48227 -0.43161 -5.87843
H -5.11214 3.69638 -4.72772
C -3.69459 -1.48657 -4.14448
H -2.62912 -1.64830 -4.37541
H -3.84781 -1.83939 -3.11194
H -4.28718 -2.12512 -4.81559
C -6.43611 2.05371 -6.47817
H -6.07007 1.81812 -7.49188
H -7.37505 1.49196 -6.34161
H -6.67508 3.12692 -6.44791
C -3.31261 3.41618 -2.75553
H -4.02506 3.66736 -1.94999
H -2.36678 3.14485 -2.26726
H -3.15298 4.33686 -3.33808
C -3.73279 -2.38817 3.58307
H -3.88425 -2.51863 2.49941
H -2.66303 -2.57147 3.77318
H -4.30810 -3.16712 4.10403
C -3.44424 2.70325 3.28618
H -2.45461 2.57240 2.82722
H -4.11602 3.06590 2.48815
H -3.37825 3.50434 4.03833
C -6.57559 0.51146 6.58301
H -7.43796 -0.14832 6.39513
H -6.15526 0.21571 7.55988
H -6.94729 1.54226 6.67999
C 3.32376 -2.74443 3.62879
H 2.24287 -2.82485 3.82837
H 3.45131 -2.88510 2.54357
H 3.82606 -3.57660 4.14300
C 3.54857 2.35033 3.32701
H 4.25734 2.64300 2.53219
H 2.55307 2.31884 2.86359
H 3.55951 3.15498 4.07813
C 6.42875 -0.14231 6.63984
H 6.05242 -0.62242 7.55862
H 7.33070 -0.70047 6.33713
H 6.73590 0.88254 6.89501
C 3.34897 -1.98417 -4.12125
H 3.44578 -2.35192 -3.08726
H 2.27243 -1.99852 -4.35739
H 3.85091 -2.70066 -4.78750
C 3.65524 2.92210 -2.73595
H 3.71075 3.86996 -3.29286
H 2.64360 2.81965 -2.31934
H 4.34139 3.01342 -1.87535
C 6.55832 1.13378 -6.45976
H 7.42078 0.46413 -6.30558
H 6.17126 0.92475 -7.47135
H 6.92722 2.16990 -6.44759
Cl 0.09320 2.74964 0.23013
O -0.19914 -1.96372 -0.25755
C 0.38472 -3.04640 0.42644
H 0.95608 -2.68344 1.30513
C 1.32430 -3.73564 -0.52798
H 2.30507 -3.27623 -0.69915
C 0.77481 -4.65490 -1.57440
H 0.34672 -4.05100 -2.40563
H 1.58411 -5.24803 -2.03562
C -0.32999 -5.57700 -1.02741
H -0.81439 -6.11989 -1.85696
H 0.12998 -6.34314 -0.37637
C -1.36683 -4.79210 -0.21377
H -1.88799 -4.07569 -0.87308
H -2.13786 -5.47582 0.18145
C -0.69887 -4.02148 0.93104
H -1.44500 -3.45034 1.50804
H -0.23014 -4.74033 1.62958

$^{3\beta}$TS$_{Ep}$

Fe -0.09174 -0.24592 -0.21310
N -0.09158 -0.41635 1.80248
N 1.92628 -0.37737 -0.20897
N -2.10725 0.01560 -0.20552
N -0.07910 0.10221 -2.21524
C -1.19271 -0.38273 2.62020
C 2.74840 -0.29934 -1.30367
C 1.00103 -0.52332 2.62597
C 2.74594 -0.51965 0.88080
C -2.92925 -0.05389 0.88814
C 1.02320 0.11521 -3.02864
C -2.91633 0.24690 -1.28613
C -1.16187 0.33632 -3.02136
C -0.78273 -0.48585 4.00527
C 4.13306 -0.43109 -0.89498
C 0.57746 -0.56811 4.00888
C 4.13122 -0.56808 0.45987
C -4.31045 0.12576 0.48387
C 0.62451 0.36500 -4.39954
C -4.30220 0.31502 -0.86462
C -0.73096 0.50135 -4.39505
H -1.45739 -0.48518 4.85799
H 4.98783 -0.41027 -1.56663
H 1.24392 -0.64972 4.86413
H 4.98269 -0.68388 1.12642
H -5.16511 0.11002 1.15627
H 1.30345 0.42355 -5.24708
H -5.14834 0.48784 -1.52551
H -1.39070 0.69583 -5.23735
C -2.53068 -0.22561 2.22235
C 2.35774 -0.05842 -2.63092
C -2.50323 0.41858 -2.61621
C 2.34482 -0.57123 2.22392
C -3.58298 -0.15717 3.29470
C -3.98448 1.10310 3.79998
C -4.16645 -1.33696 3.80750
C -4.95069 1.15518 4.81412
C -5.13460 -1.23795 4.81923
C -5.54061 -0.00315 5.33955
H -5.25141 2.13234 5.20562
H -5.58248 -2.15615 5.21145
C 3.40519 -0.59599 3.29011
C 3.97693 0.61828 3.73095
C 3.82987 -1.82096 3.86069
C 4.95202 0.58719 4.74246
C 4.81043 -1.80542 4.86023
C 5.38476 -0.61046 5.32038
H 5.38509 1.53231 5.08484
H 5.13427 -2.75611 5.29561
C 3.43699 0.11660 -3.66435
C 3.97715 -1.00140 -4.34485
C 3.92293 1.41235 -3.94897
C 4.99421 -0.80265 -5.28706
C 4.94815 1.56473 -4.89760
C 5.49802 0.47398 -5.57906
H 5.40784 -1.67222 -5.80759
H 5.32643 2.57033 -5.10665
C -3.54482 0.73782 -3.65313
C -4.19400 -0.29601 -4.36302
C -3.87808 2.08837 -3.91599
C -5.16286 0.03726 -5.32313
C -4.85066 2.37633 -4.88270
C -5.50603 1.36568 -5.60116
H -5.66306 -0.76908 -5.86826
H -5.10438 3.42279 -5.07960
C -3.86198 -1.74674 -4.10181
H -2.79734 -1.95696 -4.29340
H -4.05035 -2.02043 -3.05105
H -4.46092 -2.41243 -4.74017
C -6.53639 1.70902 -6.65043
H -7.27155 2.43661 -6.26992
H -6.06478 2.16737 -7.53687
H -7.08270 0.81629 -6.98915
C -3.20273 3.21377 -3.16662
H -3.37934 3.13968 -2.08129
H -2.10926 3.19032 -3.30018
H -3.56906 4.19335 -3.50652
C -3.76716 -2.69642 3.28227
H -3.92409 -2.76997 2.19402
H -2.69867 -2.90048 3.45773
H -4.34900 -3.49473 3.76553
C -3.41610 2.39007 3.24508
H -2.34169 2.31415 3.02170
H -3.90975 2.65765 2.29467
H -3.57124 3.22538 3.94385
C -6.58147 0.08833 6.42994
H -7.46516 0.65613 6.09304
H -6.92265 -0.90763 6.74860
H -6.18764 0.61186 7.31710
C 3.23974 -3.13614 3.40813
H 2.16425 -3.19666 3.64170
H 3.32822 -3.26749 2.31817
H 3.74022 -3.98410 3.89798
C 3.59468 1.94817 3.11933
H 4.23617 2.17407 2.24917
H 2.55880 1.96669 2.75294
H 3.72780 2.76792 3.84143
C 6.43676 -0.62961 6.40357
H 6.76262 0.38666 6.66984
H 6.06081 -1.11622 7.31905
H 7.32749 -1.19748 6.08573
C 3.47085 -2.39771 -4.06838
H 3.63461 -2.68740 -3.01808
H 2.38634 -2.47574 -4.24761
H 3.97599 -3.13647 -4.70744
C 3.34519 2.64323 -3.28578
H 2.47257 3.01567 -3.85088
H 2.99212 2.44962 -2.26295
H 4.08374 3.45842 -3.25458
C 6.58957 0.65552 -6.60667
H 6.98077 1.68363 -6.60451
H 7.43196 -0.03149 -6.42439
H 6.21882 0.44112 -7.62385
Cl 0.15231 2.20674 0.12007
O -0.36620 -1.93277 -0.51308
C 0.43572 -3.42204 0.39384
H 0.69102 -2.83277 1.27538
C 1.47662 -3.81026 -0.43921
H 2.42322 -3.26380 -0.38775
C 1.29925 -4.80628 -1.55054
H 1.10763 -4.26123 -2.49940
H 2.24231 -5.35446 -1.72458
C 0.14483 -5.78690 -1.29093
H -0.08458 -6.35487 -2.20814
H 0.46175 -6.52779 -0.53414
C -1.10081 -5.05382 -0.77985
H -1.44055 -4.33280 -1.54336
H -1.92909 -5.76453 -0.61966
C -0.79741 -4.29252 0.51518
H -1.65439 -3.67176 0.81666
H -0.63030 -5.01519 1.33792

$^{3\beta}$IM$_{Ep}$

Fe -0.01248 0.08124 0.00881
N -0.02021 -0.13585 2.01731
N 2.00736 -0.05580 0.02012
N -2.02942 0.30439 -0.00221
N 0.00018 0.39927 -1.99860
C -1.12340 -0.08602 2.83112
C 2.83378 0.06351 -1.06828
C 1.06780 -0.25732 2.84514
C 2.82377 -0.20508 1.11214
C -2.85222 0.25316 1.09215
C 1.10874 0.43977 -2.80318
C -2.83954 0.50737 -1.08800
C -1.08117 0.59527 -2.81663
C -0.72034 -0.20300 4.21755
C 4.21772 -0.04571 -0.65280
C 0.63799 -0.30937 4.22588
C 4.21120 -0.21494 0.69899
C -4.23329 0.42024 0.68363
C 0.71453 0.66567 -4.17999
C -4.22552 0.57625 -0.66938
C -0.64431 0.75853 -4.18871
H -1.39812 -0.19646 5.06775
H 5.07601 0.00733 -1.31825
H 1.30000 -0.40656 5.08293
H 5.06113 -0.32845 1.36780
H -5.08831 0.41490 1.35570
H 1.39902 0.73728 -5.02203
H -5.07230 0.72791 -1.33461
H -1.30246 0.92433 -5.03834
C -2.45766 0.09128 2.42919
C 2.44537 0.30459 -2.39631
C -2.42645 0.65321 -2.42120
C 2.41401 -0.29430 2.45063
C -3.51044 0.18948 3.49926
C -3.88977 1.46303 3.98841
C -4.11579 -0.97283 4.02642
C -4.85562 1.54547 5.00082
C -5.08256 -0.84348 5.03614
C -5.46665 0.40479 5.54049
H -5.13893 2.53282 5.37948
H -5.54715 -1.74842 5.43959
C 3.46835 -0.34891 3.52121
C 4.03137 0.84981 4.01133
C 3.89650 -1.59345 4.04613
C 5.00381 0.78400 5.02426
C 4.87283 -1.61215 5.04915
C 5.44041 -0.43276 5.55670
H 5.43102 1.71724 5.40473
H 5.19946 -2.57728 5.44923
C 3.52568 0.50908 -3.42356
C 4.09614 -0.58972 -4.10867
C 3.97982 1.81910 -3.69808
C 5.11082 -0.35807 -5.04711
C 5.00173 2.00506 -4.64293
C 5.58123 0.93245 -5.33045
H 5.54835 -1.21338 -5.57168
H 5.35397 3.02144 -4.84464
C -3.47161 0.91557 -3.47047
C -4.08919 -0.15761 -4.14974
C -3.84082 2.24738 -3.77713
C -5.06335 0.11824 -5.12267
C -4.81735 2.47760 -4.75522
C -5.44226 1.42718 -5.44315
H -5.53870 -0.71839 -5.64387
H -5.09906 3.50990 -4.98600
C -3.71702 -1.58978 -3.84354

H -2.64636 -1.77544 -4.02679
H -3.90002 -1.83692 -2.78525
H -4.29524 -2.29126 -4.46232
C -6.47921 1.70936 -6.50412
H -7.24499 2.41385 -6.14075
H -6.02123 2.17006 -7.39638
H -6.98766 0.78941 -6.82857
C -3.19838 3.41427 -3.06335
H -3.36721 3.36485 -1.97544
H -2.10559 3.42195 -3.20478
H -3.59777 4.37169 -3.42821
C -3.74211 -2.34607 3.51875
H -3.90445 -2.43203 2.43223
H -2.67672 -2.56615 3.69333
H -4.33593 -3.12728 4.01513
C -3.29770 2.73246 3.41818
H -2.22209 2.63802 3.20798
H -3.77690 2.99055 2.45783
H -3.44870 3.58148 4.10112
C -6.50671 0.52893 6.62843
H -7.38189 1.10388 6.28155
H -6.86250 -0.45674 6.96274
H -6.10594 1.06105 7.50729
C 3.31436 -2.89244 3.53903
H 2.23284 -2.95562 3.74146
H 3.43252 -2.99061 2.44810
H 3.79974 -3.75673 4.01530
C 3.64367 2.20282 3.45578
H 4.34693 2.51343 2.66282
H 2.64144 2.20685 3.00595
H 3.68073 2.97585 4.23865
C 6.48808 -0.48915 6.64279
H 6.81936 0.51709 6.93875
H 6.10512 -0.99847 7.54298
H 7.37613 -1.05410 6.31274
C 3.62775 -2.00093 -3.84130
H 3.81497 -2.29754 -2.79666
H 2.54305 -2.10413 -4.00464
H 4.14191 -2.71999 -4.49543
C 3.36876 3.02141 -3.01436
H 2.37922 3.25696 -3.44275
H 3.20351 2.85263 -1.93975
H 4.00356 3.91144 -3.13580
C 6.66635 1.15036 -6.35783
H 7.06496 2.17478 -6.31468
H 7.50455 0.44983 -6.21299
H 6.28551 0.98434 -7.38051
Cl 0.20862 2.46115 0.35976
O -0.27320 -1.71951 -0.32603
C 0.39499 -2.78008 0.33090
H 0.96256 -2.40667 1.20069
C 1.34887 -3.44889 -0.62623
H 2.34687 -3.01608 -0.75428
C 0.80771 -4.35451 -1.68795
H 0.34884 -3.73829 -2.49397
H 1.62035 -4.91862 -2.17782
C -0.26933 -5.31416 -1.14729
H -0.75169 -5.85088 -1.98217
H 0.21735 -6.08233 -0.51846
C -1.31350 -4.57066 -0.30484
H -1.86425 -3.85789 -0.94354
H -2.05887 -5.28172 0.09169
C -0.64977 -3.79753 0.84090
H -1.40365 -3.25941 1.43812
H -0.14696 -4.51194 1.51974

$S = 2$

^{5}**RC**

Fe -0.02646 -0.10473 0.05427
N -0.02628 -0.08078 2.14012
N 2.06173 -0.04177 0.06076
N -2.10434 0.10026 0.05554
N -0.01247 0.13854 -2.02133
C -1.13445 -0.04789 2.93897
C 2.86613 -0.00229 -1.04328
C 1.07837 -0.15341 2.94071
C 2.85806 -0.13148 1.16822
C -2.90514 0.10719 1.16259
C 1.09695 0.15126 -2.81901
C -2.89798 0.22296 -1.04928
C -1.11598 0.24442 -2.82041
C -0.71254 -0.10175 4.32883
C 4.25405 -0.06571 -0.61637
C 0.65121 -0.17114 4.32978
C 4.24899 -0.14782 0.74659
C -4.29040 0.22737 0.73929
C 0.67741 0.26318 -4.20627
C -4.28584 0.30237 -0.62407
C -0.68670 0.32158 -4.20697
H -1.37919 -0.08721 5.18810
H 5.11576 -0.04947 -1.28001
H 1.31531 -0.22375 5.18964
H 5.10572 -0.21149 1.41379
H -5.15002 0.25494 1.40532
H 1.34638 0.29468 -5.06336
H -5.14112 0.40522 -1.28801
H -1.34952 0.40868 -5.06501
C -2.47808 0.04759 2.50848
C 2.44253 0.09976 -2.38820
C -2.46133 0.30192 -2.39203
C 2.42613 -0.17919 2.51333
C -3.53359 0.15314 3.57597
C -3.96894 1.42996 4.00481
C -4.08515 -1.00987 4.15855
C -4.93601 1.51622 5.01605
C -5.05571 -0.87662 5.16371
C -5.49407 0.37596 5.61070
H -5.26354 2.50656 5.34850
H -5.47916 -1.78134 5.61052
C 3.48730 -0.23528 3.57949
C 4.02151 0.96615 4.10447
C 3.95201 -1.47917 4.05985
C 5.00652 0.89817 5.09846
C 4.94133 -1.50110 5.05631
C 5.48252 -0.32608 5.59058
H 5.41461 1.83092 5.50056
H 5.29714 -2.46850 5.42372
C 3.51047 0.20202 -3.44409
C 4.02907 -0.96055 -4.05903
C 3.99357 1.47476 -3.82653
C 5.01940 -0.82883 -5.04340
C 4.98419 1.56057 -4.81622
C 5.51406 0.42196 -5.43704
H 5.41378 -1.73300 -5.51759
H 5.35074 2.54902 -5.11008
C -3.51267 0.53390 -3.44362
C -4.21524 -0.55471 -4.01463
C -3.80104 1.85248 -3.86057
C -5.19393 -0.30249 -4.98426
C -4.79537 2.05949 -4.83121
C -5.50455 0.99933 -5.40586
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H -5.01809 3.08370 -5.14647
C -3.92090 -1.97571 -3.59326
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H -4.15425 -2.13691 -2.52825
H -4.51025 -2.69391 -4.18157
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H -6.44241 0.59339 -7.31989
H -7.58123 1.01079 -6.03042
H -6.59041 2.28506 -6.77736
C -3.04151 3.04116 -3.31451
H -2.74530 2.90816 -2.26405
H -2.10775 3.20164 -3.88176
H -3.63661 3.96286 -3.39824
C -3.64701 -2.38653 3.71515
H -3.79108 -2.52633 2.63170
H -2.57529 -2.55221 3.91150
H -4.21295 -3.17050 4.23903
C -3.43958 2.69722 3.37127
H -2.37448 2.62447 3.10724
H -3.97573 2.91738 2.43149
H -3.57820 3.56117 4.03810
C -6.53311 0.50435 6.69911
H -7.41193 1.07136 6.34919
H -6.88150 -0.48018 7.04434
H -6.13297 1.04666 7.57230
C 3.40215 -2.77840 3.51823
H 2.31558 -2.85735 3.68458
H 3.55770 -2.86013 2.43033
H 3.88350 -3.64336 3.99728
C 3.54639 2.31078 3.60426
H 3.75565 2.43754 2.52956
H 2.45675 2.42521 3.71997
H 4.03744 3.13200 4.14626
C 6.54429 -0.36392 6.66372
H 6.81641 -1.39632 6.92824
H 7.46120 0.15544 6.33833
H 6.20266 0.14172 7.58255
C 3.53074 -2.33319 -3.67183
H 3.69356 -2.53350 -2.60053
H 2.44756 -2.43669 -3.84511
H 4.04331 -3.11828 -4.24650
C 3.45597 2.73490 -3.18819
H 2.36949 2.83560 -3.34238
H 3.61088 2.73351 -2.09713
H 3.94466 3.62892 -3.60191
C 6.60303 0.53484 -6.47711
H 7.60157 0.41536 -6.02076
H 6.50731 -0.24431 -7.24921
H 6.58784 1.51674 -6.97390
Cl 0.02568 2.36892 0.18862
O -0.07436 -1.73063 -0.02919
C 0.56156 -4.69470 -1.68172
H 1.01675 -3.86765 -1.12605
C 1.33350 -5.60148 -2.30019
H 2.42440 -5.49920 -2.25672
C 0.78115 -6.77670 -3.07051
H 0.94076 -6.60974 -4.15418
H 1.36306 -7.68501 -2.83264
C -0.71016 -7.00875 -2.78716
H -1.13380 -7.70799 -3.52689
H -0.82093 -7.49251 -1.79949
C -1.48651 -5.68599 -2.78339
H -1.38916 -5.20918 -3.77594
H -2.56289 -5.86727 -2.62812
C -0.94624 -4.73169 -1.70990
H -1.33016 -3.70804 -1.85960
H -1.31969 -5.02992 -0.71029

$^{5\alpha}$**TS**$_{H}$

Fe 0.22664 -0.13303 0.34042
N 0.27228 0.24300 2.40207
N 2.30362 0.15459 0.28035
N -1.86065 -0.02318 0.37961
N 0.18002 -0.12120 -1.75086
C -0.81893 0.30229 3.22387
C 3.07791 0.13480 -0.84685
C 1.39542 0.31258 3.17868
C 3.13138 0.24767 1.36454
C -2.63597 0.12758 1.49440
C 1.26599 -0.07926 -2.57815
C -2.68388 -0.08143 -0.70990
C -0.94510 -0.18413 -2.52418
C -0.36680 0.41833 4.59992
C 4.47565 0.22748 -0.45992
C 0.99881 0.41920 4.57262
C 4.50894 0.29135 0.90410
C -4.03328 0.15067 1.09634
C 0.81037 -0.14105 -3.95702
C -4.06288 0.01973 -0.26299
C -0.55333 -0.20984 -3.92340
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H 5.31853 0.23681 -1.14753
H 1.68172 0.49124 5.41625
H 5.38347 0.36699 1.54654
H -4.87793 0.26175 1.77251
H 1.45441 -0.12664 -4.83340
H -4.93654 0.00272 -0.91048
H -1.23784 -0.26354 -4.76713
C -2.17419 0.27701 2.82332
C 2.61800 0.04880 -2.18081
C -2.28155 -0.16336 -2.06375
C 2.73322 0.31671 2.72002
C -3.21449 0.48217 3.89084
C -3.56506 1.79367 4.28168
C -3.84546 -0.62784 4.50282
C -4.54915 1.97148 5.26833
C -4.81644 -0.40393 5.48719
C -5.18834 0.88958 5.88362
H -4.82023 2.98997 5.56369
H -5.29755 -1.26642 5.95915
C 3.81998 0.42209 3.75648
C 4.28841 1.69135 4.16565
C 4.37261 -0.74820 4.32750
C 5.29909 1.76689 5.13635
C 5.38102 -0.62678 5.29403
C 5.86218 0.62137 5.71288
H 5.65454 2.75308 5.45059
H 5.80149 -1.53674 5.73355
C 3.64397 0.16497 -3.27537
C 4.20088 -0.99526 -3.86686
C 4.04699 1.44311 -3.72097
C 5.14273 -0.85338 -4.89318
C 4.99057 1.53824 -4.75809
C 5.55057 0.40625 -5.35891
H 5.57109 -1.75407 -5.34422
H 5.29441 2.53149 -5.10334
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C -3.77837 1.08994 -3.66508
C -5.02007 -1.29085 -4.46471
C -4.81378 1.09525 -4.61606
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H -5.12907 2.05217 -5.04400
C -3.57467 -2.67305 -2.93148
H -2.49912 -2.85655 -3.08621
H -3.74471 -2.71369 -1.84330
H -4.13218 -3.50097 -3.39309
C -6.56675 -0.05688 -6.04473
H -6.72792 0.95385 -6.44768
H -6.35393 -0.73102 -6.89086
H -7.51728 -0.39704 -5.59956
C -3.11534 2.40134 -3.30271
H -2.59607 2.36652 -2.33577
H -2.35878 2.67455 -4.05943
H -3.85111 3.22006 -3.27646
C -3.47878 -2.04142 4.11379
H -3.69562 -2.23789 3.05132
H -2.40218 -2.23202 4.25155
H -4.03511 -2.77504 4.71513
C -2.88260 3.00797 3.69130
H -1.95542 3.24134 4.24402
H -2.58827 2.86251 2.64196
H -3.53079 3.89491 3.75461
C -6.25895 1.09858 6.92790
H -7.26232 0.89226 6.51626
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C 3.89039 -2.11884 3.91203
H 2.81302 -2.24516 4.10652
H 4.03294 -2.28577 2.83215
H 4.42958 -2.90976 4.45334
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H 3.85565 2.99508 2.48317
H 2.63090 3.03381 3.75156
H 4.19415 3.84984 4.00973
C 6.97027 0.72239 6.73381
H 6.86796 -0.04380 7.51826
H 7.95804 0.57079 6.26397
H 6.98650 1.71072 7.21731
C 3.79475 -2.37472 -3.40234
H 3.97103 -2.50489 -2.32241
H 2.72031 -2.55600 -3.56725
H 4.35658 -3.15444 -3.93691
C 3.51730 2.71244 -3.09018
H 2.50946 2.59100 -2.66890
H 4.16814 3.03389 -2.25781
H 3.49639 3.53628 -3.81974
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H 6.89377 1.56104 -6.61471
H 7.43403 -0.10955 -6.30507
H 6.11231 0.19485 -7.44263
O 0.31646 -1.85757 0.50212
C 0.62709 -4.79491 2.06783
H 1.59889 -4.69636 2.56461
C -0.42927 -5.26593 2.76891
H -0.29095 -5.57237 3.81188
C -1.80407 -5.41988 2.17350
H -2.00875 -6.49821 2.01742
H -2.56480 -5.08908 2.90262
C -1.95845 -4.65064 0.85312
H -2.88190 -4.95866 0.33668
H -2.05624 -3.57346 1.07254
C -0.73658 -4.83703 -0.05509
H -0.64068 -5.90357 -0.33921
H -0.86433 -4.27374 -0.99377
C 0.53084 -4.38528 0.65730
H 1.45657 -4.55895 0.08569
H 0.48831 -3.12591 0.64403
Cl 0.03400 2.51645 0.04280

$^{5\alpha}$**IM**$_{H}$

Fe 0.03901 -0.01645 -0.21730
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N -2.04820 0.13473 -0.16649
N -0.01317 0.07114 -2.29732
C -0.99639 0.24994 2.69575
C 2.89937 0.19581 -1.38903
C 1.22002 0.25741 2.64529
C 2.95516 0.24658 0.82479
C -2.81833 0.22570 0.95970
C 1.07730 0.12190 -3.12348
C -2.87494 0.17269 -1.25451
C -1.13968 0.11592 -3.07330
C -0.54016 0.34280 4.07084
C 4.29721 0.28079 -1.00150
C 0.82629 0.34638 4.03984
C 4.33167 0.31354 0.36368
C -4.21500 0.30863 0.56809
C 0.62031 0.16837 -4.50020
C -4.24991 0.27517 -0.79705
C -0.74621 0.16320 -4.46916
H -1.18581 0.40262 4.94414
H 5.13930 0.31347 -1.68927
H 1.51037 0.40941 4.88323
H 5.20718 0.38071 1.00550
H -5.05641 0.38888 1.25255
H 1.26496 0.20929 -5.37516
H -5.12497 0.32248 -1.44117
H -1.43040 0.19713 -5.31408
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C -4.04890 -0.62846 3.94657

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H -4.91039 2.97844 5.13432
H -5.51729 -1.27236 5.38391
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C 3.99127 1.76611 3.64306
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C 5.02176 1.91546 4.58626
C 5.33629 -0.46239 4.67898
C 5.70824 0.81780 5.11654
H 5.29228 2.92372 4.91509
H 5.85526 -1.33713 5.08350
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C 4.93044 -0.67251 -5.47629
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H -2.66209 -2.27454 3.64044
H -4.31599 -2.77359 4.07418
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H -2.04404 3.18958 3.81702
H -2.68831 2.88500 2.20416
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H 4.53684 -2.80945 3.85120
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H 6.69467 0.33182 6.98707
H 7.80345 0.74578 5.67062
H 6.88112 2.03154 6.48235
C 3.54872 -2.21699 -4.04110
H 3.71877 -2.39148 -2.96651
H 2.47067 -2.36685 -4.21460
H 4.09335 -2.98927 -4.60350
C 3.39571 2.86127 -3.53506
H 2.40710 2.73569 -3.07215
H 4.08538 3.16539 -2.72783
H 3.34567 3.69911 -4.24728
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H 7.26106 0.10914 -6.83508
H 5.93998 0.39771 -7.97715
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C 0.29877 -4.67484 3.21988
H 0.92117 -4.36949 4.06815
C -1.04374 -4.97480 3.44342
H -1.45202 -4.92951 4.45741
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H -2.00868 -6.51265 2.30396
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H 0.44412 -4.67504 -0.13810
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H 0.37654 -2.23912 0.73422
Cl 0.01355 2.64203 -0.28512

$^{5\beta}$**TS**$_{H}$

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C 2.84059 -0.10323 1.57760
C -2.81847 0.44950 1.61249
C 1.05381 -0.15165 -2.35188
C -2.86429 0.06363 -0.55619
C -1.14722 -0.17461 -2.31574
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C 4.20116 -0.21193 -0.21908
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C 4.21651 -0.17882 1.14441
C -4.20699 0.46745 1.21271
C 0.61364 -0.22653 -3.72783
C -4.23635 0.21402 -0.12795
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H 5.07936 -0.18358 1.80592
H -5.04625 0.64599 1.88075
H 1.27296 -0.26443 -4.59186
H -5.10460 0.14787 -0.77916
H -1.43375 -0.31974 -4.54686
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C -2.48496 -0.12034 -1.89589
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C -4.95923 0.45635 5.73571
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C 4.94479 -0.73802 5.69154
C 5.55960 0.50207 5.92590
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H 5.25057 -1.60645 6.28347
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C 5.06478 -1.04538 -4.55224
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H -2.20729 3.21210 2.79805
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H 7.03094 1.66490 7.01979
H 6.22636 0.40531 7.98740
H 7.46331 -0.05002 6.80634
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H 3.93654 -2.71429 -2.02119
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H 4.23501 -3.35158 -3.65580
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H 2.19134 2.66319 -3.55494
H 2.88525 2.45342 -1.94997
H 3.77386 3.37999 -3.19118
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H 6.42387 -0.40493 -6.86988
H 6.54211 1.34255 -6.53243
H 7.53847 0.18361 -5.62585
Cl 0.24129 2.69546 0.37072
O -0.44838 -1.95214 0.74885
C 1.51076 -4.66414 1.31425
H 2.12326 -4.37919 2.17735
C 0.88360 -5.85746 1.31825
H 1.01915 -6.53635 2.16822
C 0.00286 -6.32803 0.18862
H 0.52362 -7.13772 -0.36108
H -0.90649 -6.80308 0.59845
C -0.37338 -5.19094 -0.77242
H -0.80795 -5.60274 -1.69812
H -1.14794 -4.55870 -0.30569
C 0.83337 -4.29741 -1.08443
H 1.61741 -4.89428 -1.58921
H 0.54695 -3.49688 -1.78494
C 1.39627 -3.68973 0.19853
H 2.32965 -3.12814 0.03687
H 0.61363 -2.85089 0.54341

$^{5\beta}$**IM**$_{H}$

Fe -0.16367 0.16832 -0.00529
N -0.12504 0.45571 2.00840
N 1.87053 0.12398 -0.02948
N -2.17498 0.40594 0.00029
N -0.18472 0.13877 -2.03500
C -1.20197 0.69732 2.82083
C 2.67546 0.05782 -1.13844
C 0.98592 0.46920 2.81242
C 2.70401 0.16466 1.06040
C -2.97103 0.63004 1.09712
C 0.90696 0.07751 -2.86531
C -3.01285 0.33442 -1.08488
C -1.29372 0.11598 -2.84267
C -0.75943 0.85860 4.18913
C 4.06395 0.02807 -0.73554
C 0.59550 0.71122 4.18496
C 4.08132 0.08620 0.62684
C -4.35783 0.68719 0.69283
C 0.47273 0.02006 -4.24428
C -4.38483 0.49289 -0.65670
C -0.88999 0.03361 -4.22982
H -1.41079 1.05916 5.03620
H 4.91045 -0.02594 -1.41575
H 1.27945 0.76862 5.02815
H 4.94495 0.08912 1.28738
H -5.19674 0.85272 1.36449
H 1.13568 -0.03235 -5.10462
H -5.25012 0.46985 -1.31481
H -1.57144 -0.00158 -5.07643
C -2.54413 0.79917 2.42230
C 2.25495 0.06203 -2.47843
C -2.63258 0.18921 -2.42855
C 2.31998 0.32787 2.40000
C -3.56635 1.16839 3.46083
C -3.90763 2.52508 3.65051
C -4.18299 0.16747 4.25189
C -4.85173 2.85837 4.63736
C -5.12265 0.54510 5.21785
C -5.47049 1.88853 5.43151
H -5.10831 3.91227 4.78429
H -5.59701 -0.23265 5.82459
C 3.39920 0.45024 3.43890
C 3.98740 1.70709 3.69576
C 3.82393 -0.69068 4.16453
C 4.98667 1.80289 4.68041
C 4.82472 -0.54901 5.13202
C 5.42071 0.69209 5.40904
H 5.43623 2.78090 4.87951
H 5.14989 -1.43383 5.68829
C 3.30669 0.11358 -3.55149
C 3.89670 -1.07605 -4.04291
C 3.70852 1.36464 -4.07004
C 4.88050 -0.98989 -5.03575
C 4.70515 1.40387 -5.05958
C 5.30529 0.24207 -5.55623
H 5.33021 -1.91347 -5.41362
H 5.01667 2.37623 -5.45376
C -3.70983 0.16008 -3.47729
C -4.27557 -1.07275 -3.88053
C -4.15981 1.36541 -4.06074
C -5.27839 -1.07507 -4.85902
C -5.16791 1.31655 -5.03678
C -5.74094 0.10880 -5.45199
H -5.71220 -2.03185 -5.16635
H -5.51300 2.25356 -5.48426
C -3.81438 -2.37579 -3.26998
H -2.73500 -2.53464 -3.42453
H -3.97881 -2.39127 -2.18035
H -4.35082 -3.23038 -3.70710
C -6.82008 0.07059 -6.50753
H -7.10921 1.08226 -6.82804
H -6.48544 -0.48338 -7.40094
H -7.72443 -0.44056 -6.13777
C -3.57450 2.69691 -3.65023
H -3.70381 2.88085 -2.57155
H -2.49008 2.73877 -3.84199
H -4.04948 3.52424 -4.19707
C -3.84011 -1.29200 4.06269
H -4.00188 -1.61300 3.02115
H -2.78003 -1.49048 4.29002
H -4.45172 -1.93065 4.71639
C -3.31621 3.63126 2.80351
H -2.36393 3.35276 2.33218
H -4.00695 3.90257 1.98555
H -3.15714 4.54167 3.40193
C -6.47630 2.26252 6.49381
H -7.42284 1.71310 6.36068
H -6.10354 2.01292 7.50183
H -6.70240 3.33881 6.47668
C 3.21145 -2.04771 3.90551
H 2.13037 -2.05070 4.11979
H 3.32018 -2.34790 2.85081
H 3.68285 -2.82043 4.52995
C 3.59945 2.95442 2.93069
H 4.37231 3.20601 2.18346
H 2.65061 2.84956 2.38792
H 3.51863 3.81970 3.60733
C 6.49154 0.81056 6.46703
H 6.89030 1.83386 6.52727
H 6.10053 0.54134 7.46282
H 7.33366 0.12876 6.26222
C 3.47993 -2.42741 -3.51153
H 3.74656 -2.54181 -2.44809
H 2.38981 -2.57085 -3.57640
H 3.96683 -3.24009 -4.06983
C 3.06805 2.65907 -3.61919
H 2.18374 2.89106 -4.23889
H 2.71596 2.62404 -2.57863
H 3.76688 3.50253 -3.72467
C 6.38782 0.30233 -6.60718
H 6.19864 -0.41631 -7.42094
H 6.46837 1.30652 -7.04899
H 7.37255 0.04654 -6.17917
Cl 0.06650 2.90372 -0.13032
O -0.27083 -1.76581 0.15507
C 2.47250 -5.62947 0.91960
H 3.34022 -5.61481 1.58834
C 1.54977 -6.66704 1.03793
H 1.71110 -7.46131 1.77303
C 0.34849 -6.73676 0.13727
H 0.56138 -7.42773 -0.70580
H -0.50579 -7.18971 0.67003
C -0.03520 -5.35444 -0.41431
H -0.81790 -5.45413 -1.18383
H -0.46862 -4.74456 0.39674
C 1.17194 -4.58798 -0.97804
H 1.47282 -5.01330 -1.95846
H 0.87747 -3.54308 -1.16968
C 2.34256 -4.62263 -0.03547
H 3.11564 -3.85271 -0.12171
H 0.55479 -2.09598 0.53722

$^{5\alpha}$**TS**$_{Ep}$

Fe 0.04674 -0.45552 -0.20109
N 0.03071 -0.45423 1.89484
N 2.14173 -0.31032 -0.16330
N -2.02120 -0.11876 -0.19333
N 0.07654 0.02557 -2.24155
C -1.07802 -0.40150 2.69150
C 2.95557 -0.14050 -1.24643
C 1.13154 -0.52902 2.70258
C 2.92975 -0.41711 0.94781

C -2.83219 -0.14556 0.90926
C 1.19602 0.13113 -3.02147
C -2.81237 0.04816 -1.29707
C -1.01765 0.17416 -3.04796
C -0.66448 -0.46682 4.08294
C 4.34085 -0.16108 -0.80619
C 0.69885 -0.54871 4.08950
C 4.32487 -0.33586 0.54826
C -4.21341 -0.00052 0.48332
C 0.79187 0.34875 -4.40011
C -4.20169 0.11479 -0.87760
C -0.57351 0.37161 -4.41721
H -1.33364 -0.44292 4.94006
H 5.20865 -0.04756 -1.45195
H 1.35812 -0.60460 4.95277
H 5.17672 -0.39401 1.22220
H -5.07644 0.01219 1.14539
H 1.46995 0.46900 -5.24215
H -5.05308 0.24236 -1.54249
H -1.22610 0.51666 -5.27524
C -2.41608 -0.25552 2.25509
C 2.53740 0.07235 -2.58112
C -2.36955 0.18413 -2.63256
C 2.48249 -0.51933 2.28490
C -3.47142 -0.12283 3.31987
C -3.86367 1.16571 3.75520
C -4.06266 -1.26939 3.89725
C -4.82896 1.27881 4.76620
C -5.02945 -1.10886 4.90148
C -5.42656 0.15581 5.35391
H -5.12236 2.27802 5.10426
H -5.48346 -2.00101 5.34359
C 3.53249 -0.52986 3.36309
C 4.03132 0.68708 3.87467
C 4.02024 -1.76017 3.87132
C 5.00437 0.65313 4.88964
C 4.99150 -1.74653 4.87831
C 5.49886 -0.54763 5.40545
H 5.38385 1.60079 5.28518
H 5.36398 -2.70028 5.26542
C 3.61339 0.33306 -3.60056
C 4.25907 -0.74247 -4.25849
C 3.98929 1.66250 -3.89296
C 5.26826 -0.46703 -5.18892
C 5.01183 1.89217 -4.82957
C 5.66415 0.84579 -5.48913
H 5.76250 -1.30294 -5.69412
H 5.30411 2.92439 -5.04692
C -3.41591 0.41012 -3.69093
C -3.96732 -0.68332 -4.39699
C -3.84351 1.72540 -3.98691
C -4.93354 -0.44209 -5.38492
C -4.81018 1.92137 -4.98423
C -5.37167 0.85220 -5.69493
H -5.35320 -1.29334 -5.93000
H -5.13213 2.94229 -5.21224
C -3.52641 -2.09911 -4.10639
H -2.45104 -2.23573 -4.30605
H -3.68262 -2.36192 -3.04778
H -4.08072 -2.82172 -4.72271
C -6.43468 1.08458 -6.74207
H -6.41258 0.30630 -7.52014
H -7.44390 1.06667 -6.29390
H -6.31508 2.06413 -7.22986
C -3.28216 2.91334 -3.23972
H -3.58247 2.89583 -2.17879
H -2.18092 2.91946 -3.24604
H -3.63588 3.85915 -3.67523
C -3.67245 -2.65806 3.44711
H -3.83663 -2.79184 2.36572
H -2.60383 -2.85686 3.62803
H -4.25495 -3.42513 3.97778
C -3.29580 2.42388 3.13502
H -2.27593 2.28884 2.74841
H -3.91348 2.74632 2.27815
H -3.29064 3.25253 3.85929
C -6.46480 0.31351 6.43931
H -7.33785 0.88282 6.07842
H -6.82387 -0.66135 6.80070
H -6.06032 0.86713 7.30315
C 3.50528 -3.07737 3.33869
H 2.42102 -3.18418 3.50533
H 3.66369 -3.16252 2.25141
H 4.00899 -3.92576 3.82441
C 3.57329 2.03392 3.35676
H 4.36402 2.50282 2.74543
H 2.67480 1.97111 2.72937
H 3.36673 2.72403 4.19043
C 6.54366 -0.56895 6.49550
H 6.17473 -1.09243 7.39354
H 7.45207 -1.10236 6.16868
H 6.83809 0.44780 6.79448
C 3.86965 -2.17388 -3.97029
H 4.05137 -2.43745 -2.91564
H 2.79664 -2.34422 -4.15431
H 4.43948 -2.87407 -4.59828
C 3.29923 2.84788 -3.25384
H 2.44663 3.17987 -3.87250
H 2.89126 2.62188 -2.25875
H 3.98618 3.70334 -3.16595
C 6.76192 1.10805 -6.49233
H 7.71043 0.63978 -6.17977
H 6.51052 0.68641 -7.47998
H 6.94369 2.18520 -6.62100
Cl 0.26764 2.31885 0.17654
O -0.03918 -2.16983 -0.40033
C 0.22846 -4.12625 0.01930
H 0.95894 -3.87134 0.79029
C 0.69082 -4.50949 -1.22042
H 1.74137 -4.32995 -1.47185
C -0.21028 -5.02910 -2.30195
H -0.42246 -4.20078 -3.00920
H 0.32288 -5.78660 -2.90309
C -1.52997 -5.59550 -1.75601
H -2.24397 -5.74944 -2.58157
H -1.34198 -6.59115 -1.31469
C -2.12956 -4.67760 -0.68412
H -2.34169 -3.68914 -1.12636
H -3.08872 -5.08178 -0.32077
C -1.15801 -4.48955 0.48628
H -1.52280 -3.72124 1.18419
H -1.08685 -5.42777 1.07136

$^{5\alpha}$**IM**$_{Ep}$

Fe -0.04920 -0.06302 -0.03069
N -0.05904 -0.16253 2.06302
N 2.04560 -0.04036 -0.00386
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N -0.02543 0.37434 -2.07703
C -1.16594 -0.08222 2.86207
C 2.85611 0.12407 -1.09179
C 1.04359 -0.25046 2.86746
C 2.83693 -0.16497 1.10445
C -2.92490 0.23909 1.08915
C 1.09464 0.46064 -2.85896
C -2.91099 0.47049 -1.11448
C -1.11946 0.57149 -2.87400
C -0.74872 -0.15307 4.25121
C 4.24204 0.07267 -0.65808
C 0.61396 -0.25867 4.25425
C 4.22994 -0.10934 0.69613
C -4.30474 0.42218 0.67259
C 0.69053 0.71075 -4.23147
C -4.29665 0.56124 -0.68661
C -0.67438 0.77591 -4.24132
H -1.41385 -0.11482 5.11091
H 5.10905 0.17199 -1.30717
H 1.27382 -0.32324 5.11645
H 5.08459 -0.18828 1.36442
H -5.16491 0.44167 1.33822
H 1.36732 0.82294 -5.07563
H -5.14865 0.71849 -1.34438
H -1.32531 0.95356 -5.09450
C -2.50300 0.09681 2.43114
C 2.43623 0.35846 -2.42343
C -2.46920 0.61353 -2.45103
C 2.39414 -0.26684 2.44363
C -3.55193 0.23197 3.50238
C -3.92011 1.51967 3.96068
C -4.16171 -0.91351 4.06223
C -4.88040 1.63291 4.97626
C -5.12271 -0.75276 5.07210
C -5.49630 0.51084 5.54676
H -5.15480 2.63129 5.33218
H -5.59111 -1.64409 5.50059
C 3.44753 -0.29647 3.51839
C 3.98870 0.91291 4.00614
C 3.89392 -1.53227 4.04945
C 4.95906 0.86607 5.02248
C 4.86679 -1.53170 5.05566
C 5.41355 -0.34126 5.56075
H 5.36966 1.80761 5.40087
H 5.20770 -2.48999 5.46023
C 3.51518 0.59593 -3.44596
C 4.12157 -0.49269 -4.11934
C 3.93370 1.91543 -3.72588
C 5.13510 -0.24017 -5.05178
C 4.95871 2.12192 -4.66495
C 5.57311 1.06190 -5.33925
H 5.59873 -1.08628 -5.56887
H 5.28393 3.14626 -4.87233
C -3.51392 0.88152 -3.50121
C -4.09600 -0.18788 -4.21937
C -3.91014 2.21113 -3.77649
C -5.06175 0.09115 -5.19784
C -4.87738 2.44499 -4.76490
C -5.46947 1.40011 -5.48689
H -5.50559 -0.74165 -5.75215
H -5.17500 3.47673 -4.97671
C -3.68743 -1.61791 -3.95153
H -2.61826 -1.77808 -4.16600
H -3.83771 -1.88995 -2.89430
H -4.26653 -2.31863 -4.57034
C -6.53256 1.67432 -6.52378
H -6.54580 0.89852 -7.30446
H -7.53771 1.69219 -6.06656
H -6.38170 2.65059 -7.00964
C -3.31375 3.37451 -3.01792
H -3.60114 3.34758 -1.95368
H -2.21281 3.35620 -3.03872
H -3.65130 4.33456 -3.43470
C -3.79792 -2.30134 3.58785
H -3.96831 -2.41502 2.50504
H -2.73246 -2.52224 3.76128
H -4.39216 -3.06640 4.10829
C -3.33023 2.77687 3.35989
H -2.30590 2.63263 2.98859
H -3.93019 3.11251 2.49561
H -3.32711 3.59944 4.09094
C -6.52977 0.66876 6.63663
H -7.40071 1.24506 6.28154
H -6.89372 -0.30586 6.99374
H -6.11929 1.21547 7.50194
C 3.33498 -2.84233 3.54460
H 2.25327 -2.92189 3.74032
H 3.46211 -2.94344 2.45486
H 3.83074 -3.69690 4.02765
C 3.58065 2.25964 3.44913
H 4.31581 2.60885 2.70258
H 2.60550 2.23671 2.94449
H 3.54677 3.02021 4.24458
C 6.45788 -0.37705 6.65088
H 6.07722 -0.88331 7.55380
H 7.35328 -0.93480 6.32865
H 6.77673 0.63517 6.93996
C 3.68675 -1.91376 -3.84581
H 3.86001 -2.19421 -2.79418
H 2.60884 -2.04838 -4.03092
H 4.23386 -2.62507 -4.48143
C 3.28474 3.11425 -3.06958
H 2.41651 3.45730 -3.65966
H 2.90746 2.89649 -2.06045
H 3.98778 3.95861 -3.00727
C 6.67545 1.29871 -6.34375
H 7.61244 0.80635 -6.03328
H 6.41230 0.88523 -7.33171
H 6.88412 2.37120 -6.47040
Cl 0.20330 2.58350 0.37823
O -0.20857 -1.92645 -0.28077
C 0.28275 -3.07914 0.36987
H 0.84383 -2.78590 1.27915
C 1.20701 -3.77433 -0.59209
H 2.21966 -3.37147 -0.70818
C 0.63881 -4.61401 -1.69287
H 0.28267 -3.94859 -2.51093
H 1.42614 -5.23802 -2.15078
C -0.54259 -5.48309 -1.22494
H -1.02924 -5.95710 -2.09407
H -0.15732 -6.30411 -0.59289
C -1.55562 -4.66545 -0.41405
H -2.00045 -3.88574 -1.05709
H -2.38551 -5.31044 -0.07836
C -0.88205 -3.99599 0.78923
H -1.60758 -3.40063 1.36773
H -0.48746 -4.77465 1.46840

$^{5\beta}$**TS**$_{Ep}$

Fe -0.09331 -0.30953 -0.21441
N -0.09343 -0.44827 1.88844
N 1.97786 -0.37442 -0.21120
N -2.14529 -0.07788 -0.20561
N -0.05685 0.06475 -2.29501
C -1.20019 -0.41625 2.68593
C 2.79016 -0.27480 -1.30976
C 1.00808 -0.53298 2.68757
C 2.77526 -0.48721 0.89674
C -2.94897 -0.11539 0.89960
C 1.05017 0.09314 -3.08796
C -2.92845 0.16775 -1.29881
C -1.15164 0.27826 -3.07901
C -0.78302 -0.50882 4.07634
C 4.17651 -0.36603 -0.88116
C 0.58201 -0.57691 4.07775
C 4.16751 -0.49469 0.47757
C -4.32677 0.09767 0.48467
C 0.64194 0.33662 -4.46379
C -4.31385 0.27359 -0.86891
C -0.71968 0.45083 -4.45801
H -1.44983 -0.51287 4.93609
H 5.04084 -0.32614 -1.54045
H 1.24383 -0.64714 4.93831
H 5.02260 -0.58108 1.14440
H -5.18714 0.11902 1.14970
H 1.31181 0.40978 -5.31790
H -5.16107 0.46763 -1.52276
H -1.37580 0.63446 -5.30624
C -2.53542 -0.26779 2.24562
C 2.38734 -0.05476 -2.64763
C -2.49205 0.34330 -2.63419
C 2.35296 -0.54755 2.24583
C -3.60417 -0.18036 3.30204
C -3.88819 1.06124 3.91204
C -4.33278 -1.33385 3.68351
C -4.90257 1.13021 4.88257
C -5.33112 -1.22042 4.65859
C -5.63633 0.00503 5.27114
H -5.12251 2.09711 5.34609
H -5.88951 -2.11625 4.94843
C 3.42010 -0.54177 3.30792
C 3.95470 0.68934 3.74941
C 3.88453 -1.75286 3.87604
C 4.93278 0.68831 4.75814
C 4.86618 -1.70773 4.87411
C 5.40384 -0.49610 5.33426
H 5.33698 1.64614 5.10042
H 5.22043 -2.64830 5.30789
C 3.46872 0.12135 -3.68048
C 3.91076 -0.97254 -4.46047
C 4.04031 1.39970 -3.87859
C 4.90965 -0.76766 -5.42298
C 5.03494 1.56070 -4.85561
C 5.48412 0.49214 -5.64149
H 5.24882 -1.62029 -6.01964
H 5.47128 2.55347 -5.00431
C -3.53897 0.69458 -3.65722
C -4.26552 -0.32343 -4.32293
C -3.79910 2.05015 -3.95474
C -5.23761 0.03494 -5.26444
C -4.78837 2.36454 -4.90263
C -5.51873 1.37609 -5.56934
H -5.79453 -0.75703 -5.77525
H -4.98990 3.41761 -5.12316
C -4.00067 -1.78230 -4.03153
H -2.94340 -2.04146 -4.20272
H -4.21612 -2.02959 -2.97940
H -4.61951 -2.43251 -4.66699
C -6.57822 1.72781 -6.58630
H -6.34384 1.29596 -7.57381
H -7.56391 1.32973 -6.29219
H -6.67646 2.81649 -6.70878
C -3.02067 3.17418 -3.30656
H -2.61603 2.89866 -2.32300
H -2.15727 3.46115 -3.93266
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C -4.04514 -2.67734 3.05431
H -4.22269 -2.66046 1.96693
H -2.99218 -2.97093 3.19366
H -4.67899 -3.46316 3.49036
C -3.10768 2.31271 3.57475
H -2.23510 2.41914 4.24332
H -2.71457 2.30398 2.54858
H -3.72777 3.21243 3.70652
C -6.72770 0.09426 6.31109
H -6.81304 1.11077 6.72262
H -7.70802 -0.18141 5.88686
H -6.53969 -0.59696 7.14953
C 3.33759 -3.08575 3.42055
H 2.25949 -3.17309 3.63205
H 3.45366 -3.22061 2.33335
H 3.85024 -3.91763 3.92517
C 3.52430 2.00439 3.13856
H 4.09380 2.21096 2.21530
H 2.46257 2.01036 2.85292
H 3.70777 2.84077 3.82952
C 6.45707 -0.48306 6.41642
H 7.35996 -1.03360 6.10262
H 6.76023 0.54238 6.67428
H 6.09269 -0.97018 7.33637
C 3.32747 -2.35288 -4.26666
H 3.45991 -2.70430 -3.23096
H 2.24333 -2.36568 -4.46382
H 3.80356 -3.08241 -4.93783
C 3.62248 2.58502 -3.03783
H 2.53319 2.62738 -2.88836
H 4.06866 2.53035 -2.02977
H 3.95022 3.53028 -3.49497
C 6.53303 0.69312 -6.70919
H 7.16959 1.56428 -6.49230
H 7.18113 -0.19125 -6.81040
H 6.06784 0.86627 -7.69573
Cl 0.02983 2.14907 0.08565
O -0.33910 -2.00901 -0.46814

C 0.63701 -3.44417 0.30007
H 1.08282 -2.83945 1.09082
C 1.46439 -3.84566 -0.74197
H 2.40008 -3.30295 -0.90790
C 1.04313 -4.85756 -1.76841
H 0.63919 -4.32447 -2.65531
H 1.92509 -5.40545 -2.14497
C -0.01656 -5.83635 -1.23871
H -0.44739 -6.41549 -2.07242
H 0.46931 -6.56771 -0.56726
C -1.11620 -5.10084 -0.46387
H -1.63072 -4.39500 -1.13843
H -1.87759 -5.81362 -0.10499
C -0.52931 -4.31631 0.71465
H -1.29921 -3.69394 1.19469
H -0.17059 -5.02248 1.48880

$^{5}\beta$**IM**$_{Ep}$

Fe -0.03209 -0.05396 -0.01586
N -0.03317 -0.12635 2.01553
N 1.99871 -0.05096 0.00197
N -2.04618 0.21016 -0.00523
N -0.01162 0.28822 -2.01819
C -1.13634 -0.10461 2.83343
C 2.82611 0.04187 -1.09008
C 1.06192 -0.21106 2.83943
C 2.81456 -0.15627 1.10174
C -2.86822 0.17968 1.09354
C 1.09565 0.34484 -2.82694
C -2.85182 0.44624 -1.09017
C -1.09738 0.51833 -2.82533
C -0.72541 -0.20183 4.21635
C 4.20725 -0.03830 -0.66950
C 0.63638 -0.26279 4.22032
C 4.20009 -0.15946 0.68833
C -4.24116 0.38300 0.68630
C 0.69438 0.59602 -4.19403
C -4.23047 0.55065 -0.66643
C -0.66425 0.70295 -4.19274
H -1.40075 -0.21306 5.06843
H 5.06534 0.00020 -1.33612
H 1.30338 -0.33317 5.07603
H 5.05051 -0.24025 1.36111
H -5.09556 0.40310 1.35819
H 1.37377 0.68481 -5.03808
H -5.07404 0.73517 -1.32705
H -1.32418 0.89547 -5.03511
C -2.47242 0.03939 2.43282
C 2.43532 0.23870 -2.42239
C -2.43663 0.60899 -2.42047
C 2.40824 -0.21780 2.44261
C -3.52948 0.14751 3.49607
C -3.79591 1.40119 4.08845
C -4.26535 -0.99434 3.89743
C -4.80395 1.49324 5.06371
C -5.25632 -0.85684 4.87633
C -5.54606 0.38082 5.47217
H -5.01160 2.46849 5.51508
H -5.82123 -1.74280 5.18302
C 3.46428 -0.20652 3.51279
C 3.98401 1.02582 3.96601
C 3.93526 -1.41963 4.07310
C 4.95591 1.02385 4.98150
C 4.90926 -1.37386 5.07731
C 5.43312 -0.16053 5.55073
H 5.34973 1.98237 5.33387
H 5.26926 -2.31459 5.50572
C 3.50487 0.45180 -3.45727
C 3.95695 -0.62258 -4.26184
C 4.05215 1.74178 -3.63301
C 4.94179 -0.38347 -5.22755
C 5.03461 1.93657 -4.61897
C 5.49422 0.89157 -5.42643
H 5.28819 -1.21806 -5.84524
H 5.45080 2.93959 -4.75587
C -3.46975 0.97912 -3.44777
C -4.17894 -0.03019 -4.14639
C -3.73599 2.33895 -3.71474
C -5.13996 0.34228 -5.09223
C -4.71323 2.66642 -4.67176
C -5.42572 1.68895 -5.37109
H -5.68424 -0.44149 -5.62843
H -4.91833 3.72291 -4.87207
C -3.90650 -1.49271 -3.88229
H -2.85106 -1.74680 -4.07196
H -4.10761 -1.75811 -2.83174
H -4.53145 -2.13397 -4.52065
C -6.47207 2.05559 -6.39612
H -6.22010 1.64581 -7.38863
H -7.45906 1.64486 -6.12479
H -6.57578 3.14593 -6.49705
C -2.99437 3.46498 -3.02566
H -2.39024 3.12974 -2.17236
H -2.30977 3.96508 -3.73257
H -3.69749 4.23479 -2.66912
C -3.99153 -2.34927 3.28706
H -4.17033 -2.34775 2.19973
H -2.94143 -2.65141 3.43027
H -4.63227 -3.12235 3.73534
C -3.00481 2.64133 3.73260
H -2.16464 2.77866 4.43615
H -2.56531 2.59780 2.72633
H -3.63300 3.54249 3.80220
C -6.63152 0.49553 6.51561
H -6.69354 1.51426 6.92566
H -7.61879 0.24077 6.09435
H -6.45590 -0.19884 7.35397
C 3.40273 -2.75275 3.60182
H 2.32315 -2.85011 3.80080
H 3.53133 -2.87843 2.51489
H 3.91646 -3.58441 4.10544
C 3.55409 2.34803 3.36852
H 4.25192 2.65782 2.57049
H 2.55486 2.30940 2.91364
H 3.56219 3.14444 4.12836
C 6.47824 -0.14802 6.64047
H 7.38349 -0.69764 6.33224
H 6.77839 0.87719 6.90243
H 6.10701 -0.63719 7.55659
C 3.39274 -2.01366 -4.08936
H 3.49696 -2.36605 -3.05085
H 2.31584 -2.04605 -4.32219
H 3.90255 -2.73218 -4.74737
C 3.63915 2.91278 -2.76800
H 2.62217 2.81184 -2.36384
H 4.31329 3.00810 -1.89839
H 3.70171 3.85772 -3.32891
C 6.54794 1.11662 -6.48431
H 6.90259 2.15777 -6.48758
H 7.42026 0.46088 -6.32590
H 6.15873 0.88908 -7.49108
Cl 0.10510 2.73652 0.23097
O -0.20830 -1.97559 -0.21205
C 0.47306 -3.02814 0.41814
H 1.03906 -2.65190 1.29550
C 1.45074 -3.66597 -0.54390
H 2.42810 -3.18974 -0.68272
C 0.93445 -4.58640 -1.60542
H 0.45095 -3.98407 -2.40773
H 1.76258 -5.12228 -2.10125
C -0.10779 -5.58239 -1.06215
H -0.57416 -6.13438 -1.89618
H 0.40658 -6.33416 -0.43552
C -1.17449 -4.87546 -0.21622
H -1.74935 -4.18052 -0.85349
H -1.89580 -5.61125 0.17964
C -0.53384 -4.08309 0.92905
H -1.30355 -3.56908 1.52904
H -0.00634 -4.78147 1.60617

3. [Fe^{IV}(O)(TPFPP$^{+\bullet}$)(Cl)] (1b)

^{2}**1b**

Fe -0.00044 0.02280 0.00674
N 0.01320 -0.04998 2.03281
N 2.02191 0.18405 0.00249
N -2.02637 0.09328 0.02691
N -0.01810 0.27352 -2.00736
C -1.06967 -0.12554 2.86247
C 2.83558 0.34197 -1.08738
C 1.11336 -0.13268 2.84390
C 2.85402 0.13054 1.08547
C -2.84133 0.07934 1.12774
C 1.06599 0.33627 -2.83637
C -2.85731 0.20650 -1.05144
C -1.11519 0.25277 -2.82672
C -0.64646 -0.27789 4.23695
C 4.22036 0.41707 -0.67788
C 0.71319 -0.27474 4.22614
C 4.23329 0.27003 0.67360
C -4.22551 0.21771 0.73374
C 0.64779 0.33084 -4.22084
C -4.23575 0.29537 -0.62358
C -0.71049 0.27445 -4.21469
H -1.30268 -0.37557 5.09730
H 5.07087 0.56408 -1.33771
H 1.38431 -0.35062 5.07730
H 5.09828 0.25635 1.33083
H -5.07565 0.26763 1.40848
H 1.30777 0.35052 -5.08358
H -5.09572 0.42223 -1.27539
H -1.37768 0.23953 -5.07145
C -2.41629 -0.05020 2.45961
C 2.41035 0.39846 -2.42473
C -2.45274 0.24124 -2.39944
C 2.44921 -0.04727 2.42109
C -3.46426 -0.10901 3.52182
C -3.64376 0.94552 4.42692
C -4.30367 -1.22347 3.65175
C -4.61870 0.89846 5.42361
C -5.43827 -0.22707 5.53219
C 3.51504 -0.13823 3.46479
C 4.23468 0.99205 3.87166
C 3.82873 -1.36063 4.07180
C 5.23099 0.91470 4.84539
C 4.82462 -1.46176 5.04382
C 5.52708 -0.31840 5.43034
C 3.45388 0.53285 -3.48451
C 4.33496 -0.51612 -3.77921
C 3.58654 1.71617 -4.22342
C 5.30976 -0.39840 -4.77032
C 4.55860 1.85772 -5.21396
C 5.42097 0.79410 -5.48841
C -3.52085 0.28897 -3.44117
C -4.36125 -0.80929 -3.66920
C -3.73017 1.43595 -4.21897
C -5.36813 -0.77487 -4.63406
C -4.73605 1.49434 -5.18388
C -5.55593 0.38312 -5.39178
F -4.91889 2.59799 -5.90144
F -2.96472 2.51125 -4.03853
F 4.66812 2.99421 -5.89431
F 6.34557 0.91640 -6.43100
F 2.77522 2.74485 -3.98148
F 6.12852 -1.41145 -5.03467
F 4.24973 -1.66474 -3.10944
F 5.89607 2.00350 5.21807
F 6.47490 -0.40330 6.35415
F 5.10751 -2.63517 5.60044
F 3.16989 -2.46436 3.72111
F 3.97111 2.17871 3.32599
F -4.17354 -2.25459 2.81819
F -2.87471 2.03035 4.34429
F -4.77261 1.91541 6.26539
F -6.36616 -0.28247 6.47778
F -6.51261 0.42734 -6.30868
F -6.14595 -1.83353 -4.83540
F -4.20487 -1.92471 -2.95764
C -5.28074 -1.29400 4.64510
F -6.05799 -2.36686 4.75199
Cl -0.05499 2.42465 0.19657
O 0.04082 -1.59827 -0.12693

^{4}**1b**

Fe -0.00527 0.02616 0.00765
N 0.01429 -0.01992 2.03518
N 2.01771 0.15186 -0.00485
N -2.02918 0.13267 0.03328
N -0.02537 0.23419 -2.00941
C -1.06876 -0.12556 2.86320
C 2.82753 0.30868 -1.09665
C 1.11448 -0.12680 2.84190
C 2.84914 0.15271 1.08085
C -2.83974 0.13789 1.13598
C 1.05813 0.24525 -2.84376
C -2.86109 0.26928 -1.04322
C -1.12504 0.22136 -2.82403
C -0.64360 -0.33644 4.22930
C 4.20702 0.45069 -0.68725
C 0.71609 -0.33813 4.21580
C 4.22082 0.35147 0.66881
C -4.22056 0.32082 0.74827
C 0.63415 0.20324 -4.22560
C -4.23390 0.40298 -0.60893
C -0.72533 0.18710 -4.21322
H -1.29903 -0.47750 5.08434
H 5.05147 0.62013 -1.34959
H 1.38825 -0.48059 5.05752
H 5.07855 0.42446 1.33192
H -5.06583 0.39465 1.42705
H 1.29078 0.17693 -5.09077
H -5.09253 0.55707 -1.25668
H -1.39675 0.14534 -5.06635
C -2.41388 -0.02347 2.46556
C 2.40241 0.31504 -2.43637
C -2.46149 0.26886 -2.39201
C 2.45019 -0.02098 2.41829
C -3.45968 -0.08665 3.52904
C -3.61082 0.94677 4.46337
C -4.32498 -1.18417 3.63218
C -4.58264 0.89535 5.46286
C -5.42791 -0.21328 5.54458
C 3.51894 -0.08817 3.45848
C 3.69174 0.94129 4.39339
C 4.38846 -1.18451 3.53463
C 4.68974 0.88768 5.36667
C 5.38811 -1.26194 4.50463
C 5.53890 -0.21961 5.42171
C 3.44812 0.41129 -3.49735
C 4.34424 -0.64020 -3.73328
C 3.57466 1.55936 -4.29127
C 5.32628 -0.55922 -4.72076
C 4.55386 1.66394 -5.27937
C 5.43090 0.59871 -5.49432
C -3.53021 0.33693 -3.43193
C -4.41480 -0.73105 -3.63550
C -3.69421 1.47436 -4.23440
C -5.42166 -0.67622 -4.59944
C -4.69858 1.55270 -5.19943
C -5.56350 0.47166 -5.38203
F -4.83800 2.64719 -5.94055
F -2.88544 2.52131 -4.07796
F 4.65784 2.76806 -6.01197
F 6.36283 0.68634 -6.43349
F 2.75251 2.59088 -4.10475
F 6.15837 -1.57441 -4.92961
F 4.26573 -1.75602 -3.00959
F 4.83765 1.88149 6.23681
F 6.48883 -0.28112 6.34482
F 6.19380 -2.31762 4.56078
F 4.26555 -2.19167 2.67125
F 2.89583 2.00918 4.36124
F -4.22183 -2.19562 2.77126
F -2.81767 2.01568 4.40632
F -4.70974 1.89257 6.33236
F -6.35295 -0.27288 6.49274
F -6.51942 0.53484 -6.29873
F -6.24237 -1.70646 -4.77719
F -4.30168 -1.83719 -2.90161
C -5.29867 -1.25931 4.62847
F -6.10014 -2.31652 4.71038
Cl -0.01457 2.42558 0.15267
O 0.00158 -1.59886 -0.09265

CHE + 1b

$S = 1/2$

^{2}**RC**

Fe 0.05870 0.22642 -0.30317
N 0.08605 0.13209 1.72407
N 2.08436 0.31925 -0.32113
N -1.96439 0.35582 -0.26576
N 0.03340 0.50583 -2.31204
C -0.99438 0.03021 2.55604
C 2.89351 0.47529 -1.41271
C 1.18753 0.01483 2.52640
C 2.92104 0.26333 0.75960
C -2.77171 0.31099 0.83794
C 1.11375 0.52859 -3.15059
C -2.80048 0.53052 -1.33363
C -1.06928 0.55208 -3.12038
C -0.56597 -0.17354 3.92208
C 4.27979 0.55278 -1.00882
C 0.79358 -0.18308 3.90346
C 4.29721 0.41700 0.34413
C -4.15577 0.49171 0.46147
C 0.68307 0.55893 -4.53059
C -4.17330 0.63269 -0.89094
C -0.67625 0.57381 -4.51175
H -1.21941 -0.30353 4.78034
H 5.12646 0.70743 -1.67193
H 1.46879 -0.32323 4.74300
H 5.16015 0.43784 1.00417
H -4.99945 0.52647 1.14543
H 1.33536 0.55568 -5.39938
H -5.03492 0.80599 -1.52968
H -1.35194 0.58540 -5.36237
C -2.34022 0.12174 2.16181
C 2.46124 0.54282 -2.74903
C -2.40436 0.59222 -2.68181
C 2.52309 0.08527 2.09574
C -3.38392 0.01189 3.22454
C -3.59152 1.04028 4.15252
C -4.18722 -1.13043 3.33222
C -4.56254 0.94178 5.14957
C -5.34699 -0.21047 5.23504
C 3.59416 -0.03701 3.12950
C 3.84250 0.99030 4.04868
C 4.38400 -1.19032 3.21738
C 4.84121 0.88075 5.01681
C 5.38216 -1.32482 4.18244
C 5.61191 -0.28202 5.08256
C 3.50321 0.64822 -3.81290
C 4.36160 -0.42176 -4.09993

C 3.66145 1.82324 -4.56028
C 5.33754 -0.33285 -5.09282
C 4.63568 1.93601 -5.55234
C 5.47414 0.85167 -5.81975
C -3.47394 0.71694 -3.71577
C -4.36206 -0.33613 -3.97390
C -3.63145 1.89342 -4.46107
C -5.36582 -0.22983 -4.93680
C -4.63286 2.02344 -5.42360
C -5.50111 0.95593 -5.66195
F -4.76577 3.15358 -6.11026
F -2.81807 2.92746 -4.25146
F 4.77012 3.06499 -6.24061
F 6.40023 0.94681 -6.76388
F 2.87498 2.87233 -4.32437
F 6.13354 -1.36549 -5.35050
F 4.25211 -1.56282 -3.42103
F 5.06309 1.87321 5.87247
F 6.56155 -0.39629 6.00105
F 6.11038 -2.43448 4.25066
F 4.17911 -2.20228 2.37283
F 3.11860 2.10790 4.00742
F -4.02130 -2.14283 2.47928
F -2.85339 2.14768 4.09268
F -4.74532 1.93478 6.01375
F -6.27030 -0.31448 6.18116
F -6.45391 1.06794 -6.57719
F -6.18988 -1.24676 -5.16723
F -4.25477 -1.47786 -3.29575
C -5.15809 -1.25397 4.32620
F -5.89955 -2.35346 4.41308
Cl 0.08279 2.61923 -0.08663
O 0.04244 -1.39574 -0.45608
C 0.00733 -4.33750 3.10210
H -0.02614 -4.17929 4.18664
C 1.17097 -4.18902 2.45032
H 2.06712 -3.88673 3.00407
C 1.32391 -4.40589 0.96493
H 1.42746 -3.42286 0.46755
H 2.26621 -4.94541 0.76245
C 0.12891 -5.16098 0.36601
H 0.16179 -5.11078 -0.73498
H 0.19811 -6.23133 0.63446
C -1.19442 -4.59154 0.89174
H -1.25257 -3.52608 0.60798
H -2.05316 -5.09624 0.41869
C -1.28555 -4.71404 2.41990
H -1.56035 -5.74849 2.70675
H -2.10616 -4.08171 2.80205

^{2}**TS**$_H$

Fe -0.11478 0.14113 -0.07458
N -0.17205 0.06491 1.94047
N 1.91356 0.24278 -0.01339
N -2.12057 0.21080 -0.13013
N -0.04980 0.34924 -2.09375
C -1.28869 0.04527 2.73250
C 2.76367 0.43753 -1.06933
C 0.89791 -0.10555 2.78025
C 2.70120 0.13570 1.10157
C -2.97292 0.30267 0.94238
C 1.07257 0.42337 -2.87532
C -2.90688 0.29830 -1.25147
C -1.11175 0.26987 -2.95299
C -0.91755 -0.16800 4.11289
C 4.13125 0.49616 -0.60056
C 0.43841 -0.27240 4.14104
C 4.09380 0.29616 0.74376
C -4.33124 0.47645 0.48424
C 0.70780 0.37018 -4.27470
C -4.29176 0.46236 -0.87547
C -0.64657 0.26179 -4.32273
H -1.60842 -0.24522 4.94831
H 5.00481 0.67230 -1.22246
H 1.07299 -0.44768 5.00554
H 4.93009 0.27948 1.43774
H -5.20215 0.60308 1.12192
H 1.40297 0.39131 -5.10987
H -5.12319 0.57785 -1.56574
H -1.27618 0.17887 -5.20459
C -2.61077 0.20041 2.29186
C 2.39415 0.51949 -2.41909
C -2.46392 0.26026 -2.58114
C 2.25038 -0.07373 2.41182
C -3.69449 0.24250 3.31880
C -3.83609 1.33828 4.18077
C -4.60991 -0.80830 3.46191
C -4.84685 1.39416 5.14121
C -5.74417 0.33104 5.25889
C 3.27806 -0.24688 3.48314
C 3.52328 0.75187 4.43412
C 4.03963 -1.41937 3.57073
C 4.48368 0.59570 5.43440
C 5.00372 -1.59886 4.56353
C 5.22512 -0.58562 5.49816
C 3.47405 0.68906 -3.43797
C 4.37092 -0.34466 -3.73714
C 3.62486 1.89319 -4.13826
C 5.37776 -0.19293 -4.69130
C 4.62564 2.06878 -5.09481
C 5.50427 1.01967 -5.37159
C -3.49457 0.25254 -3.66226
C -4.31447 -0.86320 -3.87784
C -3.68444 1.35800 -4.50277
C -5.27741 -0.88868 -4.88716
C -4.64241 1.35683 -5.51729
C -5.44014 0.22734 -5.71011
F -4.80180 2.42275 -6.29649
F -2.94137 2.45288 -4.34148
F 4.74777 3.22537 -5.74061
F 6.45907 1.17472 -6.28059
F 2.79908 2.91127 -3.89575
F 6.21277 -1.19380 -4.95730
F 4.27341 -1.51498 -3.10557
F 4.69787 1.56272 6.32241
F 6.14026 -0.74476 6.44642
F 5.70770 -2.72590 4.62607
F 3.84927 -2.40321 2.69124
F 2.83154 1.89102 4.39659
F -4.52406 -1.88239 2.67368
F -2.99435 2.36789 4.09136
F -4.96131 2.45088 5.94068
F -6.70836 0.37310 6.16974
F -6.35288 0.21519 -6.67323
F -6.03512 -1.96606 -5.07108
F -4.18481 -1.94657 -3.10877
C -5.62667 -0.77640 4.41679
F -6.47858 -1.79130 4.53122
Cl -0.08762 2.48978 0.06809
O 0.02144 -1.49252 -0.23261
C -1.95879 -5.13304 -1.24675
H -2.42807 -5.54919 -2.14487
C -2.40502 -3.94560 -0.75458
H -3.18758 -3.40349 -1.29390
C -1.85814 -3.33983 0.46941
H -2.62310 -2.79603 1.04833
C -1.00522 -4.27949 1.32071
H -0.42380 -3.69998 2.05485
H -1.67247 -4.94353 1.90234
C -0.07630 -5.12194 0.43903
H 0.61937 -4.44512 -0.08685
H 0.54041 -5.79598 1.05409
C -0.87032 -5.93125 -0.59561
H -1.33443 -6.82041 -0.12083
H -0.20325 -6.34751 -1.37109
H -1.15621 -2.46540 0.11751

^{2}**PC**$_H$

Fe -0.10817 0.27481 0.02384
N -0.23128 0.05267 2.02202
N 1.89471 0.10508 0.16454
N -2.12157 0.34194 -0.12919
N 0.00499 0.40287 -1.98685
C -1.38663 -0.01976 2.75867
C 2.77928 0.10993 -0.88311
C 0.80089 0.01419 2.92758
C 2.65716 0.09843 1.30669
C -3.01358 0.24924 0.91089
C 1.14868 0.29757 -2.73799
C -2.87158 0.60355 -1.25102
C -1.01926 0.60114 -2.87782
C -1.07346 -0.12931 4.16653
C 4.13862 0.10230 -0.38825
C 0.28312 -0.10461 4.27088
C 4.06222 0.10701 0.97023
C -4.36362 0.43576 0.42697
C 0.83084 0.40279 -4.14560
C -4.27317 0.67771 -0.90870
C -0.51155 0.60546 -4.23116
H -1.80010 -0.20415 4.97153
H 5.03433 0.11493 -1.00399
H 0.88214 -0.16978 5.17553
H 4.88309 0.12029 1.68263
H -5.26441 0.39584 1.03383
H 1.54382 0.32646 -4.96243
H -5.08431 0.88209 -1.60270
H -1.11029 0.72321 -5.13063
C -2.69478 0.04410 2.25956
C 2.45194 0.14866 -2.24558
C -2.37589 0.73477 -2.55389
C 2.16597 0.05309 2.61701
C -3.81915 -0.07671 3.23945
C -4.53940 1.04308 3.67302
C -4.19117 -1.32004 3.76475
C -5.58710 0.93697 4.58906
C -5.93581 -0.31731 5.09322
C 3.14740 0.00707 3.74291
C 3.36469 1.11553 4.57060
C 3.88097 -1.15358 4.01898
C 4.27342 1.07754 5.62931
C 4.79442 -1.21615 5.07201
C 4.99022 -0.09401 5.87940
C 3.57257 0.05502 -3.23164
C 4.21613 -1.16407 -3.47839
C 4.02654 1.17409 -3.94039
C 5.26536 -1.27375 -4.39197
C 5.07451 1.09017 -4.85836
C 5.69439 -0.14010 -5.08472
C -3.34172 1.00342 -3.66216
C -4.23035 0.02167 -4.11900
C -3.38762 2.25211 -4.29579
C -5.12982 0.26538 -5.15789
C -4.27763 2.51946 -5.33697
C -5.15181 1.52042 -5.76881
F -4.29940 3.71699 -5.91718
F -2.56453 3.22659 -3.90647
F 5.48666 2.17186 -5.51495
F 6.69184 -0.23159 -5.95672
F 3.45475 2.36294 -3.74457
F 5.85540 -2.44699 -4.60769
F 3.82969 -2.26581 -2.83075
F 4.46096 2.14750 6.39807
F 5.85674 -0.14138 6.88468
F 5.47462 -2.33445 5.31278
F 3.71144 -2.24217 3.26578
F 2.69145 2.24695 4.35828
F -3.53897 -2.42488 3.39357
F -4.22989 2.25401 3.20767
F -6.25273 2.01961 4.98367
F -6.93223 -0.43044 5.96390
F -6.00271 1.76374 -6.75890
F -5.96007 -0.68942 -5.57095
F -4.23161 -1.18908 -3.55869
C -5.23388 -1.45215 4.68299
F -5.56422 -2.64807 5.16420
Cl 0.01194 2.50959 0.23166
O -0.24035 -1.73986 -0.22877
C -1.18128 -4.84903 0.78899
H -2.00324 -5.35316 1.30987
C -0.82294 -3.61688 1.18433
H -1.36522 -3.11656 1.99203
C 0.30868 -2.85868 0.54487
H 0.92260 -2.36896 1.31195
C 1.19117 -3.73882 -0.34259
H 1.83540 -3.09769 -0.96289
H 1.85900 -4.31617 0.32096
C 0.36294 -4.69919 -1.20143
H -0.28326 -4.11615 -1.88200
H 1.02141 -5.30332 -1.84468
C -0.50758 -5.60547 -0.32356
H 0.10649 -6.41220 0.12273
H -1.26902 -6.12557 -0.92939
H -1.06052 -2.00599 -0.67334

^{2}**TS**$_{Ep}$

Fe -0.09116 0.01442 0.10980
N -0.07119 0.02038 2.11370
N 1.91582 0.01858 0.08549
N -2.11173 0.20208 0.12576
N -0.11308 0.17378 -1.91803
C -1.15785 -0.12234 2.93962
C 2.71867 -0.04532 -1.02149
C 1.02830 0.06573 2.92913
C 2.75514 0.15513 1.16206
C -2.92471 0.09484 1.21810
C 0.95043 -0.03090 -2.75526
C -2.93182 0.44521 -0.94419
C -1.21012 0.33093 -2.71950
C -0.72515 -0.20669 4.31640
C 4.10813 0.06251 -0.63538
C 0.62863 -0.06877 4.31149
C 4.12914 0.20777 0.71719
C -4.30622 0.29618 0.83549
C 0.50745 -0.03078 -4.13324
C -4.30766 0.53663 -0.50305
C -0.82957 0.21645 -4.11199
H -1.37470 -0.34560 5.17633
H 4.95474 0.06057 -1.31702
H 1.30071 -0.07939 5.16553
H 4.99672 0.34249 1.35767
H -5.15761 0.28497 1.51113
H 1.13918 -0.19481 -5.00216
H -5.16216 0.75457 -1.13811
H -1.50606 0.28858 -4.95971
C -2.50093 -0.12088 2.53863
C 2.28867 -0.14812 -2.35455
C -2.52998 0.52476 -2.28466
C 2.36178 0.17389 2.50629
C -3.55358 -0.32383 3.57967
C -3.86787 0.66316 4.52200
C -4.27419 -1.52361 3.63917
C -4.85557 0.46872 5.48864
C -5.55471 -0.73928 5.52538
C 3.42446 0.26059 3.55218
C 3.58814 1.41515 4.32841
C 4.29380 -0.80962 3.80018
C 4.57890 1.50975 5.30665
C 5.29017 -0.73906 4.77424
C 5.43190 0.42703 5.52913
C 3.33099 -0.34870 -3.40543
C 4.01296 -1.56806 -3.51313
C 3.67704 0.66240 -4.31118
C 4.99310 -1.78225 -4.48261
C 4.65667 0.47264 -5.28687
C 5.31645 -0.75494 -5.37115
C -3.57280 0.78057 -3.32406
C -4.52314 -0.18759 -3.67234
C -3.62706 2.00674 -3.99963
C -5.49136 0.04903 -4.64910
C -4.58758 2.26684 -4.97788
C -5.52240 1.28220 -5.30305
F -4.61843 3.44292 -5.59882
F -2.74564 2.96420 -3.71086
F 4.96769 1.45256 -6.13076
F 6.24942 -0.94553 -6.29561
F 3.06945 1.84754 -4.25189
F 5.61871 -2.95317 -4.56457
F 3.72664 -2.56744 -2.67630
F 4.71611 2.62133 6.02396
F 6.37662 0.50557 6.45798
F 6.09952 -1.77226 4.98974
F 4.18011 -1.93907 3.09758
F 2.78670 2.46305 4.13816
F -4.01853 -2.49821 2.76386
F -3.21844 1.82741 4.50884
F -5.13594 1.42501 6.36961
F -6.49554 -0.93430 6.44112
F -6.43971 1.51827 -6.23298
F -6.37912 -0.89114 -4.96190
F -4.51547 -1.37645 -3.06844
C -5.26370 -1.74201 4.59832
F -5.92767 -2.89397 4.63504
Cl -0.02373 2.39087 0.15312
O -0.25286 -1.59926 -0.04689
C 0.39894 -3.46478 1.56942
H 0.38183 -2.84683 2.47148
C 1.53497 -3.49836 0.81193
H 2.38357 -2.87195 1.10154
C 1.67312 -4.34901 -0.40901
H 1.64256 -3.67547 -1.28917
H 2.68362 -4.79371 -0.43655
C 0.58519 -5.42765 -0.51571
H 0.57781 -5.85266 -1.53198
H 0.83188 -6.25837 0.16957
C -0.79528 -4.86696 -0.15384
H -1.05478 -4.05687 -0.85563
H -1.56838 -5.64505 -0.25653
C -0.80621 -4.29948 1.27139
H -0.84120 -5.12137 2.01597
H -1.71628 -3.70625 1.46382

^{2}**PC**$_{Ep}$

Fe 0.10313 0.31497 0.01233
N 0.07099 0.19498 2.02667
N 2.11720 0.23456 0.06740
N -1.91277 0.29770 -0.04794
N 0.13471 0.30020 -2.00538
C -1.04828 0.14629 2.81886
C 2.96111 0.32264 -1.01307
C 1.14370 0.12756 2.88135
C 2.92484 0.25532 1.18000
C -2.75508 0.30824 1.03416
C 1.25262 0.29992 -2.80230
C -2.71841 0.36485 -1.15618
C -0.93885 0.30245 -2.86174
C -0.67056 0.01664 4.20930
C 4.33374 0.40547 -0.56936
C 0.68900 0.00530 4.24771
C 4.31078 0.36439 0.79072
C -4.13040 0.40941 0.59586
C 0.87279 0.27142 -4.19760
C -4.10718 0.44408 -0.76364
C -0.48683 0.27174 -4.23402
H -1.35928 -0.06614 5.04605
H 5.20165 0.49708 -1.21737
H 1.32886 -0.08956 5.12112
H 5.15601 0.41631 1.47211
H -4.99897 0.45690 1.24762
H 1.56059 0.24383 -5.03885
H -4.95185 0.52489 -1.44308
H -1.12952 0.24430 -5.11015
C -2.37695 0.20819 2.37943

C 2.58180 0.32102 -2.36169
C -2.28687 0.33917 -2.48727
C 2.49312 0.16875 2.50907
C -3.46123 0.13811 3.40657
C -3.74821 1.21751 4.25103
C -4.23182 -1.02113 3.56290
C -4.75909 1.15334 5.21142
C -5.51061 -0.01576 5.34266
C 3.52816 0.09590 3.58400
C 3.75933 1.16359 4.46041
C 4.30442 -1.05700 3.75988
C 4.72007 1.09323 5.47043
C 5.27041 -1.15142 4.76224
C 5.47743 -0.06983 5.62056
C 3.66528 0.32283 -3.39183
C 4.41077 -0.83338 -3.65348
C 3.97943 1.47033 -4.12958
C 5.42982 -0.85447 -4.60637
C 4.99555 1.47480 -5.08663
C 5.72240 0.30681 -5.32434
C -3.32084 0.33528 -3.56642
C -4.06344 -0.81803 -3.84841
C -3.58327 1.47294 -4.33914
C -5.02723 -0.84663 -4.85709
C -4.54355 1.46967 -5.35209
C -5.26770 0.30432 -5.61008
F -4.77332 2.56669 -6.06950
F -2.90445 2.59918 -4.11741
F 5.27588 2.58176 -5.77006
F 6.69104 0.30004 -6.23284
F 3.30083 2.59984 -3.92489
F 6.12026 -1.96889 -4.83543
F 4.15097 -1.95770 -2.98230
F 4.91940 2.12496 6.28690
F 6.39389 -0.14729 6.57845
F 5.98920 -2.26192 4.90758
F 4.12648 -2.10857 2.95668
F 3.05058 2.28714 4.34303
F -4.00329 -2.08305 2.78678
F -3.04595 2.34683 4.15035
F -5.01134 2.19638 5.99849
F -6.47512 -0.08745 6.25281
F -6.18301 0.28984 -6.57217
F -5.71463 -1.95871 -5.10570
F -3.85360 -1.93346 -3.14534
C -5.24685 -1.10980 4.51627
F -5.96058 -2.22585 4.64379
Cl 0.13393 2.55884 0.06910
O -0.02724 -1.74527 -0.00139
C 0.80351 -2.76968 0.59978
H 1.77134 -2.39369 0.94834
C 0.55052 -2.77344 -0.85745
H 1.34273 -2.38374 -1.50506
C -0.45571 -3.71599 -1.48754
H -1.29740 -3.10698 -1.85958
H 0.00586 -4.17423 -2.37642
C -0.95571 -4.80648 -0.52356
H -1.86850 -5.26595 -0.93421
H -0.20113 -5.61123 -0.46677
C -1.21147 -4.27696 0.89255
H -1.98237 -3.48805 0.87164
H -1.60604 -5.08184 1.53235
C 0.07700 -3.72260 1.51611
H 0.77806 -4.54639 1.74000
H -0.12638 -3.21770 2.47506

$S = 3/2$

^{4}RC

Fe 0.06207 0.23435 -0.30951
N 0.08750 0.13897 1.71751
N 2.08789 0.31356 -0.32655
N -1.96053 0.36845 -0.27397
N 0.03923 0.50684 -2.31877
C -0.99417 0.03938 2.54871
C 2.89860 0.46145 -1.41813
C 1.18794 0.02009 2.52109
C 2.92376 0.25860 0.75531
C -2.76891 0.32610 0.82906
C 1.12032 0.51933 -3.15722
C -2.79521 0.54866 -1.34244
C -1.06272 0.55936 -3.12784
C -0.56729 -0.16468 3.91522
C 4.28496 0.53407 -1.01357
C 0.79223 -0.17621 3.89792
C 4.30083 0.40436 0.33998
C -4.15193 0.51320 0.45174
C 0.69026 0.54908 -4.53741
C -4.16783 0.65649 -0.90044
C -0.66890 0.57477 -4.51909
H -1.22176 -0.29332 4.77289
H 5.13278 0.68180 -1.67679
H 1.46643 -0.31708 4.73816
H 5.16345 0.42406 1.00047
H -4.99595 0.55048 1.13514
H 1.34283 0.53834 -5.40595
H -5.02826 0.83441 -1.53954
H -1.34418 0.58937 -5.37000
C -2.33917 0.13455 2.15331
C 2.46746 0.52637 -2.75508
C -2.39786 0.60897 -2.69010
C 2.52417 0.08643 2.09154
C -3.38429 0.02725 3.21495
C -3.59055 1.05606 4.14275
C -4.19048 -1.11312 3.32159
C -4.56294 0.95978 5.13868
C -5.35025 -0.19059 5.22315
C 3.59378 -0.03550 3.12687
C 3.84321 0.99377 4.04357
C 4.38078 -1.19040 3.21917
C 4.84038 0.88466 5.01336
C 5.37741 -1.32445 4.18588
C 5.60836 -0.27965 5.08337
C 3.51086 0.62174 -3.81850
C 4.36310 -0.45438 -4.10084
C 3.67720 1.79324 -4.56962
C 5.34084 -0.37475 -5.09275
C 4.65338 1.89676 -5.56077
C 5.48562 0.80649 -5.82343
C -3.46556 0.74116 -3.72510
C -4.35988 -0.30605 -3.98550
C -3.61427 1.91909 -4.46991
C -5.36129 -0.19271 -4.95006
C -4.61310 2.05613 -5.43415
C -5.48772 0.99433 -5.67469
F -4.73755 3.18753 -6.12035
F -2.79448 2.94766 -4.25831
F 4.79556 3.02260 -6.25264
F 6.41355 0.89290 -6.76660
F 2.89684 2.84791 -4.33831
F 6.13090 -1.41307 -5.34591
F 4.24595 -1.59237 -3.41806
F 5.06333 1.87898 5.86659
F 6.55654 -0.39350 6.00344
F 6.10300 -2.43557 4.25820
F 4.17460 -2.20437 2.37733
F 3.12182 2.11284 3.99834
F -4.02603 -2.12582 2.46869
F -2.84972 2.16172 4.08386
F -4.74433 1.95315 6.00275
F -6.27492 -0.29246 6.16820
F -6.43817 1.11298 -6.59158
F -6.19141 -1.20423 -5.18264
F -4.26085 -1.44905 -3.30818
C -5.16278 -1.23446 4.31445
F -5.90698 -2.33218 4.40036
Cl 0.09597 2.62026 -0.09516
O 0.03845 -1.38884 -0.45955
C -0.00848 -4.33019 3.10052
H -0.04182 -4.17048 4.18484
C 1.15569 -4.18541 2.44885
H 2.05244 -3.88456 3.00242
C 1.30852 -4.40453 0.96377
H 1.41551 -3.42242 0.46530
H 2.24924 -4.94720 0.76232
C 0.11153 -5.15675 0.36517
H 0.14477 -5.10749 -0.73584
H 0.17779 -6.22708 0.63443
C -1.21042 -4.58352 0.89023
H -1.26607 -3.51815 0.60563
H -2.07034 -5.08646 0.41746
C -1.30208 -4.70448 2.41846
H -1.57918 -5.73810 2.70612
H -2.12136 -4.07004 2.79991

^{4}TS$_H$

Fe -0.08014 0.16816 -0.12554
N -0.17532 0.05915 1.90192
N 1.90474 0.22350 -0.04201
N -2.12001 0.22632 -0.18822
N -0.01502 0.37175 -2.11783
C -1.30134 0.08984 2.68104
C 2.77240 0.48251 -1.07481
C 0.87111 -0.17849 2.74532
C 2.68482 0.04712 1.07895
C -2.97572 0.34597 0.87516
C 1.10358 0.51400 -2.89230
C -2.89372 0.25435 -1.31073
C -1.07461 0.25701 -2.98915
C -0.95243 -0.14696 4.06471
C 4.13244 0.50551 -0.58668
C 0.39568 -0.33137 4.10243
C 4.08000 0.21328 0.74025
C -4.33534 0.48434 0.40318
C 0.74990 0.47292 -4.29430
C -4.28686 0.40868 -0.95535
C -0.59610 0.29144 -4.35356
H -1.65299 -0.19046 4.89461
H 5.01417 0.71712 -1.18558
H 1.01354 -0.54855 4.96965
H 4.90986 0.14369 1.43875
H -5.21249 0.62435 1.02944
H 1.44862 0.54532 -5.12373
H -5.11488 0.47952 -1.65589
H -1.21394 0.19121 -5.24188
C -2.61582 0.27944 2.22894
C 2.41896 0.63283 -2.42107
C -2.42620 0.19552 -2.63650
C 2.22673 -0.20242 2.37623
C -3.69960 0.37510 3.25330
C -3.82127 1.50509 4.07289
C -4.63107 -0.65447 3.43852
C -4.82829 1.61383 5.03289
C -5.74262 0.57091 5.19244
C 3.24489 -0.46334 3.43870
C 3.55372 0.49181 4.41534
C 3.93433 -1.68166 3.48921
C 4.50945 0.25139 5.40346
C 4.89218 -1.94539 4.46921
C 5.17955 -0.97327 5.42925
C 3.49946 0.88280 -3.42158
C 4.42747 -0.10702 -3.77025
C 3.61229 2.12323 -4.06356
C 5.42891 0.12204 -4.71475
C 4.60621 2.37577 -5.00988
C 5.51708 1.36924 -5.33606
C -3.44420 0.11813 -3.72753
C -4.19258 -1.04806 -3.93478
C -3.69840 1.20189 -4.57863
C -5.14935 -1.14204 -4.94598
C -4.65146 1.13234 -5.59558
C -5.37776 -0.04567 -5.77970
F -4.87268 2.17893 -6.38599
F -3.02389 2.34166 -4.42631
F 4.69124 3.56515 -5.59969
F 6.46608 1.59788 -6.23550
F 2.75434 3.10166 -3.77400
F 6.29410 -0.83869 -5.02840
F 4.36556 -1.31010 -3.19845
F 4.78608 1.17907 6.31599
F 6.08930 -1.21309 6.36570
F 5.52825 -3.11356 4.49570
F 3.67927 -2.62785 2.58509
F 2.93112 1.67080 4.41354
F -4.56278 -1.76056 2.69359
F -2.96241 2.51613 3.94327
F -4.92359 2.70211 5.79170
F -6.70377 0.66311 6.10309
F -6.28527 -0.12258 -6.74506
F -5.83908 -2.26564 -5.12167
F -3.99725 -2.11394 -3.15505
C -5.64438 -0.57013 4.39390
F -6.51172 -1.56648 4.54923
Cl -0.18660 2.48669 0.10420
O -0.08473 -1.51651 -0.24692
C -2.03019 -5.13378 -1.01296
H -2.53289 -5.57214 -1.88176
C -2.45343 -3.92718 -0.53835
H -3.25153 -3.39616 -1.06589
C -1.86053 -3.29338 0.63916
H -2.58326 -2.69686 1.21909
C -0.96866 -4.19586 1.48703
H -0.34922 -3.58699 2.16430
H -1.60729 -4.82889 2.13272
C -0.08536 -5.08045 0.59932
H 0.59385 -4.42993 0.02141
H 0.55025 -5.73738 1.21349
C -0.92645 -5.91917 -0.37296
H -1.38256 -6.78318 0.15326
H -0.29334 -6.37317 -1.15546
H -1.14643 -2.42131 0.20599

^{4}IM$_H$

Fe 0.11214 0.27161 0.04910
N 0.03564 0.21839 2.06739
N 2.11662 0.29882 0.11804
N -1.90023 0.27358 -0.01991
N 0.18169 0.38174 -1.96508
C -1.09113 0.22731 2.84858
C 2.97639 0.50487 -0.93377
C 1.09608 0.01992 2.91507
C 2.89729 0.20216 1.24439
C -2.75981 0.40702 1.04642
C 1.30792 0.46108 -2.74271
C -2.68062 0.28958 -1.15166
C -0.87749 0.24665 -2.82814
C -0.73173 0.02279 4.23284
C 4.33436 0.57051 -0.45144
C 0.62038 -0.12181 4.27167
C 4.28714 0.36550 0.89358
C -4.11463 0.52926 0.56969
C 0.95032 0.36498 -4.13939
C -4.06736 0.44082 -0.78863
C -0.40054 0.21545 -4.19123
H -1.43123 -0.02896 5.06313
H 5.21223 0.75191 -1.06575
H 1.24428 -0.31023 5.14124
H 5.11838 0.35072 1.59366
H -4.99189 0.66946 1.19566
H 1.65057 0.38304 -4.97046
H -4.89735 0.49807 -1.48802
H -1.02318 0.09120 -5.07322
C -2.40834 0.37611 2.40029
C 2.62495 0.58129 -2.28578
C -2.23010 0.21063 -2.47454
C 2.44821 0.01177 2.55625
C -3.49573 0.46045 3.42102
C -3.65002 1.59969 4.22211
C -4.39966 -0.59074 3.62184
C -4.66056 1.69624 5.17978
C -5.54730 0.63214 5.35413
C 3.47037 -0.17455 3.63009
C 3.73221 0.82263 4.57855
C 4.21162 -1.35977 3.72376
C 4.68763 0.65300 5.58146
C 5.17154 -1.55246 4.71821
C 5.40877 -0.54047 5.65022
C 3.70890 0.75992 -3.29825
C 4.61894 -0.26401 -3.59167
C 3.84922 1.96371 -4.00139
C 5.62885 -0.10275 -4.54112
C 4.85158 2.14840 -4.95465
C 5.74407 1.10928 -5.22434
C -3.25020 0.13022 -3.56355
C -3.99922 -1.03465 -3.77521
C -3.49718 1.21324 -4.41778
C -4.95218 -1.12652 -4.79038
C -4.44526 1.14578 -5.43950
C -5.17384 -0.03039 -5.62613
F -4.65888 2.19195 -6.23274
F -2.81734 2.34991 -4.26509
F 4.96263 3.30459 -5.60354
F 6.70137 1.27324 -6.12941
F 3.01031 2.97286 -3.76587
F 6.47721 -1.09436 -4.80036
F 4.53255 -1.43421 -2.95804
F 4.91674 1.61910 6.46707
F 6.31966 -0.71231 6.60060
F 5.85642 -2.69117 4.78513
F 4.00652 -2.34345 2.84731
F 3.06145 1.97432 4.53653
F -4.30100 -1.70601 2.89374
F -2.81804 2.63123 4.07816
F -4.78598 2.79329 5.92157
F -6.51222 0.71294 6.26201
F -6.07716 -0.10568 -6.59571
F -5.64408 -2.24853 -4.96841
F -3.81101 -2.10157 -2.99436
C -5.41678 -0.51854 4.57422
F -6.25793 -1.53492 4.74379
Cl 0.07892 2.54152 0.14631
O 0.14708 -1.50324 -0.00810
C -1.91373 -4.46547 -1.37150
H -2.33427 -4.40166 -2.37893
C -2.44724 -3.67886 -0.35124
H -3.27107 -2.99867 -0.58824
C -1.98121 -3.74588 0.96237
H -2.47514 -3.16274 1.74466
C -0.86810 -4.68392 1.33707
H -0.26762 -4.25749 2.15848
H -1.30554 -5.61718 1.74966
C 0.02878 -5.01688 0.13372
H 0.61969 -4.11924 -0.11626
H 0.74526 -5.81069 0.39800
C -0.79075 -5.42631 -1.10111
H -1.21044 -6.44349 -0.95258
H -0.13748 -5.51160 -1.98642
H -0.72695 -1.90158 0.17833

^{4}TS$_{Ep}$

Fe -0.11783 0.04923 0.09416
N -0.09286 0.05666 2.12890
N 1.91795 0.01789 0.08912
N -2.10925 0.21280 0.11588
N -0.12127 0.14731 -1.90203
C -1.17508 -0.07691 2.95139
C 2.72426 -0.06728 -1.00644
C 1.01047 0.07977 2.93890
C 2.74725 0.13208 1.17437
C -2.92703 0.12933 1.21766
C 0.95609 -0.05509 -2.73594

C -2.93173 0.45140 -0.95498
C -1.21046 0.31061 -2.71681
C -0.74601 -0.16527 4.32987
C 4.11469 0.00995 -0.61258
C 0.61042 -0.04915 4.32336
C 4.12788 0.15156 0.74080
C -4.30462 0.33462 0.82748
C 0.51865 -0.05651 -4.11434
C -4.30494 0.55739 -0.51389
C -0.81793 0.19252 -4.10394
H -1.39769 -0.29499 5.18983
H 4.96620 -0.01259 -1.28783
H 1.28335 -0.07126 5.17665
H 4.99330 0.26314 1.38881
H -5.15675 0.33813 1.50229
H 1.15592 -0.22235 -4.97886
H -5.15806 0.77258 -1.15185
H -1.48764 0.26479 -4.95705
C -2.51820 -0.06922 2.54066
C 2.29198 -0.16911 -2.34091
C -2.53085 0.51555 -2.29514
C 2.34618 0.16032 2.51651
C -3.57803 -0.25289 3.57806
C -3.88818 0.74595 4.50917
C -4.30640 -1.44734 3.65049
C -4.87962 0.56933 5.47546
C -5.58722 -0.63321 5.52397
C 3.40744 0.22603 3.56677
C 3.60539 1.38527 4.32764
C 4.24057 -0.86741 3.83508
C 4.59391 1.46196 5.30985
C 5.23421 -0.81562 4.81324
C 5.41008 0.35559 5.55268
C 3.33352 -0.36917 -3.39354
C 4.00736 -1.59167 -3.51270
C 3.69005 0.64804 -4.28823
C 4.98891 -1.80353 -4.48137
C 4.67010 0.46090 -5.26417
C 5.32184 -0.77006 -5.35902
C -3.56878 0.76751 -3.34007
C -4.51999 -0.20077 -3.68576
C -3.62000 1.98948 -4.02344
C -5.48541 0.03132 -4.66645
C -4.57669 2.24497 -5.00676
C -5.51241 1.26016 -5.32851
F -4.60346 3.41732 -5.63554
F -2.73809 2.94801 -3.73856
F 4.98942 1.44687 -6.09835
F 6.25598 -0.95819 -6.28334
F 3.08995 1.83680 -4.22032
F 5.60717 -2.97802 -4.57261
F 3.71383 -2.59798 -2.68569
F 4.76309 2.57874 6.01269
F 6.35256 0.41684 6.48562
F 6.00904 -1.87149 5.04697
F 4.09566 -2.00302 3.14719
F 2.83918 2.45614 4.11934
F -4.05515 -2.43451 2.78789
F -3.23086 1.90592 4.48549
F -5.15554 1.53741 6.34540
F -6.53228 -0.81142 6.43931
F -6.42670 1.49191 -6.26295
F -6.37445 -0.90929 -4.97557
F -4.51715 -1.38586 -3.07388
C -5.30066 -1.64790 4.60874
F -5.97280 -2.79514 4.65662
Cl 0.07401 2.38119 0.22472
O -0.18393 -1.63057 0.07144
C 0.33237 -3.36384 1.46203
H 0.26857 -2.72119 2.34276
C 1.55470 -3.52096 0.84127
H 2.40003 -2.91737 1.18351
C 1.76005 -4.43900 -0.31462
H 1.85132 -3.80504 -1.22120
H 2.74633 -4.92779 -0.22602
C 0.63266 -5.46877 -0.48579
H 0.69960 -5.93081 -1.48312
H 0.77458 -6.28277 0.24710
C -0.74726 -4.83471 -0.27371
H -0.91222 -4.04707 -1.02805
H -1.54181 -5.58513 -0.40965
C -0.85404 -4.20463 1.11961
H -0.92498 -4.99489 1.89557
H -1.77209 -3.60666 1.23499

^{4}**PC**$_{Ep}$

Fe 0.10325 0.48753 0.00282
N 0.05426 0.28493 2.01627
N 2.11878 0.33348 0.05163
N -1.91142 0.33361 -0.05122
N 0.15438 0.34318 -2.01545
C -1.06375 0.19001 2.80998
C 2.97181 0.38653 -1.02574
C 1.13164 0.24016 2.86847
C 2.91719 0.38349 1.17066
C -2.76416 0.31839 1.02544
C 1.27289 0.30108 -2.81374
C -2.70953 0.38369 -1.16816
C -0.92271 0.31253 -2.86877
C -0.67959 0.05807 4.19512
C 4.33834 0.48591 -0.57400
C 0.68091 0.09225 4.23171
C 4.30416 0.48741 0.78722
C -4.13452 0.39015 0.57579
C 0.88984 0.21735 -4.20262
C -4.10045 0.43234 -0.78428
C -0.47114 0.22595 -4.23688
H -1.36343 -0.05758 5.03189
H 5.21139 0.55781 -1.21751
H 1.32377 0.00857 5.10407
H 5.14443 0.56115 1.47264
H -5.00957 0.41375 1.22004
H 1.57536 0.14874 -5.04328
H -4.94194 0.49636 -1.46932
H -1.11431 0.16519 -5.11095
C -2.39308 0.21757 2.37168
C 2.60155 0.33611 -2.37498
C -2.27191 0.35015 -2.49713
C 2.48058 0.31167 2.49891
C -3.47799 0.10650 3.39350
C -3.79185 1.16524 4.25452
C -4.22180 -1.07301 3.52781
C -4.80393 1.06175 5.21011
C -5.52870 -0.12643 5.31924
C 3.51060 0.27506 3.58051
C 3.71278 1.36159 4.44077
C 4.30591 -0.86047 3.78228
C 4.66519 1.32615 5.46039
C 5.26371 -0.91978 4.79513
C 5.44236 0.17988 5.63685
C 3.68740 0.29713 -3.40079
C 4.44595 -0.86326 -3.60013
C 3.99012 1.40838 -4.19693
C 5.46608 -0.92302 -4.55009
C 5.00747 1.37354 -5.15195
C 5.74735 0.20261 -5.32709
C -3.30135 0.31586 -3.58013
C -4.02821 -0.85134 -3.84641
C -3.57051 1.43677 -4.37467
C -4.98397 -0.90896 -4.86138
C -4.52336 1.40410 -5.39411
C -5.23197 0.22583 -5.63633
F -4.76025 2.48506 -6.13276
F -2.90510 2.57357 -4.16855
F 5.27682 2.44584 -5.89208
F 6.71716 0.15885 -6.23283
F 3.29867 2.53907 -4.05210
F 6.16843 -2.04018 -4.72048
F 4.19737 -1.95305 -2.87077
F 4.83738 2.37453 6.26126
F 6.35054 0.13539 6.60425
F 6.00142 -2.01381 4.96601
F 4.15404 -1.92793 2.99544
F 2.98245 2.46799 4.29854
F -3.96559 -2.11605 2.73533
F -3.11518 2.31139 4.17444
F -5.08263 2.08535 6.01314
F -6.49409 -0.23507 6.22432
F -6.13969 0.18363 -6.60439
F -5.65655 -2.03295 -5.09513
F -3.81007 -1.95101 -3.12190
C -5.23725 -1.20063 4.47619
F -5.92520 -2.33456 4.58298
Cl 0.10283 2.83417 0.03419
O -0.00413 -1.89206 0.01262
C 0.80095 -2.90669 0.64312
H 1.76700 -2.53599 1.00897
C 0.57363 -2.92761 -0.81666
H 1.38024 -2.55674 -1.46073
C -0.42151 -3.88184 -1.45261
H -1.26192 -3.27960 -1.83976
H 0.04996 -4.35027 -2.33138
C -0.93285 -4.96378 -0.48550
H -1.83648 -5.43411 -0.90505
H -0.17516 -5.76407 -0.40557
C -1.21415 -4.41791 0.91923
H -1.98335 -3.62830 0.87300
H -1.62220 -5.21452 1.56147
C 0.06300 -3.85540 1.55818
H 0.75833 -4.67765 1.80555
H -0.16135 -3.34158 2.50840