

Supporting Information

A Six-Coordinate High-Spin Fe^{IV}=O Species of Cucurbit[5]uril: A Highly Potent Catalyst for C-H Hydroxylation of Methane, If synthesised

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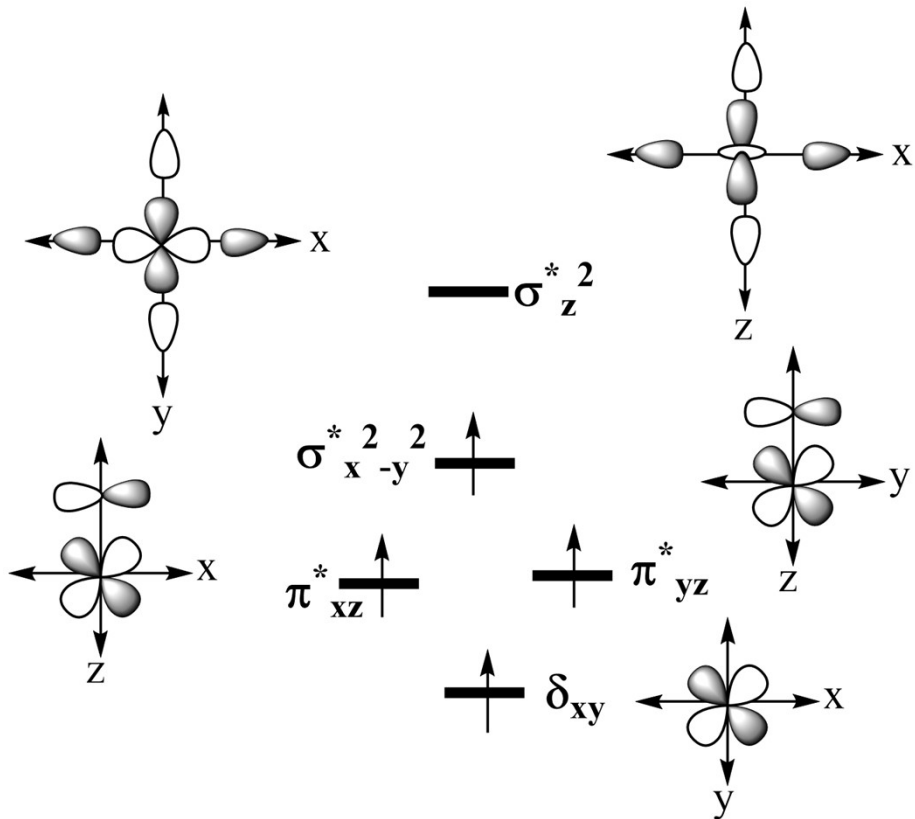
Computational details

In the present work, all the calculations were performed using established procedures.^[1] Geometry optimization is carried out with Gaussian 09 Revision D.01,^[2] whereas all spectroscopic parameters are calculated with the ORCA 4.0.1 program package incorporating COSMO solvation effects.^[3] The geometries were optimized by using the Grimme's dispersion corrected unrestricted B3LYP functional (UB3LYP-D3).^[4] We were carried out optimizations and frequency calculations with LANL2DZ ECP encompasses a double ζ -quality basis set with the Los Alamos effective core potential for Fe and a 6-31G* basis set for C, H, O;^[5] then perform single-point energy calculations using a TZVP basis set for C, H, O, Fe.^[6] Frequency calculations were performed on the optimized structures to verify that they are minima on the potential-energy surface (PES) and also to obtain free energy corrections. The quoted DFT energies are UB3LYP-D3 solvation including free-energy corrections with TZVP basis set at the temperature of 298.15 K, unless otherwise mentioned. The optimized geometries were verified by animating frequency by using Chemcraft software.^[7] The solvation energies were computed at the UB3LYP-D3 level by using polarisable continuum model (PCM) with acetonitrile as a solvent.^[8] In short, the DFT calculations were performed at B3LYP-D3/TZVP(PCM)//B3LYP-D3/LACVP* level. We have also performed calculations using water as solvent (see Table S5) and found the energies being similar to MeCN. All spectroscopic parameter calculations incorporate a relativistic effect via a zeroth-order regular approximation method (ZORA) as implemented in ORCA suite.^[3, 9] The Mössbauer isomer shift (δ) were calculated based on the calibration constants reported by Römelt et al. and 0.16 barn was used for the calculation of quadrupole moment of ^{57}Fe nuclei.^[10] We have performed the state average complete active space self-consistent field (SA-CASSCF) calculations incorporating the required excited states. We employed the def2-TZVP basis set during the zero field splitting (ZFS) calculations. The active space for CASSCF calculations comprises five Fe^{IV} -based orbitals with four electrons in them (d^4 system; CAS(4,5) setup). We considered five quintet excited states, thirty five triplet excited states and twenty two singlet excited states in our calculations. The zero-field splitting are then extracted using effective Hamiltonian approach implemented in ORCA program.^[11] Further Domain localised pair natural orbital CCSD(T) method, termed DLPNO-CCSD(T) was used to estimate accurate energies employing cc-pvTZ and No Frozen core and TIGHTPNO approximations with the optimized coordinates from DFT calculation using ORCA program.^[1d, 3, 12]

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(a)

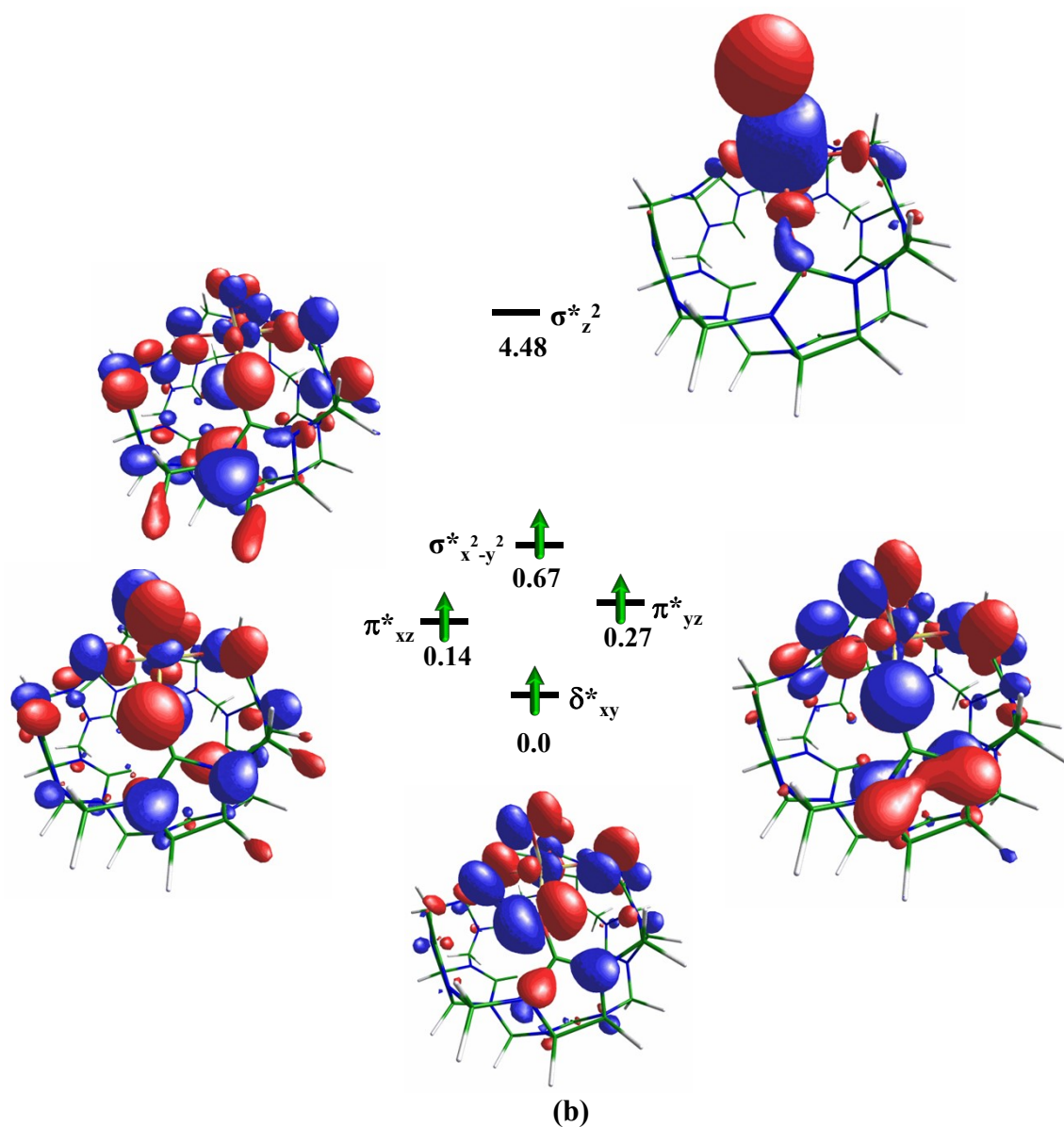


Figure S1. (a) Qualitative MO diagram for high-spin iron(IV)-oxo species and (b) Electronic structure and molecular orbitals of ground state (S=1) of the species **1** (in eV). The contour value used here is 0.03 a.u.

Table S1. Reported Fe-O bond distance in Fe^{IV}=O and Fe^V=O moieties (in Å).

Species	Fe-O	reference
CPO-I	1.65 (exp.)	<i>Proc. Natl. Acad. Sci. U.S.A</i> 2005 , 102 (46), 16563-16565.
TauD-J	1.62 (exp.)	<i>Inorg. Chem.</i> 2005 , 44 (4), 742-757.
[(H ₂ O) ₅ Fe ^{IV} =O] ²⁺	1.62 (DFT)	<i>Angew. Chem. Int. Ed.</i> 2005 , 44, 6871–6874
[(TMG ₃ tren)Fe ^{IV} =O] ²⁺	1.648 (DFT) and 1.65 (exp.)	<i>Angew. Chem. Int. Ed.</i> 2009 , 48, 3622–3626; <i>J. Am. Chem. Soc.</i> 2010 , 132, 8635–8644
[(H ₃ buea)Fe ^{IV} =O] ⁻	1.68 (exp.)	<i>J. Am. Chem. Soc.</i> 2010 , 132, 12188–12190
[(Me ₄ cy)Fe ^{IV} =O(CH ₃ CN)] ²⁺	1.64 (DFT) and 1.646 (exp.)	<i>Science</i> 2003 , 299, 1037–1039
[(Me ₄ cyS)Fe ^{IV} =O] ⁺	1.68 (DFT) and 1.70 (exp.)	<i>Science</i> 2005 , 310, 1000–1002
[(TAML)Fe ^V =O] ⁻	1.60 (DFT) and 1.58 (exp.)	<i>Science</i> 2007 , 315, 835–838

$[(CB5)Fe^{IV}=O(H_2O)]^{2+}(1)$	1.60 (DFT)	This Work
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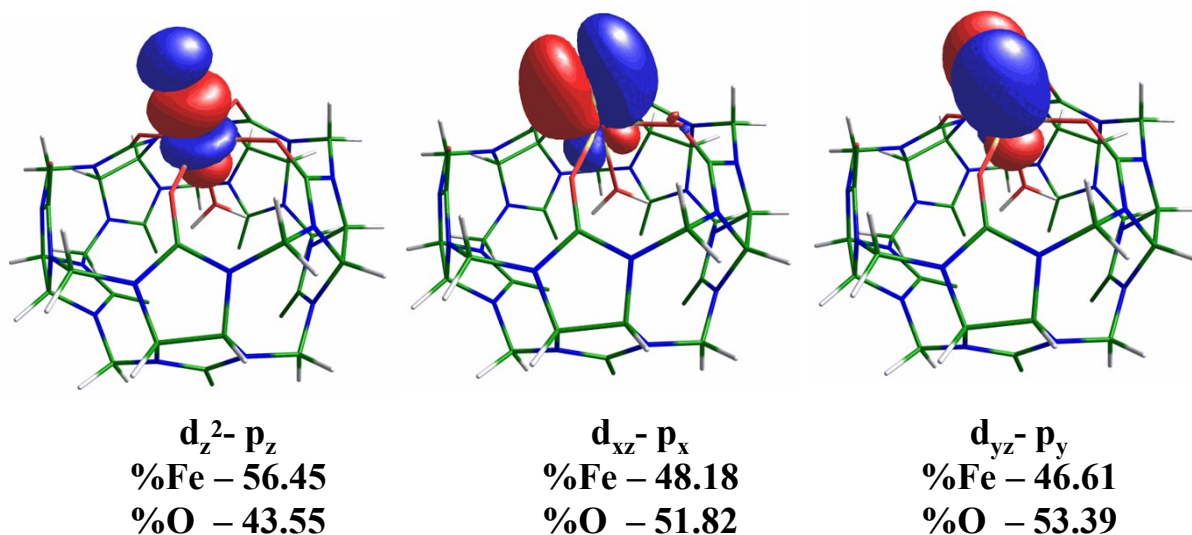


Figure S2. NBO diagram for selective bonds for the ground state of **1** showing σ -bonding and π -bonding interaction between Fe^{IV} and O atoms of $Fe^{IV}=O$ moiety. The contour value used here is 0.03 a.u.

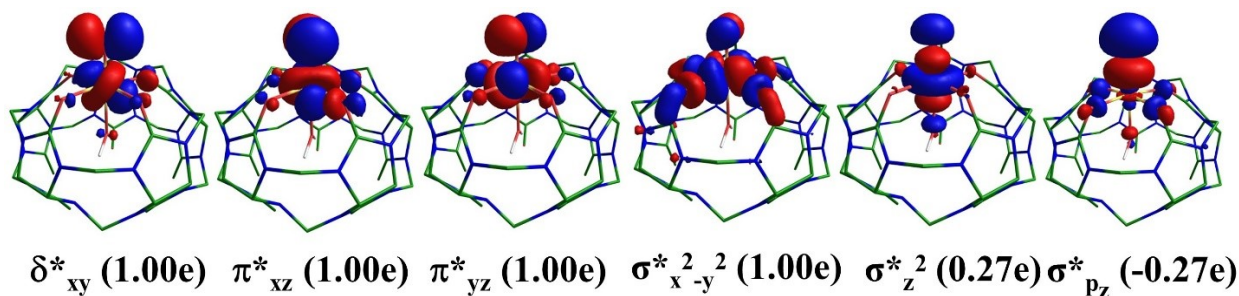
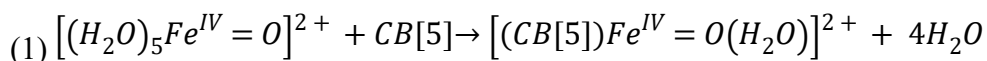
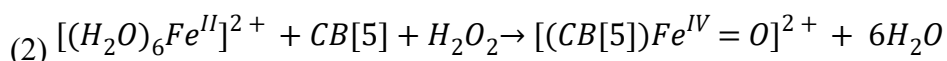


Figure S3. Spin natural orbitals (SNOs) and their occupations in species **1**. Here, negative sign in the occupation number signifies the β spin electrons and others are α spin electrons. The contour value used here is 0.03 a.u.

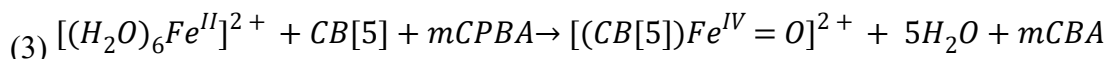
Thermodynamic Analysis of formation of $[(CB)Fe^{IV}(=O)(H_2O)]^{2+}$ (**1**)



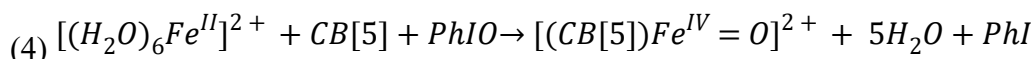
$$\Delta G = -71.8 \text{ kJ/mol}$$



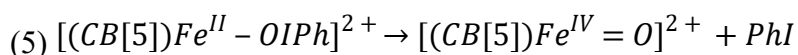
$$\Delta G = -73.6 \text{ kJ/mol}$$



$$\Delta G = -70.4 \text{ kJ/mol}$$



$$\Delta G = -134.9 \text{ kJ/mol}$$



$$\Delta G = -30.8 \text{ kJ/mol}$$

Table S2: Previous reports on C-H activation of DHA, methane and ethane by Fe^{IV}=O

Complex	Substrate	ΔG^\ddagger (kJ/mol)	Reference
$[(TMC)Fe^{IV}=O(CH_3CN)]^{2+}$	DHA	70.6	Siegbahn & Coworkers, <i>J. Phys. Chem. C</i> 2007 , <i>111</i> , 12397-12406.
$[(TMC)Fe^{IV}=O(CF_3CO_2)]^+$		60.6	
$[(H_3buea)Fe^{IV}=O]^-$		109.1	Borovik, Shaik & Coworkers, <i>J. Am. Chem. Soc.</i> 2013 , <i>135</i> , 17090–17104.
$[(H1^{cyp})Fe^{IV}=O]^-$		88.2	
$[(N4Py)Fe^{IV}=O]^{2+}$		36.8	
Cpd-I of HRP		59.4	Eldik & Coworkers, <i>Chem. Eur. J.</i> 2014 , <i>20</i> , 14437 – 14450.
Cpd-II of HRP		68.6	
$[(TMC)Fe^{IV}=O(CH_3CN)]^{2+}$		108.3	Shaik & Coworker, <i>J. Am. Chem. Soc.</i>

$[(\text{TMC})\text{Fe}^{\text{IV}}=\text{O}(\text{CH}_2\text{S})]^+$		110.4	2015 , 137, 722–733.
$[(\text{TMC})\text{Fe}^{\text{IV}}=\text{O}(\text{N}_3)]^+$		106.2	
Cpd I		38.9	Visser & Coworker <i>Chem. Eur. J.</i> 2015 , 21, 9083-9092.
$[(\text{Bn-TPEN})\text{Fe}^{\text{IV}}=\text{O}]^{2+}$		60.2	Shaik & Coworker, <i>J. Am. Chem. Soc.</i> 2016 , 138, 2094–2097.
$[(\text{TMG3tren})\text{Fe}^{\text{IV}}=\text{O}]^{2+}$		60.2	Que, Cramer & Coworker <i>Chem. Commun.</i> , 2016 , 52, 10509—10512.
$[\text{TMG}_2\text{dien}(\text{MeCN})\text{Fe}^{\text{IV}}=\text{O}]^{2+}$		45.6	
$[(6\text{-PhTPA})\text{Fe}^{\text{IV}}=\text{O}]^{2+}$		58.3	Rajraman & Coworker <i>Chem. Commun.</i> 2017 , 53, 3193-3196.
$[(\text{TPFPP})\text{Fe}^{\text{IV}}=(\text{O})]^{2+}$		73.6	Shaik & Coworker, <i>J. Am. Chem. Soc.</i> 2017 , 139, 11451- 11459.
$[(\text{TMP})\text{Fe}^{\text{IV}}=(\text{O})]^{2+}$		84.9	
$[(\text{CB5})\text{Fe}^{\text{IV}}=\text{O}(\text{H}_2\text{O})]^{2+}$		2.2	This work
Cpd I	Ethane	88.3	Yoshizawa & Coworkers, <i>J. Phys. Chem. B</i> 2000 , 104, 12365-12370.
$\text{Fe}_{0.1}\text{Mg}_{1.9}(\text{dobdc})\text{Fe}^{\text{IV}}=\text{O}$		58.0	Gagliardi, Truhler & Coworkers, <i>J. Am. Chem. Soc.</i> 2015 , 137,

			5770-5781.
MIL-type MOF Fe ^{IV} =O		40.0	Gagliardi & Coworkers, <i>ACS Catal.</i> 2019 , <i>9</i> , 2870-2879.
[(CB5)Fe ^{IV} =O(H ₂ O)] ²⁺		28.7	This work
Cpd I	Methane	110.8	Yoshizawa & Coworkers, <i>J. Am. Chem. Soc.</i> 2001 , <i>123</i> , 9806-9816; Shaik & Coworker, <i>J. Am. Chem. Soc.</i> 2000 , <i>122</i> , 8977-8989.
sMMO		81.6	Yoshizawa & Coworkers, <i>Dalton Trans.</i> 2013 , <i>42</i> , 1011-1023.
Fe _{0.1} Mg _{1.9} (dobdc)Fe ^{IV} =O		69	Gagliardi, Truhler & Coworkers, <i>J. Am. Chem. Soc.</i> 2015 , <i>137</i> , 5770-5781
MIL-type MOF Fe ^{IV} =O		60	Gagliardi & Coworkers, <i>ACS Catal.</i> 2019 , <i>9</i> , 2870-2879
[(CB5)Fe ^{IV} =O(H ₂ O)] ²⁺		44.0	This work

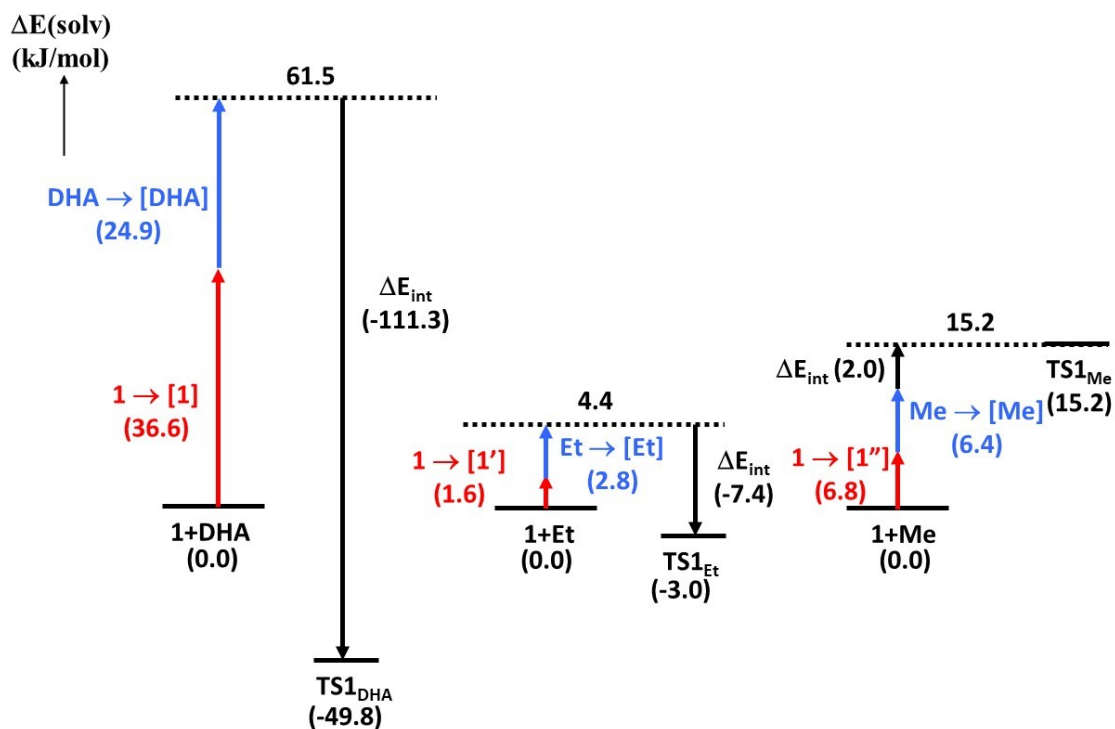


Figure S4. Fragment energy decomposition analysis of TS1_{DHA} , TS1_{Et} and TS1_{Me} .

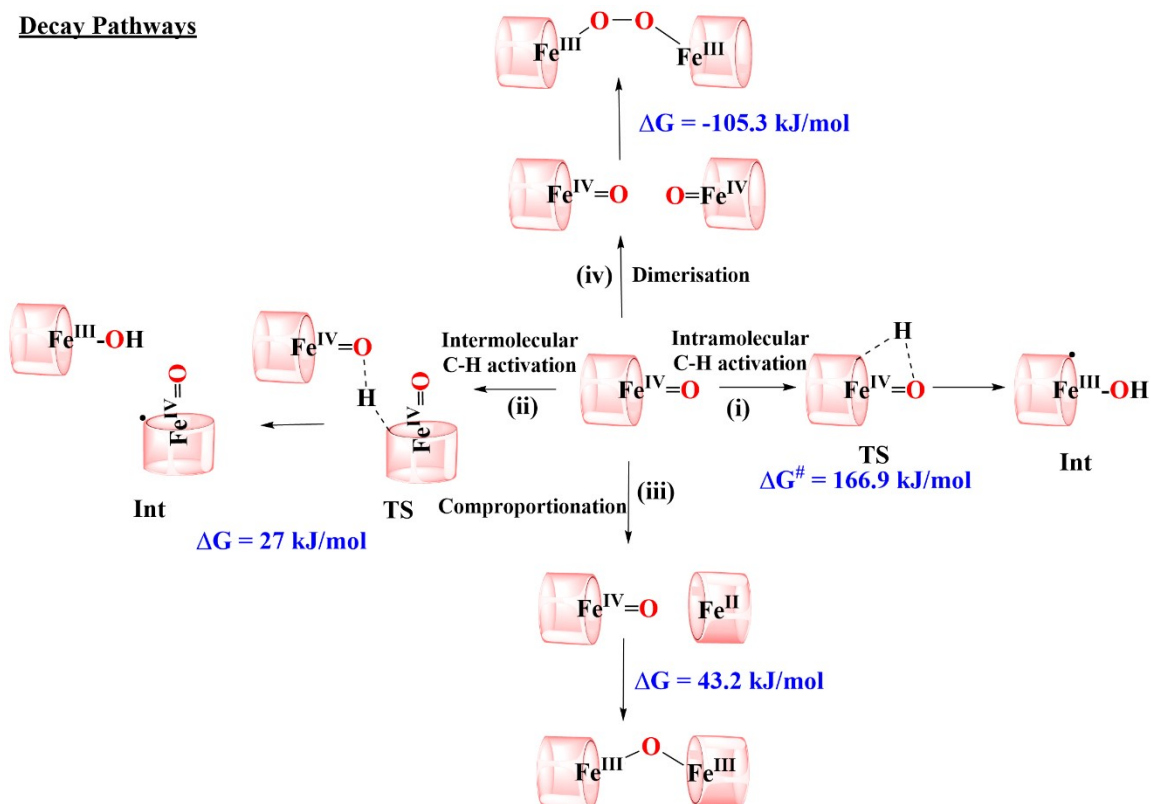


Figure S5. Various possible decay pathways. Here, ΔG is Gibbs free energy and ΔG^\ddagger is activation barrier. These are not the exhausted decomposition pathways but the most important pathways discussed in other papers.

Table S3. B3LYP-D3 computed structural parameters; bond lengths (Å) and bond angles (°).

Spin states	Fe-O	Fe-OH ₂	Fe-O1	Fe-O2	Fe-O3	Fe-O4	O-H _{ts}	H _{ts} -C	O-C _{ts}	O-Fe-OH ₂	O1-Fe-O3	O2-Fe-O4	Fe-O-H	O-H-C	Fe-O-C
⁵ I	1.600	2.205	2.051	2.125	2.069	2.065	-	-	-	177.4	167.3	166.9	-	-	-
³ I	1.609	2.188	2.026	1.967	1.993	2.043	-	-	-	175.2	174.6	174.8	-	-	-
⁵ TS1 _{DHA}	1.696	2.442	2.141	2.135	2.201	2.182	1.841 (1.856)	1.145 (1.140)	-	174.2	161.6	160.6	115.8 (131.7)	149.8 (148.7)	-
³ TS1 _{DHA}	1.610	2.200	2.176	2.198	2.151	2.263	2.005 (2.021)	1.131 (1.124)	-	174.0	168.0	165.7	108.4 (116.5)	138.0 (137.7)	-
⁵ P _{DHA}	2.093	2.286	2.163	2.108	2.263	2.098	0.981 (0.977)	4.301 (3.874)	-	161.5	163.0	163.6	105.6 (120.6)	109.5 (131.4)	-
³ P _{DHA}	1.964	2.089	2.132	2.111	2.315	2.041	0.980 (0.980)	4.030 (3.800)	-	173.7	161.6	163.1	107.9 (115.1)	120.7 (133.4)	-
⁵ TS1 _{Et}	1.632	2.285	2.092	2.077	2.122	2.068	1.753	1.126	-	177.0	165.7	166.5	159.7	149.9	-
³ TS1 _{Et}	1.694	2.188	2.121	1.986	2.038	2.051	1.246	1.299	-	174.5	171.2	175.0	116.4	172.0	-
⁵ P _{Et}	2.072	2.272	2.123	2.131	2.285	2.108	0.970	-	1.469	175.8	162.6	162.9	112.9	-	125.2
³ P _{Et}	1.957	2.103	2.143	2.086	2.343	2.065	0.973	-	1.477	176.3	162.8	163.0	106.4	-	123.1
⁵ TS1 _{Me}	1.658	2.317	2.104	2.070	2.119	2.092	1.569	1.114	-	175.7	165.5	165.5	150.1	163.6	-
³ TS1 _{Me}	1.767	2.221	2.090	2.080	2.186	2.073	1.249	1.290	-	178.8	165.5	166.6	119.2	176.2	-
⁵ Int1 _{Me}	1.762	2.392	2.110	2.077	2.140	2.125	1.002	1.874	-	175.0	162.7	163.0	129.0	170.6	-
³ Int1 _{Me}	1.753	2.179	2.085	2.103	2.159	2.050	0.998	2.017	-	178.9	166.0	166.9	111.8	163.5	-
⁵ P _{Me}	2.087	2.282	2.147	2.099	2.246	2.134	0.982	-	1.443	159.8	163.9	162.9	104.0	-	122.3

³ P _{Me}	1.994	2.135	2.096	2.163	2.247	2.113	0.983	-	1.447	168.2	162.3	161.0	103.4	-	120.2
	Fe-O	Fe-X	Fe-O1	Fe-O2	Fe-O3	Fe-O4	O-H_{ts}	H_{ts}-C	O-C_{ts}	O-Fe-X	O1-Fe-O3	O2-Fe-O4	Fe-O-H	O-H-C	Fe-O-C
⁵ 1a	1.639	2.412	2.151	2.174	2.152	2.170	-	-	-	176.7	162.5	162.7	-	-	-
³ 1a	1.736	2.362	2.133	2.206	2.166	2.168	-	-	-	178.2	161.3	161.6	-	-	-
⁵ 1b	1.621	2.339	2.139	2.149	2.148	2.141	-	-	-	176.6	164.0	164.0	-	-	-
³ 1b	1.628	2.354	2.130	1.992	1.992	2.131	-	-	-	173.8	172.5	172.5	-	-	-
⁵ 1c	1.628	2.027	2.155	2.144	2.145	2.155	-	-	-	170.1	174.4	170.1	-	-	-
³ 1c	1.639	2.025	2.165	1.994	1.994	2.165	-	-	-	172.3	172.7	172.7	-	-	-
⁵ 1d	1.636	1.875	2.174	2.126	2.127	2.172	-	-	-	179.3	169.0	169.0	-	-	-
³ 1d	1.675	1.804	2.247	2.165	2.166	2.247	-	-	-	178.4	169.1	169.1	-	-	-
⁵ 1e	1.630	1.979	2.146	2.148	2.121	2.192	-	-	-	177.9	169.2	167.2	-	-	-
³ 1e	1.677	1.924	2.159	2.193	2.138	2.279	-	-	-	178.4	169.9	166.6	-	-	-

Table S4. B3LYP-D3 computed spin densities.

Species	Fe	O	O1	O2	O3	O4	OH ₂	C _{ts}
⁵ 1	3.146	0.608	0.050	0.038	0.044	0.050	0.000	-
³ 1	1.061	0.986	-0.007	-0.012	-0.010	-0.006	-0.002	-
⁵ TS1 _{DHA}	3.977	0.544	0.028	0.027	0.022	0.026	0.003	-0.700
³ TS1 _{DHA}	2.675	0.063	0.005	0.003	0.003	0.003	-0.002	-0.792
⁵ P _{DHA}	3.827	0.032	0.013	0.019	0.006	0.020	0.010	0.000
³ P _{DHA}	1.941	-0.022	0.014	0.009	0.005	0.013	-0.011	0.000
⁵ TS1 _{Et}	3.483	0.354	0.049	0.045	0.038	0.049	0.004	-0.091
³ TS1 _{Et}	2.818	-0.389	0.015	0.021	0.026	0.020	-0.003	-0.569
⁵ P _{Et}	3.824	0.034	0.017	0.015	0.006	0.021	0.011	0.000
³ P _{Et}	1.951	-0.026	0.014	0.010	0.005	0.012	-0.010	-0.002
⁵ TS1 _{Me}	3.704	0.195	0.049	0.047	0.039	0.049	0.007	-0.162
³ TS1 _{Me}	0.859	0.668	-0.012	-0.005	-0.001	-0.003	-0.001	0.510
⁵ Int1 _{Me}	4.190	0.446	0.047	0.052	0.039	0.048	0.010	-0.976
³ Int1 _{Me}	2.906	-0.111	0.041	0.020	0.030	0.021	-0.001	-1.044
⁵ P _{Me}	3.821	0.036	0.014	0.020	0.006	0.018	0.010	0.000
³ P _{Me}	1.945	-0.025	-0.010	0.014	0.009	0.006	0.011	0.000
	Fe	O	O1	O2	O3	O4	X	C _{ts}
⁵ 1a	3.205	0.787	0.019	0.019	0.020	0.018	-0.121	-
³ 1a	0.973	1.080	-0.009	-0.011	-0.012	-0.010	0.003	-
⁵ 1b	3.154	0.680	0.029	0.029	0.029	0.029	0.002	-
³ 1b	1.096	0.955	-0.007	-0.017	-0.017	-0.007	0.015	-
⁵ 1c	3.081	0.809	0.026	0.028	0.028	0.026	-0.095	-
³ 1c	1.041	1.029	-0.004	-0.017	-0.017	-0.004	-0.065	-
⁵ 1d	3.134	0.699	0.021	0.028	0.028	0.021	0.020	-

³ I _d	2.664	-0.769	-0.002	0.001	0.001	-0.002	0.070	-
⁵ I _e	3.150	0.723	0.024	0.030	0.027	0.023	-0.028	-
³ I _e	1.024	0.989	-0.006	-0.018	-0.013	0.001	0.013	-

Table S4. The comparative Gibbs free energies (ΔG , kJ/mol) of acetonitrile and water as a solvent.

Species	ΔG (Acetonitrile) (kJ/mol)	ΔG (Water) (kJ/mol)
⁵ I	0.0	0.0
³ I	87.2	87.5
⁵ TSI _{DHA}	2.2	2.4
⁵ P _{DHA}	-359.7	-357.3
⁵ TSI _{Et}	28.7	29.3
⁵ P _{Et}	-281.0	-279.8
⁵ TSI _{Me}	44.0	44.5
⁵ IntI _{Me}	-11.5	-10.8
⁵ P _{Me}	-257.3	-256.1

Optimized geometries Cartesian coordinates:

⁵R

```

Fe  0.050769000  -0.435628000  -2.481890000
C   -0.053044000  3.694717000  -1.791948000
N    1.053578000  4.004242000  -1.006502000
C    0.705105000  4.336912000  0.366928000
C   -0.869133000  4.307845000  0.353037000
N   -1.182108000  3.966653000  -1.026594000
N   -1.190750000  3.255272000  1.286539000
C   -0.060626000  2.518157000  1.622226000
N    1.047335000  3.299062000  1.309334000
C    2.304014000  3.234234000  2.042375000
N    3.219094000  2.225961000  1.575595000
C    3.398413000  1.048785000  2.299027000
N    4.109722000  0.170789000  1.468378000
C    4.309266000  0.712224000  0.151349000
C    3.787493000  2.185688000  0.256179000

```

N	2.805963000	2.283845000	-0.827451000
C	2.539511000	1.063850000	-1.359821000
N	3.434976000	0.147409000	-0.878115000
C	4.271947000	-1.216445000	1.842964000
N	3.207829000	-2.112563000	1.380542000
C	2.019619000	-2.244075000	2.090966000
N	1.158708000	-3.079278000	1.316141000
C	1.934864000	-3.787750000	0.305756000
C	3.243844000	-2.931200000	0.200727000
N	1.350400000	-3.684327000	-1.025214000
C	1.883354000	-2.611005000	-1.683669000
N	3.022701000	-2.224912000	-1.068304000
C	0.040321000	-3.735946000	2.016258000
N	-1.248953000	-3.378436000	1.488566000
C	-2.011729000	-2.367021000	2.088582000
N	-3.151714000	-2.195860000	1.302797000
C	-3.159198000	-3.047297000	0.146189000
C	-1.843242000	-3.905902000	0.292993000
N	-2.929709000	-2.351172000	-1.129376000
C	-1.712245000	-2.614673000	-1.647501000
N	-1.098335000	-3.595197000	-0.935450000
C	-4.264740000	-1.360435000	1.755241000
N	-4.173187000	0.037936000	1.395469000
C	-3.502782000	0.936046000	2.237851000
N	-3.332643000	2.113696000	1.511108000
C	-3.877643000	2.054591000	0.181727000
C	-4.334179000	0.561477000	0.067356000
N	-2.883977000	2.192321000	-0.883076000
C	-2.529649000	0.979944000	-1.384032000
N	-3.393680000	0.021476000	-0.920101000
C	3.757006000	-1.086355000	-1.560673000
C	0.088691000	-4.278016000	-1.423293000
C	-3.670294000	-1.214787000	-1.624096000
O	1.741674000	-1.751364000	3.151437000
O	-1.734337000	-1.786126000	3.107085000
O	-3.180070000	0.748562000	3.383795000
O	1.408371000	-2.056601000	-2.694137000
O	1.636162000	0.833955000	-2.195260000
O	-1.244835000	-2.039454000	-2.655488000
O	-1.576372000	0.796977000	-2.172758000
C	-2.459211000	3.147574000	1.996806000
C	2.351547000	3.559514000	-1.415509000
C	-2.459542000	3.482272000	-1.458359000
O	3.051004000	0.843876000	3.434866000
O	-0.041857000	1.385498000	2.082972000
O	-0.034945000	3.291308000	-2.934761000
O	0.041807000	-0.188839000	-4.062254000
O	0.035260000	-0.678948000	-0.290447000
H	0.282858000	-1.478829000	0.224026000
H	-0.028152000	0.047117000	0.369449000

H	0.066685000	-3.394434000	3.054156000
H	0.172282000	-4.823715000	1.979284000
H	-5.194056000	-1.784603000	1.362409000
H	-4.280380000	-1.392499000	2.846586000
H	4.269873000	-1.242273000	2.934616000
H	5.226070000	-1.598584000	1.468384000
H	4.163883000	-3.521065000	0.143741000
H	2.111554000	-4.834273000	0.574165000
H	-2.018940000	-4.985032000	0.354161000
H	-4.074841000	-3.642812000	0.080369000
H	-5.360373000	0.437386000	-0.295164000
H	0.065451000	-5.311951000	-1.070497000
H	0.058619000	-4.267066000	-2.513938000
H	-3.412314000	-1.099634000	-2.677927000
H	-4.740213000	-1.423810000	-1.538767000
H	3.522969000	-0.987595000	-2.622019000
H	4.829095000	-1.270740000	-1.445022000
H	2.109627000	2.995128000	3.090509000
H	2.762482000	4.227291000	1.980913000
H	-2.945205000	4.127349000	1.931172000
H	-2.275530000	2.909938000	3.047250000
H	5.354552000	0.631284000	-0.165919000
H	4.564001000	2.945506000	0.117801000
H	1.130913000	5.301534000	0.658871000
H	-1.334940000	5.255434000	0.639638000
H	-4.682490000	2.781981000	0.031451000
H	3.112136000	4.301222000	-1.154521000
H	2.313174000	3.444206000	-2.500253000
H	-2.400284000	3.373937000	-2.542864000
H	-3.246548000	4.199217000	-1.207124000

³R

Fe	-0.153943000	-0.530796000	-2.415495000
C	0.868631000	3.648098000	-1.819963000
N	2.026994000	3.642221000	-1.049582000
C	1.802424000	4.048592000	0.329476000
C	0.271065000	4.414949000	0.347889000
N	-0.141000000	4.189587000	-1.028628000
N	-0.286685000	3.462562000	1.279179000
C	0.637414000	2.477764000	1.614637000
N	1.894904000	2.961126000	1.273375000
C	3.112161000	2.575668000	1.973877000
N	3.714611000	1.358959000	1.498279000
C	3.601243000	0.179874000	2.233875000
N	4.031901000	-0.857177000	1.393972000
C	4.297088000	-0.395833000	0.060152000
C	4.202274000	1.159601000	0.159327000
N	3.246434000	1.511197000	-0.889215000
C	2.592522000	0.410534000	-1.355090000

N	3.245815000	-0.717101000	-0.909796000
C	3.823901000	-2.236760000	1.769524000
N	2.566054000	-2.830556000	1.309726000
C	1.403654000	-2.741249000	2.075026000
N	0.456224000	-3.592978000	1.485289000
C	0.937999000	-4.237097000	0.296614000
C	2.407334000	-3.672841000	0.158968000
N	0.286814000	-3.776523000	-0.941386000
C	1.094631000	-2.936940000	-1.632376000
N	2.336953000	-2.948686000	-1.123536000
C	-0.883507000	-3.673333000	2.007570000
N	-1.833027000	-2.781496000	1.318043000
C	-2.488277000	-1.772202000	2.088958000
N	-3.592252000	-1.352806000	1.353399000
C	-3.807939000	-2.142628000	0.173694000
C	-2.732125000	-3.280214000	0.287280000
N	-3.418048000	-1.506360000	-1.095131000
C	-2.377486000	-2.124453000	-1.678596000
N	-2.108798000	-3.293682000	-1.033251000
C	-4.431209000	-0.237608000	1.810655000
N	-3.962080000	1.078011000	1.441108000
C	-3.071636000	1.773704000	2.273671000
N	-2.635212000	2.881867000	1.552227000
C	-3.190137000	2.965125000	0.226161000
C	-4.001636000	1.634711000	0.115619000
N	-2.203018000	2.858030000	-0.847991000
C	-2.140774000	1.588302000	-1.336957000
N	-3.230921000	0.883750000	-0.875817000
C	3.283497000	-1.975306000	-1.619710000
C	-1.022043000	-4.166402000	-1.431906000
C	-3.833075000	-0.214461000	-1.589171000
O	1.235740000	-2.086870000	3.072490000
O	-2.124399000	-1.370499000	3.160972000
O	-2.779183000	1.490577000	3.408569000
O	0.766498000	-2.255300000	-2.637205000
O	1.574393000	0.470821000	-2.078737000
O	-1.768543000	-1.670140000	-2.677104000
O	-1.240508000	1.169201000	-2.093749000
C	-1.522308000	3.666431000	2.020889000
C	3.143691000	2.857998000	-1.480563000
C	-1.502984000	4.017808000	-1.432369000
O	3.252118000	0.079584000	3.383061000
O	0.385889000	1.386473000	2.103916000
O	0.764885000	3.281642000	-2.969619000
O	-0.078394000	-0.236069000	-3.995719000
O	-0.171851000	-0.769937000	-0.240455000
H	-0.624898000	-1.453311000	0.300712000
H	0.042496000	-0.038255000	0.377473000
H	-0.842260000	-3.351637000	3.051282000
H	-1.243527000	-4.707105000	1.951755000

H	-5.443329000	-0.396022000	1.426961000
H	-4.442993000	-0.265989000	2.902140000
H	3.818890000	-2.256562000	2.861270000
H	4.647018000	-2.853403000	1.394630000
H	3.179063000	-4.446012000	0.101795000
H	0.881556000	-5.328725000	0.356732000
H	-3.148501000	-4.262685000	0.531353000
H	-4.838808000	-2.503005000	0.105591000
H	-5.030167000	1.769152000	-0.236332000
H	-1.241765000	-5.177309000	-1.080492000
H	-0.988262000	-4.162161000	-2.522631000
H	-3.555599000	-0.173372000	-2.643690000
H	-4.920260000	-0.131819000	-1.502316000
H	3.053674000	-1.817082000	-2.674367000
H	4.291987000	-2.388510000	-1.533999000
H	2.892880000	2.404545000	3.030385000
H	3.812162000	3.413745000	1.885203000
H	-1.757921000	4.735218000	1.969779000
H	-1.378987000	3.382024000	3.065921000
H	5.262372000	-0.757571000	-0.310336000
H	5.150474000	1.678740000	-0.015533000
H	2.461489000	4.876494000	0.607949000
H	0.064159000	5.444367000	0.656215000
H	-3.790588000	3.870154000	0.087268000
H	4.085213000	3.362270000	-1.243726000
H	3.049938000	2.756561000	-2.563355000
H	-1.493383000	3.906849000	-2.518193000
H	-2.098770000	4.894635000	-1.162753000

⁵TS1_{DHA}

Fe	1.198328000	-0.629699000	-1.176351000
C	1.123769000	-1.851250000	2.884894000
N	0.024469000	-2.681949000	3.035184000
C	-1.006381000	-2.124859000	3.901951000
C	-0.391411000	-0.745798000	4.341810000
N	0.918338000	-0.750443000	3.708777000
N	-1.309984000	0.222152000	3.794572000
C	-2.291026000	-0.375946000	3.004629000
N	-2.217471000	-1.749292000	3.219790000
C	-3.355311000	-2.630961000	2.994177000
N	-3.473382000	-3.131913000	1.650252000
C	-4.413502000	-2.593598000	0.770411000
N	-4.102580000	-3.091266000	-0.500848000
C	-2.905025000	-3.885735000	-0.504118000
C	-2.515846000	-3.993727000	1.010838000
N	-1.138514000	-3.511016000	1.043231000
C	-0.758792000	-2.982528000	-0.157206000

N	-1.733163000	-3.236805000	-1.089827000
C	-4.741331000	-2.548612000	-1.678038000
N	-4.037336000	-1.435535000	-2.307804000
C	-4.300543000	-0.118392000	-1.935884000
N	-3.654791000	0.705900000	-2.864923000
C	-2.929665000	-0.024779000	-3.867834000
C	-3.179689000	-1.527022000	-3.458008000
N	-1.472281000	0.106781000	-3.791881000
C	-0.888291000	-1.026983000	-3.306989000
N	-1.820799000	-2.005515000	-3.186565000
C	-3.661203000	2.135433000	-2.706216000
N	-2.464086000	2.650795000	-2.029003000
C	-2.640238000	3.338963000	-0.797144000
N	-1.477488000	4.067169000	-0.567616000
C	-0.561332000	4.012805000	-1.674184000
C	-1.356597000	3.230485000	-2.774757000
N	0.612339000	3.156287000	-1.495759000
C	0.640171000	2.114289000	-2.365842000
N	-0.398787000	2.245856000	-3.252993000
C	-1.299288000	4.841298000	0.660848000
N	-0.769619000	4.100635000	1.784385000
C	-1.640071000	3.422107000	2.651309000
N	-0.850722000	2.589156000	3.440020000
C	0.556841000	2.694197000	3.157873000
C	0.587312000	3.635877000	1.906468000
N	1.176348000	1.465579000	2.675626000
C	1.313884000	1.473320000	1.315664000
N	1.031322000	2.733182000	0.847471000
C	-1.477534000	-3.236664000	-2.516438000
C	-0.685325000	1.236719000	-4.253792000
C	1.556215000	3.219985000	-0.409845000
O	-4.980608000	0.254263000	-1.012081000
O	-3.618769000	3.286321000	-0.098764000
O	-2.834408000	3.568897000	2.731529000
O	0.317950000	-1.166073000	-3.045536000
O	0.319715000	-2.404295000	-0.361245000
O	1.484289000	1.206456000	-2.355540000
O	1.667527000	0.505788000	0.627062000
C	-1.449712000	1.586689000	4.283371000
C	-0.192718000	-3.775787000	2.130929000
C	1.727274000	0.421764000	3.543432000
O	-5.343913000	-1.883648000	1.060152000
O	-3.068666000	0.199732000	2.268145000
O	2.106294000	-2.062227000	2.198933000
O	2.766533000	-1.244251000	-1.373847000
O	-1.026918000	0.225736000	-0.649491000
H	-1.548325000	0.897291000	-1.133117000
H	-1.484284000	0.123552000	0.205318000
H	-4.519110000	2.384148000	-2.076505000
H	-3.765445000	2.617551000	-3.685755000

H	-0.649487000	5.692837000	0.436913000
H	-2.283891000	5.199621000	0.968173000
H	-5.717554000	-2.183130000	-1.352468000
H	-4.873872000	-3.338565000	-2.424769000
H	-3.631437000	-2.132177000	-4.250973000
H	-3.269681000	0.221073000	-4.879925000
H	-1.705055000	3.862361000	-3.599215000
H	-0.247200000	5.016325000	-1.980645000
H	1.289675000	4.472118000	1.999552000
H	-1.213302000	1.713246000	-5.084230000
H	0.274104000	0.853222000	-4.604377000
H	2.419716000	2.619645000	-0.696974000
H	1.879160000	4.255985000	-0.267375000
H	-0.412373000	-3.402062000	-2.687172000
H	-2.046571000	-4.057081000	-2.963923000
H	-4.279434000	-2.081580000	3.187670000
H	-3.270496000	-3.460007000	3.705847000
H	-1.012787000	1.621805000	5.288226000
H	-2.509959000	1.843796000	4.340847000
H	-3.069118000	-4.855452000	-0.988200000
H	-2.558693000	-5.014368000	1.407846000
H	-1.213384000	-2.803200000	4.736337000
H	-0.293035000	-0.632443000	5.426793000
H	1.116980000	3.078858000	4.017866000
H	-0.574423000	-4.646676000	2.673184000
H	0.779829000	-4.014977000	1.696750000
H	2.669183000	0.080812000	3.114587000
H	1.917250000	0.891590000	4.513492000
H	3.820968000	-1.248915000	0.134704000
C	4.805855000	-0.981133000	0.654230000
C	5.793431000	-1.770186000	-0.121468000
C	4.900019000	0.499332000	0.466987000
H	4.699448000	-1.298937000	1.693258000
C	6.092374000	-1.301714000	-1.443785000
C	6.362233000	-2.964734000	0.340714000
C	5.169561000	0.958814000	-0.842193000
C	4.704080000	1.423362000	1.498353000
C	5.364004000	-0.086809000	-1.897258000
C	6.959069000	-2.034522000	-2.262015000
C	7.239709000	-3.666051000	-0.472798000
H	6.126850000	-3.321811000	1.338832000
C	5.216081000	2.332097000	-1.103327000
C	4.773681000	2.790628000	1.237531000
H	4.541550000	1.067489000	2.511873000
H	5.731567000	0.311769000	-2.846582000
H	4.311348000	-0.487274000	-2.071212000
C	7.540048000	-3.199089000	-1.777659000
H	7.183789000	-1.682050000	-3.264281000
H	7.707740000	-4.576698000	-0.111768000
C	5.028630000	3.245942000	-0.066435000

H	5.431618000	2.681772000	-2.109406000
H	4.665028000	3.505071000	2.049110000
H	8.233166000	-3.758995000	-2.397993000
H	5.108068000	4.311376000	-0.263416000

Imaginary Frequency: $i340\text{ cm}^{-1}$

³TS1_{DHA}

Fe	1.129924000	-1.039336000	-0.988817000
C	0.868175000	-1.219580000	3.292145000
N	-0.323186000	-1.876922000	3.553947000
C	-1.307416000	-1.047675000	4.231869000
C	-0.569687000	0.330618000	4.376916000
N	0.737298000	0.066153000	3.800511000
N	-1.401606000	1.243922000	3.629368000
C	-2.529042000	0.620730000	3.090590000
N	-2.481259000	-0.724208000	3.459373000
C	-3.659402000	-1.570115000	3.354538000
N	-3.727930000	-2.337869000	2.133602000
C	-4.626988000	-2.010470000	1.121898000
N	-4.335049000	-2.853894000	0.034910000
C	-3.189916000	-3.686475000	0.287421000
C	-2.877923000	-3.454158000	1.804768000
N	-1.451320000	-3.163587000	1.810948000
C	-0.975659000	-2.922658000	0.553211000
N	-1.951524000	-3.253575000	-0.362361000
C	-4.864009000	-2.558767000	-1.276653000
N	-4.030389000	-1.677651000	-2.101612000
C	-4.095155000	-0.298798000	-1.960342000
N	-3.115774000	0.259681000	-2.834388000
C	-2.699048000	-0.737549000	-3.813939000
C	-3.119173000	-2.086770000	-3.137897000
N	-1.255802000	-0.847573000	-3.939765000
C	-0.778905000	-1.844389000	-3.119845000
N	-1.824122000	-2.601627000	-2.689707000
C	-3.284438000	1.668878000	-3.222152000
N	-2.171682000	2.492760000	-2.843424000
C	-2.215986000	3.247064000	-1.665623000
N	-0.973960000	3.861195000	-1.526418000
C	-0.059549000	3.496948000	-2.576001000
C	-0.910947000	2.572722000	-3.528103000
N	1.031241000	2.605385000	-2.173128000
C	0.922368000	1.362181000	-2.709759000
N	-0.145535000	1.322457000	-3.564085000
C	-0.768712000	4.918012000	-0.534807000
N	-0.347462000	4.466851000	0.772631000
C	-1.307815000	4.094820000	1.730520000
N	-0.635098000	3.361956000	2.706526000
C	0.787697000	3.292184000	2.484928000

C	0.937646000	3.885443000	1.045800000
N	1.320618000	1.947217000	2.345301000
C	1.440317000	1.584768000	1.030975000
N	1.267593000	2.704042000	0.245227000
C	-1.619922000	-3.646565000	-1.718031000
C	-0.383567000	0.194945000	-4.454183000
C	1.911152000	2.822041000	-1.050130000
O	-4.822332000	0.330637000	-1.236759000
O	-3.169810000	3.358290000	-0.935296000
O	-2.475634000	4.393330000	1.730380000
O	0.405213000	-2.026431000	-2.814221000
O	0.158780000	-2.502717000	0.295089000
O	1.692706000	0.418215000	-2.467455000
O	1.682024000	0.439737000	0.631836000
C	-1.348763000	2.693170000	3.767618000
C	-0.595180000	-3.169321000	2.996715000
C	1.690676000	1.079011000	3.460434000
O	-5.512636000	-1.194377000	1.177837000
O	-3.397234000	1.152837000	2.435541000
O	1.859423000	-1.689003000	2.765080000
O	2.555927000	-1.784275000	-0.936496000
O	-0.780484000	0.040955000	-0.840657000
H	-1.508982000	0.198306000	-1.482167000
H	-1.148599000	0.188142000	0.046156000
H	-4.160172000	2.048661000	-2.689923000
H	-3.449020000	1.733782000	-4.304513000
H	-0.033301000	5.622618000	-0.936095000
H	-1.723342000	5.427038000	-0.386820000
H	-5.818269000	-2.053213000	-1.115347000
H	-5.026751000	-3.486425000	-1.833308000
H	-3.589999000	-2.800360000	-3.822185000
H	-3.166550000	-0.571269000	-4.790483000
H	-1.021661000	2.965345000	-4.545128000
H	0.351382000	4.381686000	-3.073598000
H	1.740814000	4.626459000	0.958398000
H	-0.809308000	0.572836000	-5.387527000
H	0.580516000	-0.274636000	-4.654222000
H	2.706748000	2.081665000	-1.125240000
H	2.351836000	3.820624000	-1.124124000
H	-0.563605000	-3.918765000	-1.767704000
H	-2.231149000	-4.515358000	-1.983981000
H	-4.547767000	-0.934210000	3.359781000
H	-3.678975000	-2.237338000	4.224322000
H	-0.894662000	2.926012000	4.738407000
H	-2.368002000	3.085725000	3.736778000
H	-3.394783000	-4.733630000	0.036214000
H	-3.083580000	-4.323514000	2.439880000
H	-1.582877000	-1.499304000	5.192293000
H	-0.462986000	0.660523000	5.417178000
H	1.347706000	3.838296000	3.252938000

H	-1.084657000	-3.811061000	3.736507000
H	0.369927000	-3.599857000	2.723225000
H	2.610262000	0.555398000	3.199017000
H	1.877243000	1.732545000	4.318610000
H	3.512464000	-1.203054000	0.726619000
C	4.572932000	-0.990096000	1.055744000
C	5.331151000	-2.070523000	0.380967000
C	4.856893000	0.398955000	0.578107000
H	4.559185000	-1.088423000	2.144082000
C	5.650591000	-1.890206000	-1.010433000
C	5.670654000	-3.270837000	1.025703000
C	5.163455000	0.577894000	-0.789515000
C	4.796727000	1.513223000	1.423444000
C	5.175237000	-0.639286000	-1.666039000
C	6.313664000	-2.906157000	-1.705284000
C	6.343084000	-4.258451000	0.327063000
H	5.417198000	-3.406193000	2.072698000
C	5.405509000	1.863142000	-1.286073000
C	5.043398000	2.790311000	0.924282000
H	4.595596000	1.371700000	2.481687000
H	5.654671000	-0.463242000	-2.633579000
H	4.092029000	-0.860568000	-1.869232000
C	6.668063000	-4.074938000	-1.044662000
H	6.558885000	-2.771756000	-2.754484000
H	6.633032000	-5.178885000	0.824269000
C	5.351916000	2.965863000	-0.434102000
H	5.658162000	1.994853000	-2.334887000
H	5.030879000	3.646579000	1.592769000
H	7.201296000	-4.858231000	-1.574658000
H	5.573596000	3.957818000	-0.817129000

Imaginary Frequency: $i260\text{ cm}^{-1}$

$^{51}\text{P}_{\text{DHA}}$

Fe	0.141947000	-0.291206000	-1.925112000
C	0.910645000	-3.380233000	0.534783000
N	-0.289496000	-3.947277000	0.931083000
C	-0.612310000	-3.684157000	2.328480000
C	0.662587000	-2.931470000	2.852948000
N	1.510843000	-2.862702000	1.670137000
N	0.150654000	-1.653077000	3.275551000
C	-1.172257000	-1.473400000	2.879167000
N	-1.669217000	-2.721587000	2.507860000
C	-3.082947000	-3.062336000	2.628178000
N	-3.870200000	-2.791182000	1.455529000
C	-4.710454000	-1.677485000	1.410450000
N	-5.114774000	-1.531417000	0.077611000
C	-4.461253000	-2.467457000	-0.796604000
C	-3.689567000	-3.428470000	0.177771000

N	-2.321123000	-3.398055000	-0.330547000
C	-2.155536000	-2.416618000	-1.261250000
N	-3.379428000	-1.903242000	-1.603757000
C	-5.784179000	-0.322346000	-0.352163000
N	-4.902820000	0.756920000	-0.792820000
C	-4.455682000	1.727484000	0.103915000
N	-3.843161000	2.734064000	-0.652097000
C	-3.848148000	2.469755000	-2.064142000
C	-4.581165000	1.076234000	-2.158460000
N	-2.528118000	2.194934000	-2.641285000
C	-2.373506000	0.872989000	-2.931547000
N	-3.553618000	0.225556000	-2.766844000
C	-3.164765000	3.823529000	-0.003292000
N	-1.715477000	3.608633000	0.134512000
C	-1.171557000	3.582227000	1.452785000
N	0.192814000	3.816185000	1.335187000
C	0.586332000	4.155135000	-0.007458000
C	-0.771825000	4.235168000	-0.782887000
N	1.289624000	3.111287000	-0.751053000
C	0.597404000	2.673161000	-1.837737000
N	-0.526163000	3.453472000	-1.983797000
C	1.071291000	3.770589000	2.506609000
N	1.572475000	2.458657000	2.848356000
C	0.853300000	1.629404000	3.717779000
N	1.460965000	0.373601000	3.670518000
C	2.575023000	0.308985000	2.761274000
C	2.596755000	1.744599000	2.130350000
N	2.362814000	-0.565636000	1.609244000
C	2.102709000	0.148845000	0.484068000
N	2.281274000	1.477341000	0.729963000
C	-3.607929000	-1.213882000	-2.857770000
C	-1.520933000	3.182456000	-2.999948000
C	2.490714000	2.443838000	-0.325684000
O	-4.593089000	1.729699000	1.301801000
O	-1.796604000	3.380886000	2.460813000
O	-0.078883000	1.949204000	4.413182000
O	-1.316358000	0.335677000	-3.312494000
O	-1.063646000	-2.077992000	-1.742054000
O	0.933571000	1.729597000	-2.566228000
O	1.775876000	-0.350044000	-0.610421000
C	0.802728000	-0.772558000	4.239593000
C	-1.271499000	-4.373839000	-0.028372000
C	2.653837000	-1.999237000	1.573715000
O	-5.057323000	-1.004923000	2.348982000
O	-1.781597000	-0.419403000	2.856765000
O	1.378486000	-3.379982000	-0.594828000
O	1.318299000	-1.644894000	-3.003422000
O	-1.092946000	0.650227000	-0.248050000
H	-1.380587000	1.584929000	-0.170281000
H	-1.307555000	0.244261000	0.614875000

H	-3.577274000	3.901571000	1.005661000
H	-3.344904000	4.755045000	-0.552782000
H	1.906710000	4.455359000	2.332194000
H	0.488276000	4.111283000	3.364767000
H	-6.341046000	0.040449000	0.514247000
H	-6.479183000	-0.556025000	-1.165046000
H	-5.473582000	1.087238000	-2.792800000
H	-4.339187000	3.268639000	-2.630348000
H	-1.072371000	5.256702000	-1.039917000
H	1.166411000	5.083944000	-0.028946000
H	3.571087000	2.237407000	2.197474000
H	-2.029435000	4.117584000	-3.250007000
H	-0.988037000	2.812886000	-3.877182000
H	2.902903000	1.930692000	-1.194386000
H	3.216438000	3.178620000	0.032725000
H	-2.841109000	-1.516184000	-3.572915000
H	-4.590947000	-1.508317000	-3.237070000
H	-3.530121000	-2.468907000	3.428945000
H	-3.138823000	-4.124932000	2.890973000
H	1.517814000	-1.383251000	4.802255000
H	0.052241000	-0.373722000	4.925798000
H	-5.180291000	-2.979553000	-1.445906000
H	-4.064042000	-4.458100000	0.176652000
H	-0.826817000	-4.619717000	2.855106000
H	1.181316000	-3.445836000	3.668422000
H	3.510832000	0.038231000	3.260181000
H	-1.773222000	-5.278598000	0.328037000
H	-0.731481000	-4.599984000	-0.949344000
H	3.140390000	-2.223853000	0.625201000
H	3.351296000	-2.199951000	2.392389000
H	1.503621000	-2.384709000	-2.386184000
C	5.305617000	-1.748443000	-0.478658000
C	4.896653000	-1.758189000	-1.818532000
C	5.581707000	-0.554377000	0.201610000
H	5.428930000	-2.696332000	0.041603000
C	4.778380000	-0.503501000	-2.524883000
C	4.602504000	-2.973365000	-2.514468000
C	5.482691000	0.699242000	-0.511703000
C	5.971512000	-0.532158000	1.578584000
C	5.088227000	0.688464000	-1.857120000
C	4.365416000	-0.524766000	-3.895510000
C	4.228429000	-2.955875000	-3.833053000
H	4.691732000	-3.914676000	-1.979172000
C	5.807869000	1.908352000	0.182057000
C	6.254261000	0.650645000	2.214270000
H	6.069727000	-1.478377000	2.106002000
H	5.045562000	1.627446000	-2.406203000
H	2.179049000	-1.369989000	-3.375439000
C	4.107807000	-1.714848000	-4.533650000
H	4.282062000	0.417400000	-4.431137000

H	4.021037000	-3.884038000	-4.356403000
C	6.179053000	1.887746000	1.503293000
H	5.785330000	2.846054000	-0.369018000
H	6.572613000	0.651797000	3.252802000
H	3.815633000	-1.719798000	-5.579607000
H	6.449392000	2.809920000	2.010118000

³P_{DHA}

Fe	0.118251000	0.036560000	-1.779390000
C	0.858633000	-3.489552000	0.018140000
N	-0.357819000	-4.091461000	0.312816000
C	-0.701535000	-4.015867000	1.726699000
C	0.590735000	-3.406036000	2.379258000
N	1.451528000	-3.166862000	1.230433000
N	0.115186000	-2.196424000	3.001369000
C	-1.167853000	-1.878423000	2.567852000
N	-1.718628000	-3.035456000	2.019588000
C	-3.144372000	-3.338966000	2.095468000
N	-3.913959000	-2.894017000	0.966660000
C	-4.761164000	-1.791791000	1.079978000
N	-5.146639000	-1.443648000	-0.221501000
C	-4.457530000	-2.224014000	-1.214460000
C	-3.730059000	-3.342570000	-0.389054000
N	-2.354252000	-3.275843000	-0.868885000
C	-2.137719000	-2.143385000	-1.595551000
N	-3.340014000	-1.540449000	-1.867443000
C	-5.777172000	-0.163427000	-0.469390000
N	-4.861866000	0.953981000	-0.696016000
C	-4.407524000	1.735911000	0.365244000
N	-3.752251000	2.841580000	-0.190025000
C	-3.739276000	2.835234000	-1.627653000
C	-4.496310000	1.496544000	-1.978269000
N	-2.414820000	2.641492000	-2.223393000
C	-2.273215000	1.383079000	-2.731511000
N	-3.468415000	0.740594000	-2.699592000
C	-3.047306000	3.766577000	0.652350000
N	-1.600140000	3.493253000	0.740848000
C	-1.064670000	3.235256000	2.040580000
N	0.299871000	3.484030000	1.977421000
C	0.704262000	4.054049000	0.718533000
C	-0.647348000	4.282281000	-0.036586000
N	1.401476000	3.152109000	-0.195674000
C	0.713010000	2.925743000	-1.350339000
N	-0.396915000	3.741291000	-1.361277000
C	1.167991000	3.247870000	3.134396000
N	1.655030000	1.893568000	3.272391000
C	0.913576000	0.948680000	3.993273000
N	1.480006000	-0.297883000	3.723516000
C	2.594056000	-0.238330000	2.814057000

C	2.643758000	1.278390000	2.424499000
N	2.362797000	-0.910784000	1.537219000
C	2.096930000	-0.019894000	0.548917000
N	2.291462000	1.251173000	1.006648000
C	-3.528465000	-0.666339000	-3.009729000
C	-1.394559000	3.661239000	-2.409212000
C	2.561078000	2.365388000	0.120426000
O	-4.567514000	1.530615000	1.542678000
O	-1.697606000	2.859482000	2.992127000
O	-0.004626000	1.171482000	4.742955000
O	-1.218644000	0.892963000	-3.170117000
O	-1.022151000	-1.753614000	-1.974571000
O	1.039919000	2.113345000	-2.223510000
O	1.749927000	-0.329492000	-0.609766000
C	0.786884000	-1.502764000	4.095114000
C	-1.338211000	-4.321203000	-0.713695000
C	2.614760000	-2.330762000	1.276981000
O	-5.125888000	-1.274499000	2.106289000
O	-1.706952000	-0.785776000	2.638778000
O	1.338787000	-3.315532000	-1.089179000
O	1.171760000	-0.744552000	-3.241311000
O	-1.060112000	0.652770000	-0.167658000
H	-1.299881000	1.582251000	0.050187000
H	-1.214669000	0.134620000	0.650669000
H	-3.459543000	3.655967000	1.658362000
H	-3.202560000	4.792440000	0.297559000
H	2.010847000	3.942711000	3.072208000
H	0.583111000	3.456456000	4.032510000
H	-6.361200000	0.064612000	0.424494000
H	-6.443331000	-0.244886000	-1.333972000
H	-5.371511000	1.637660000	-2.620827000
H	-4.207211000	3.732588000	-2.047043000
H	-0.945374000	5.334629000	-0.094910000
H	1.291045000	4.966823000	0.867090000
H	3.633370000	1.728481000	2.547963000
H	-1.889353000	4.632276000	-2.495737000
H	-0.863334000	3.439314000	-3.335794000
H	2.953808000	1.980299000	-0.819922000
H	3.321487000	2.992563000	0.593992000
H	-2.743463000	-0.862647000	-3.741900000
H	-4.502716000	-0.890699000	-3.454305000
H	-3.578750000	-2.839315000	2.964564000
H	-3.234835000	-4.424102000	2.222718000
H	1.480161000	-2.220309000	4.547529000
H	0.047570000	-1.200344000	4.840168000
H	-5.149546000	-2.612012000	-1.970347000
H	-4.133018000	-4.348793000	-0.548548000
H	-0.972693000	-5.003832000	2.112185000
H	1.080827000	-4.063922000	3.103895000
H	3.523587000	-0.607641000	3.258723000

H	-1.875161000	-5.253573000	-0.515608000
H	-0.789224000	-4.412445000	-1.652422000
H	3.098181000	-2.414173000	0.304749000
H	3.302513000	-2.673089000	2.055580000
H	1.537868000	-1.596692000	-2.925904000
C	5.083907000	-1.728091000	-1.015548000
C	4.654317000	-1.360597000	-2.296890000
C	5.472692000	-0.774033000	-0.064961000
H	5.128979000	-2.784607000	-0.758880000
C	4.648145000	0.036978000	-2.661658000
C	4.230898000	-2.328296000	-3.262943000
C	5.471457000	0.624083000	-0.431965000
C	5.875417000	-1.135216000	1.260136000
C	5.072554000	0.989005000	-1.725589000
C	4.217319000	0.401126000	-3.978478000
C	3.842265000	-1.943235000	-4.520816000
H	4.233047000	-3.378125000	-2.982941000
C	5.882415000	1.588411000	0.542955000
C	6.245122000	-0.179079000	2.172129000
H	5.908314000	-2.189859000	1.523831000
H	5.107286000	2.037296000	-2.016740000
H	1.948882000	-0.217136000	-3.522378000
C	3.836959000	-0.560016000	-4.884488000
H	4.221688000	1.451514000	-4.258055000
H	3.538485000	-2.686207000	-5.251765000
C	6.252217000	1.202148000	1.806989000
H	5.924651000	2.635919000	0.252569000
H	6.570297000	-0.468281000	3.167436000
H	3.532426000	-0.274134000	-5.886884000
H	6.585356000	1.941931000	2.529482000

⁵TS1_{Et}

Fe	0.201829000	0.203378000	2.373682000
C	1.931028000	-3.345160000	0.908735000
N	2.862584000	-3.002404000	-0.063655000
C	2.430835000	-3.341616000	-1.411959000
C	1.074807000	-4.105208000	-1.174171000
N	0.925631000	-4.065160000	0.273880000
N	0.110018000	-3.295042000	-1.875687000
C	0.650529000	-2.067542000	-2.245990000
N	2.035399000	-2.195254000	-2.193766000
C	2.930425000	-1.455935000	-3.075595000
N	3.347040000	-0.175561000	-2.569969000
C	2.816569000	1.000924000	-3.097544000
N	3.203601000	2.036895000	-2.236085000
C	3.878150000	1.544609000	-1.066832000
C	4.100754000	0.023283000	-1.361359000
N	3.539984000	-0.639845000	-0.185280000
C	2.820790000	0.229345000	0.575513000

N	3.055868000	1.510986000	0.145885000
C	2.606929000	3.348715000	-2.362322000
N	1.376471000	3.552344000	-1.598004000
C	0.128870000	3.256248000	-2.148307000
N	-0.837554000	3.740768000	-1.256240000
C	-0.275259000	4.378064000	-0.099014000
C	1.277500000	4.205556000	-0.322291000
N	-0.516064000	3.662513000	1.161349000
C	0.602630000	3.016278000	1.583490000
N	1.662486000	3.376349000	0.828970000
C	-2.238054000	3.514610000	-1.496340000
N	-2.774051000	2.358111000	-0.759929000
C	-3.309506000	1.276187000	-1.517288000
N	-4.126258000	0.543840000	-0.661693000
C	-4.261157000	1.149873000	0.633515000
C	-3.525008000	2.525827000	0.475754000
N	-3.481544000	0.526999000	1.711214000
C	-2.523543000	1.346721000	2.198821000
N	-2.666811000	2.591394000	1.652291000
C	-4.757383000	-0.701828000	-1.103230000
N	-3.928556000	-1.880704000	-0.991801000
C	-3.121181000	-2.287043000	-2.063152000
N	-2.312159000	-3.317217000	-1.584963000
C	-2.531016000	-3.625738000	-0.198218000
C	-3.597505000	-2.561032000	0.230732000
N	-1.389422000	-3.341728000	0.674370000
C	-1.569008000	-2.184298000	1.363643000
N	-2.857039000	-1.750502000	1.197338000
C	2.913449000	2.675671000	0.994757000
C	-1.742085000	3.671216000	1.941103000
C	-3.523039000	-0.855784000	2.116799000
O	-0.093057000	2.714314000	-3.201396000
O	-3.076899000	1.053203000	-2.675671000
O	-3.153289000	-1.862211000	-3.190688000
O	0.667548000	2.220519000	2.544044000
O	2.091635000	-0.106143000	1.530733000
O	-1.654478000	1.000181000	3.022514000
O	-0.696491000	-1.633641000	2.068812000
C	-1.181456000	-3.769505000	-2.353577000
C	3.863684000	-2.016653000	0.222471000
C	-0.310604000	-4.306249000	0.955540000
O	2.191808000	1.108770000	-4.122670000
O	0.026276000	-1.062188000	-2.546018000
O	1.994281000	-3.094207000	2.094560000
O	0.684591000	-0.146317000	3.893177000
O	-0.389029000	0.617927000	0.205784000
H	-1.049506000	1.266236000	-0.118562000
H	-0.179848000	0.054823000	-0.568769000
H	-2.349040000	3.298802000	-2.562039000
H	-2.812296000	4.411822000	-1.236848000

H	-5.682233000	-0.836212000	-0.534138000
H	-4.991116000	-0.590578000	-2.164068000
H	2.361941000	3.470349000	-3.419419000
H	3.329405000	4.113899000	-2.061475000
H	1.836718000	5.146127000	-0.300441000
H	-0.597509000	5.419877000	0.001558000
H	-4.200136000	3.387080000	0.439343000
H	-5.310186000	1.234186000	0.934375000
H	-4.485670000	-2.988025000	0.709455000
H	-2.255479000	4.621025000	1.772488000
H	-1.470533000	3.588096000	2.994637000
H	-3.044098000	-0.917570000	3.095448000
H	-4.565969000	-1.173843000	2.207093000
H	2.971520000	2.370637000	2.040803000
H	3.736732000	3.361264000	0.775181000
H	2.426677000	-1.249806000	-4.022858000
H	3.799006000	-2.097388000	-3.262327000
H	-1.138394000	-4.863991000	-2.364139000
H	-1.351828000	-3.408365000	-3.370345000
H	4.802538000	2.098855000	-0.870308000
H	5.152240000	-0.259942000	-1.478965000
H	3.191642000	-3.936076000	-1.927235000
H	1.074008000	-5.136843000	-1.539113000
H	-2.853338000	-4.662526000	-0.054054000
H	4.801527000	-2.270568000	-0.280253000
H	4.018350000	-2.030668000	1.302515000
H	-0.089382000	-4.276921000	2.023951000
H	-0.706469000	-5.291955000	0.693498000
C	2.720028000	-1.003147000	5.589479000
H	2.994067000	-0.267661000	6.353625000
H	2.564321000	-1.980897000	6.058075000
H	1.708760000	-0.686705000	5.209406000
C	3.701765000	-1.057935000	4.429344000
H	4.691918000	-1.377097000	4.781250000
H	3.360316000	-1.765093000	3.667362000
H	3.815644000	-0.072059000	3.961503000

Imaginary Frequency: $i190\text{ cm}^{-1}$

³TS1_{Et}

Fe	-0.087926000	-0.397132000	2.287471000
C	-1.882335000	3.374769000	1.134623000
N	-2.827184000	3.076918000	0.159457000
C	-2.410534000	3.468176000	-1.178854000
C	-1.035913000	4.192979000	-0.929529000
N	-0.866993000	4.091943000	0.512772000
N	-0.098108000	3.394005000	-1.679224000
C	-0.670732000	2.197965000	-2.099651000
N	-2.051254000	2.353561000	-2.020580000

C	-2.975272000	1.673368000	-2.917552000
N	-3.400115000	0.376427000	-2.464260000
C	-2.900250000	-0.778968000	-3.061832000
N	-3.279005000	-1.850386000	-2.241078000
C	-3.914354000	-1.405317000	-1.031242000
C	-4.123605000	0.129553000	-1.245181000
N	-3.526478000	0.726647000	-0.053033000
C	-2.789486000	-0.183612000	0.648501000
N	-3.061556000	-1.442947000	0.158280000
C	-2.704258000	-3.160988000	-2.446705000
N	-1.462989000	-3.422566000	-1.716748000
C	-0.221225000	-3.115874000	-2.273505000
N	0.754146000	-3.676333000	-1.435896000
C	0.201848000	-4.351395000	-0.295951000
C	-1.351847000	-4.146707000	-0.482216000
N	0.476758000	-3.691667000	0.989963000
C	-0.625916000	-3.051855000	1.458965000
N	-1.704099000	-3.372854000	0.718650000
C	2.153428000	-3.454777000	-1.690435000
N	2.719822000	-2.342653000	-0.907030000
C	3.262395000	-1.231392000	-1.622045000
N	4.098062000	-0.550854000	-0.743584000
C	4.256064000	-1.229254000	0.513344000
C	3.499872000	-2.588271000	0.298294000
N	3.507348000	-0.658501000	1.641717000
C	2.545992000	-1.488672000	2.092821000
N	2.667384000	-2.708249000	1.489632000
C	4.747054000	0.705655000	-1.134113000
N	3.946770000	1.894964000	-0.953291000
C	3.120714000	2.358797000	-1.987171000
N	2.326931000	3.365939000	-1.441902000
C	2.572400000	3.603213000	-0.042947000
C	3.616056000	2.492991000	0.312532000
N	1.440412000	3.302079000	0.831048000
C	1.571026000	2.074700000	1.410424000
N	2.856043000	1.623658000	1.209413000
C	-2.937001000	-2.652114000	0.939338000
C	1.716921000	-3.773370000	1.744105000
C	3.529291000	0.709330000	2.100686000
O	-0.009656000	-2.513584000	-3.295272000
O	3.015031000	-0.952197000	-2.764714000
O	3.129661000	1.990772000	-3.135365000
O	-0.671869000	-2.288225000	2.453159000
O	-2.027706000	0.101330000	1.590577000
O	1.681504000	-1.172643000	2.935239000
O	0.661996000	1.495106000	2.033031000
C	1.189425000	3.869020000	-2.166160000
C	-3.828506000	2.085564000	0.422182000
C	0.387647000	4.269597000	1.182216000
O	-2.304009000	-0.846101000	-4.107483000

O	-0.073775000	1.195325000	-2.458823000
O	-1.948340000	3.095135000	2.313518000
O	-0.498997000	-0.013133000	3.885689000
O	0.372001000	-0.703944000	0.170707000
H	1.065465000	-1.284710000	-0.212624000
H	0.153220000	-0.055064000	-0.530547000
H	2.247748000	-3.186734000	-2.745808000
H	2.720190000	-4.370960000	-1.487533000
H	5.681847000	0.792140000	-0.572273000
H	4.964399000	0.641832000	-2.202297000
H	-2.479500000	-3.229299000	-3.513062000
H	-3.431308000	-3.932335000	-2.173546000
H	-1.925022000	-5.078789000	-0.499112000
H	0.509881000	-5.400839000	-0.241937000
H	4.163866000	-3.452737000	0.196924000
H	5.310450000	-1.340734000	0.784388000
H	4.507418000	2.869908000	0.825867000
H	2.196919000	-4.729462000	1.521344000
H	1.467493000	-3.731511000	2.805495000
H	3.045505000	0.722105000	3.078964000
H	4.567818000	1.035461000	2.209839000
H	-2.971739000	-2.408067000	2.001776000
H	-3.777012000	-3.308232000	0.694799000
H	-2.495512000	1.505995000	-3.884707000
H	-3.837266000	2.335979000	-3.054297000
H	1.163574000	4.963556000	-2.128202000
H	1.332359000	3.550112000	-3.201175000
H	-4.841992000	-1.955657000	-0.838068000
H	-5.174017000	0.430426000	-1.323060000
H	-3.166780000	4.101186000	-1.653506000
H	-1.018864000	5.238445000	-1.252719000
H	2.923557000	4.623559000	0.143783000
H	-4.776905000	2.367605000	-0.044821000
H	-3.956524000	2.055244000	1.505399000
H	0.182258000	4.187570000	2.251098000
H	0.800533000	5.259809000	0.967383000
C	-2.916283000	-0.216322000	4.633698000
H	-2.840905000	-0.889090000	5.491279000
H	-1.688906000	-0.190451000	4.208820000
H	-3.428193000	-0.670468000	3.781772000
C	-3.257595000	1.218764000	4.922844000
H	-4.314980000	1.291822000	5.224070000
H	-2.656767000	1.613811000	5.747515000
H	-3.104358000	1.854033000	4.045373000

Imaginary Frequency: $i1031\text{ cm}^{-1}$

$^{55}\text{P}_{\text{Et}}$

Fe	0.026862000	-0.098301000	2.293617000
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C	-0.971892000	3.667457000	1.065720000
N	-2.091806000	3.564365000	0.253805000
C	-1.804899000	3.820522000	-1.151550000
C	-0.282094000	4.216997000	-1.138454000
N	0.067960000	4.135367000	0.273398000
N	0.335197000	3.194907000	-1.945499000
C	-0.553203000	2.161872000	-2.231337000
N	-1.834539000	2.636204000	-1.972264000
C	-3.016747000	2.139289000	-2.667211000
N	-3.624640000	0.982384000	-2.069578000
C	-3.432577000	-0.283375000	-2.626242000
N	-3.905456000	-1.208512000	-1.688743000
C	-4.315056000	-0.584703000	-0.460576000
C	-4.215663000	0.951601000	-0.759841000
N	-3.354295000	1.454256000	0.310409000
C	-2.809990000	0.436432000	1.033401000
N	-3.383803000	-0.749461000	0.656466000
C	-3.657522000	-2.622844000	-1.864634000
N	-2.420858000	-3.116135000	-1.264890000
C	-1.229057000	-3.133803000	-1.988729000
N	-0.298489000	-3.850123000	-1.226672000
C	-0.823771000	-4.313263000	0.027321000
C	-2.307005000	-3.775117000	0.007795000
N	-0.245003000	-3.663085000	1.207531000
C	-1.115530000	-2.777599000	1.769328000
N	-2.328448000	-2.882325000	1.171693000
C	1.070941000	-3.953391000	-1.651912000
N	1.949617000	-2.945940000	-1.036325000
C	2.623880000	-2.041485000	-1.905772000
N	3.696878000	-1.515628000	-1.194706000
C	3.864411000	-2.128258000	0.094487000
C	2.806606000	-3.282280000	0.093725000
N	3.429253000	-1.332908000	1.244646000
C	2.405671000	-1.910769000	1.931139000
N	2.147760000	-3.143856000	1.382680000
C	4.540516000	-0.467185000	-1.767051000
N	4.041409000	0.879085000	-1.592891000
C	3.184248000	1.444474000	-2.546108000
N	2.707188000	2.634372000	-1.998990000
C	3.217125000	2.909988000	-0.684361000
C	4.073204000	1.633295000	-0.368538000
N	2.204576000	2.917218000	0.373840000
C	2.241160000	1.769115000	1.103037000
N	3.339250000	1.035592000	0.746496000
C	-3.369859000	-1.934933000	1.490986000
C	1.038118000	-3.966787000	1.821393000
C	3.892446000	-0.012092000	1.580185000
O	-1.031794000	-2.655397000	-3.077784000
O	2.303328000	-1.789514000	-3.037435000
O	2.942852000	1.012528000	-3.645389000

O	-0.849781000	-1.997476000	2.700774000
O	-1.950645000	0.578269000	1.923153000
O	1.812973000	-1.393707000	2.888674000
O	1.421658000	1.453404000	1.989455000
C	1.616940000	3.337512000	-2.622142000
C	-3.259971000	2.864421000	0.710696000
C	1.417886000	4.099252000	0.757881000
O	-2.993488000	-0.523339000	-3.722900000
O	-0.258800000	1.045378000	-2.624987000
O	-0.917650000	3.428263000	2.257495000
O	0.011434000	0.351893000	4.315635000
O	0.209595000	-0.618513000	0.089804000
H	0.656022000	-1.420445000	-0.253375000
H	0.009135000	-0.077027000	-0.702001000
H	1.085367000	-3.778164000	-2.730502000
H	1.454569000	-4.956974000	-1.433149000
H	5.540678000	-0.555093000	-1.332070000
H	4.591545000	-0.639319000	-2.844130000
H	-3.590403000	-2.788351000	-2.941896000
H	-4.494215000	-3.197891000	-1.454983000
H	-3.063649000	-4.557080000	0.129023000
H	-0.747656000	-5.401226000	0.129475000
H	3.245850000	-4.280358000	-0.010356000
H	4.894775000	-2.467707000	0.244983000
H	5.101068000	1.852935000	-0.058860000
H	1.279869000	-5.013386000	1.618456000
H	0.937423000	-3.820128000	2.897558000
H	3.611940000	0.172217000	2.618337000
H	4.982640000	0.025386000	1.489992000
H	-3.219737000	-1.635043000	2.529237000
H	-4.340918000	-2.429607000	1.395771000
H	-2.743313000	1.840573000	-3.681820000
H	-3.731898000	2.967971000	-2.715775000
H	1.835499000	4.409743000	-2.679930000
H	1.542107000	2.931094000	-3.633311000
H	-5.315502000	-0.913169000	-0.157109000
H	-5.178947000	1.473047000	-0.733333000
H	-2.464578000	4.599512000	-1.546415000
H	-0.078565000	5.218157000	-1.531261000
H	3.786717000	3.845449000	-0.653141000
H	-4.162928000	3.356018000	0.336250000
H	-3.246525000	2.916417000	1.800511000
H	1.358877000	4.136391000	1.846719000
H	1.971647000	4.970545000	0.395383000
C	-0.176961000	1.694106000	4.883070000
H	0.261457000	2.399319000	4.175111000
H	0.367276000	1.734669000	5.830949000
H	0.662227000	-0.159909000	4.820876000
C	-1.658556000	1.946047000	5.066286000
H	-2.166471000	1.859724000	4.103025000

H	-2.093927000	1.234320000	5.774688000
H	-1.812394000	2.961507000	5.446260000

³P_{Et}

Fe	-0.054040000	0.181088000	2.218578000
C	0.767877000	-3.710460000	1.165935000
N	1.890611000	-3.703414000	0.350333000
C	1.576431000	-3.945308000	-1.051148000
C	0.034803000	-4.259593000	-1.025922000
N	-0.305821000	-4.113559000	0.382700000
N	-0.528433000	-3.229530000	-1.860129000
C	0.402185000	-2.228917000	-2.124907000
N	1.661689000	-2.761233000	-1.870032000
C	2.860958000	-2.348953000	-2.592448000
N	3.556992000	-1.233993000	-2.013999000
C	3.470025000	0.030838000	-2.596063000
N	4.007765000	0.934983000	-1.672738000
C	4.345419000	0.303630000	-0.425685000
C	4.160462000	-1.227824000	-0.707910000
N	3.281025000	-1.671369000	0.370725000
C	2.761728000	-0.613669000	1.058131000
N	3.395127000	0.538227000	0.662248000
C	3.851245000	2.359922000	-1.872317000
N	2.634756000	2.939769000	-1.308685000
C	1.457292000	3.006074000	-2.053075000
N	0.551541000	3.779853000	-1.317462000
C	1.083165000	4.248342000	-0.067781000
C	2.531214000	3.619999000	-0.046368000
N	0.444762000	3.666936000	1.116796000
C	1.242830000	2.730536000	1.702747000
N	2.468165000	2.740644000	1.126709000
C	-0.807779000	3.926969000	-1.756111000
N	-1.738210000	2.986489000	-1.103774000
C	-2.459293000	2.093965000	-1.951577000
N	-3.581284000	1.675527000	-1.245599000
C	-3.728665000	2.349305000	0.015350000
C	-2.598382000	3.430099000	-0.011048000
N	-3.364013000	1.575243000	1.203806000
C	-2.324362000	2.121552000	1.894630000
N	-1.978168000	3.311544000	1.297770000
C	-4.494912000	0.676632000	-1.800488000
N	-4.095411000	-0.697055000	-1.588280000
C	-3.279304000	-1.346330000	-2.523879000
N	-2.865865000	-2.539534000	-1.933563000
C	-3.381314000	-2.735976000	-0.606989000
C	-4.158255000	-1.401182000	-0.335731000
N	-2.363168000	-2.763228000	0.446253000
C	-2.326811000	-1.587775000	1.130334000
N	-3.380414000	-0.802228000	0.748905000

C	3.437689000	1.731398000	1.483389000
C	-0.818075000	4.074083000	1.715173000
C	-3.889000000	0.285679000	1.562453000
O	1.252520000	2.522615000	-3.138276000
O	-2.133164000	1.771367000	-3.063456000
O	-3.022461000	-0.971705000	-3.640469000
O	0.905786000	1.984599000	2.639978000
O	1.879318000	-0.697325000	1.928652000
O	-1.786404000	1.611338000	2.885074000
O	-1.486792000	-1.290105000	2.005337000
C	-1.816465000	-3.320661000	-2.532941000
C	3.103786000	-3.067369000	0.789048000
C	-1.648020000	-3.978962000	0.867971000
O	3.057329000	0.281712000	-3.700839000
O	0.155965000	-1.090598000	-2.492467000
O	0.732046000	-3.450358000	2.353375000
O	0.016294000	-0.115185000	4.152060000
O	-0.137584000	0.630992000	0.165566000
H	-0.561187000	1.432532000	-0.212335000
H	0.008516000	0.020716000	-0.588709000
H	-0.822691000	3.707721000	-2.826617000
H	-1.149035000	4.954410000	-1.582547000
H	-5.488629000	0.849354000	-1.376531000
H	-4.526271000	0.822406000	-2.882206000
H	3.818226000	2.513080000	-2.952911000
H	4.713046000	2.887699000	-1.451904000
H	3.331670000	4.355136000	0.085297000
H	1.072083000	5.341326000	0.002954000
H	-2.969440000	4.447777000	-0.173353000
H	-4.736666000	2.760993000	0.132881000
H	-5.193811000	-1.548916000	-0.009637000
H	-0.988313000	5.127562000	1.478387000
H	-0.731559000	3.954148000	2.795796000
H	-3.620729000	0.110167000	2.605224000
H	-4.979407000	0.293584000	1.467897000
H	3.240512000	1.455183000	2.520472000
H	4.440408000	2.162716000	1.408351000
H	2.590408000	-2.038053000	-3.604254000
H	3.515215000	-3.226318000	-2.649219000
H	-2.091521000	-4.380948000	-2.557332000
H	-1.722023000	-2.952335000	-3.557006000
H	5.355883000	0.575052000	-0.099777000
H	5.094198000	-1.800577000	-0.684957000
H	2.190128000	-4.757580000	-1.452681000
H	-0.223878000	-5.259139000	-1.388867000
H	-4.003992000	-3.634793000	-0.537732000
H	3.971606000	-3.618311000	0.414667000
H	3.096014000	-3.105784000	1.879443000
H	-1.588337000	-3.986369000	1.957412000
H	-2.257420000	-4.824456000	0.534456000

C	0.054009000	-1.460142000	4.761245000
H	-0.400384000	-2.152788000	4.053090000
H	-0.549727000	-1.408861000	5.671996000
H	-0.700819000	0.416722000	4.537913000
C	1.494053000	-1.819152000	5.051618000
H	2.067262000	-1.823498000	4.122853000
H	1.940699000	-1.111856000	5.757011000
H	1.533496000	-2.823780000	5.485464000

⁵TS1_{Me}

Fe	-0.028864000	-0.248878000	2.491444000
C	1.071710000	3.654136000	1.292872000
N	0.050869000	4.165349000	0.502072000
C	0.415149000	4.272211000	-0.903683000
C	1.929897000	3.843284000	-0.914497000
N	2.197622000	3.543915000	0.485535000
N	1.940820000	2.680999000	-1.767889000
C	0.650649000	2.240845000	-2.048771000
N	-0.218183000	3.282994000	-1.740439000
C	-1.484413000	3.480625000	-2.434365000
N	-2.602232000	2.790375000	-1.848261000
C	-3.128080000	1.649302000	-2.452783000
N	-4.015655000	1.078881000	-1.529035000
C	-3.987665000	1.756862000	-0.262214000
C	-3.111289000	3.028025000	-0.524977000
N	-2.099849000	2.971524000	0.529488000
C	-2.112056000	1.766581000	1.162180000
N	-3.231593000	1.067488000	0.787277000
C	-4.529398000	-0.255794000	-1.744294000
N	-3.704277000	-1.335614000	-1.203896000
C	-2.700866000	-1.927491000	-1.970780000
N	-2.256551000	-3.054120000	-1.265058000
C	-2.939537000	-3.250043000	-0.017813000
C	-3.931779000	-2.024434000	0.035832000
N	-2.099817000	-3.055120000	1.171875000
C	-2.377066000	-1.874626000	1.785125000
N	-3.470643000	-1.307108000	1.233037000
C	-1.147856000	-3.831095000	-1.751496000
N	0.136000000	-3.462136000	-1.132408000
C	1.172387000	-2.985051000	-1.987748000
N	2.369194000	-3.120778000	-1.291869000
C	2.208197000	-3.796877000	-0.034820000
C	0.707211000	-4.248712000	-0.047923000
N	2.242099000	-2.939885000	1.157160000
C	1.061959000	-2.921747000	1.816374000
N	0.218097000	-3.844953000	1.264177000
C	3.629375000	-2.624278000	-1.849464000
N	3.893586000	-1.223918000	-1.609442000
C	3.464454000	-0.250611000	-2.522801000

N	3.688599000	0.987425000	-1.921738000
C	4.241392000	0.894161000	-0.598519000
C	4.304500000	-0.653066000	-0.354919000
N	3.354938000	1.376424000	0.463245000
C	2.770342000	0.343941000	1.127241000
N	3.352015000	-0.833737000	0.739787000
C	-3.835671000	0.038388000	1.608457000
C	-1.148692000	-4.006294000	1.721183000
C	3.302851000	-2.039038000	1.535145000
O	-2.301966000	-1.569628000	-3.050019000
O	1.015663000	-2.545383000	-3.095603000
O	3.032269000	-0.444867000	-3.631053000
O	-1.741609000	-1.383673000	2.743074000
O	-1.246537000	1.387453000	1.977009000
O	0.803398000	-2.175630000	2.780777000
O	1.871342000	0.464505000	1.984330000
C	3.110885000	2.183527000	-2.478010000
C	-1.302249000	4.124885000	0.975475000
C	3.317822000	2.771385000	0.934734000
O	-2.900824000	1.260172000	-3.570628000
O	0.338849000	1.141230000	-2.475185000
O	1.003761000	3.385731000	2.475263000
O	0.099602000	0.185610000	4.086540000
O	-0.192959000	-0.688137000	0.222616000
H	-0.197914000	-1.563172000	-0.220164000
H	-0.059189000	-0.039416000	-0.497834000
H	-1.060195000	-3.626819000	-2.821615000
H	-1.339139000	-4.898726000	-1.591150000
H	4.444209000	-3.233903000	-1.447543000
H	3.578167000	-2.746485000	-2.933402000
H	-4.583269000	-0.390337000	-2.826604000
H	-5.532006000	-0.339578000	-1.313149000
H	-4.981565000	-2.308077000	0.160051000
H	-3.433715000	-4.225843000	0.037607000
H	0.571279000	-5.324613000	-0.199156000
H	2.923142000	-4.618119000	0.077908000
H	5.292124000	-1.015935000	-0.049658000
H	-1.481047000	-5.016179000	1.468679000
H	-1.141633000	-3.888346000	2.805906000
H	3.141025000	-1.776530000	2.582108000
H	4.263919000	-2.553127000	1.438070000
H	-3.526136000	0.173882000	2.645945000
H	-4.922459000	0.142674000	1.542984000
H	-1.405404000	3.101330000	-3.455855000
H	-1.670605000	4.560123000	-2.464748000
H	3.848936000	2.992931000	-2.493204000
H	2.836035000	1.929728000	-3.504344000
H	-4.997710000	1.980812000	0.098243000
H	-3.662173000	3.972473000	-0.457708000
H	0.237610000	5.286032000	-1.275768000

H	2.608384000	4.618487000	-1.283954000
H	5.211581000	1.396873000	-0.522729000
H	-1.846502000	5.016912000	0.651590000
H	-1.248561000	4.108473000	2.065413000
H	3.274523000	2.768431000	2.025339000
H	4.255463000	3.231142000	0.608324000
C	0.722253000	2.227748000	5.717072000
H	-0.119944000	2.531665000	6.342844000
H	1.602769000	1.973263000	6.310978000
H	0.940509000	2.945669000	4.925076000
H	0.400270000	1.269549000	5.180805000

Imaginary Frequency: $i312\text{ cm}^{-1}$

³TS1_{Me}

Fe	-0.023506000	-0.303890000	2.399239000
C	-0.943049000	3.664495000	1.406449000
N	-2.042845000	3.609875000	0.562263000
C	-1.722667000	3.958330000	-0.817065000
C	-0.194705000	4.329731000	-0.743909000
N	0.118003000	4.170366000	0.669198000
N	0.430822000	3.339696000	-1.585891000
C	-0.468599000	2.342268000	-1.953926000
N	-1.748266000	2.834063000	-1.716553000
C	-2.919365000	2.400406000	-2.467768000
N	-3.546343000	1.207680000	-1.966221000
C	-3.362089000	-0.013961000	-2.616980000
N	-3.844471000	-1.002702000	-1.751803000
C	-4.269129000	-0.467850000	-0.489090000
C	-4.146976000	1.082483000	-0.667705000
N	-3.287176000	1.490597000	0.445902000
C	-2.771401000	0.413898000	1.100683000
N	-3.360308000	-0.730123000	0.630286000
C	-3.638440000	-2.404514000	-2.042529000
N	-2.426418000	-2.982992000	-1.471363000
C	-1.211854000	-2.925462000	-2.154407000
N	-0.302552000	-3.712768000	-1.438248000
C	-0.861695000	-4.285469000	-0.245051000
C	-2.342701000	-3.735787000	-0.251566000
N	-0.306022000	-3.744387000	1.001568000
C	-1.175140000	-2.886435000	1.597659000
N	-2.375440000	-2.928366000	0.976336000
C	1.076293000	-3.787137000	-1.840325000
N	1.947599000	-2.843168000	-1.119197000
C	2.658989000	-1.881468000	-1.897610000
N	3.719112000	-1.431016000	-1.119139000
C	3.846223000	-2.152166000	0.118447000
C	2.779349000	-3.292356000	-0.008146000
N	3.376916000	-1.449911000	1.315308000

C	2.319324000	-2.063477000	1.904551000
N	2.086656000	-3.258485000	1.270531000
C	4.600433000	-0.358249000	-1.585205000
N	4.121998000	0.983340000	-1.330654000
C	3.294915000	1.624148000	-2.264157000
N	2.800580000	2.769049000	-1.641739000
C	3.269785000	2.940113000	-0.292841000
C	4.084807000	1.625427000	-0.043744000
N	2.218295000	2.890662000	0.723387000
C	2.165793000	1.668056000	1.318469000
N	3.268137000	0.939230000	0.959051000
C	-3.396394000	-1.982792000	1.359500000
C	0.963086000	-4.104829000	1.618209000
C	3.794926000	-0.147040000	1.761032000
O	-0.983464000	-2.338741000	-3.182503000
O	2.369874000	-1.535821000	-3.012475000
O	3.087127000	1.278525000	-3.400291000
O	-0.926489000	-2.168776000	2.586687000
O	-1.921427000	0.483663000	2.014958000
O	1.677674000	-1.598424000	2.858269000
O	1.264094000	1.292099000	2.095784000
C	1.723186000	3.514717000	-2.236958000
C	-3.208963000	2.870825000	0.950233000
C	1.454390000	4.062378000	1.180210000
O	-2.923138000	-0.174015000	-3.727628000
O	-0.186035000	1.237625000	-2.388995000
O	-0.918824000	3.358344000	2.582585000
O	-0.170415000	0.029026000	4.128511000
O	0.143426000	-0.681789000	0.216648000
H	0.649650000	-1.412673000	-0.200735000
H	-0.030860000	-0.041920000	-0.505384000
H	1.116313000	-3.518291000	-2.898832000
H	1.449486000	-4.808678000	-1.702027000
H	5.582625000	-0.499038000	-1.124382000
H	4.686376000	-0.451939000	-2.669697000
H	-3.561590000	-2.481506000	-3.129105000
H	-4.496973000	-2.986474000	-1.692252000
H	-3.107170000	-4.517164000	-0.199481000
H	-0.793045000	-5.378309000	-0.237033000
H	3.212083000	-4.281523000	-0.191363000
H	4.869019000	-2.511631000	0.271089000
H	5.092373000	1.794883000	0.351304000
H	1.202211000	-5.134220000	1.339650000
H	0.837839000	-4.041052000	2.700162000
H	3.453089000	-0.036802000	2.791615000
H	4.887271000	-0.086463000	1.735874000
H	-3.259924000	-1.780020000	2.422644000
H	-4.378697000	-2.437779000	1.204010000
H	-2.631391000	2.173829000	-3.496991000
H	-3.627005000	3.236866000	-2.469313000

H	1.946294000	4.587476000	-2.226798000
H	1.662409000	3.171802000	-3.272418000
H	-5.277852000	-0.806105000	-0.226223000
H	-5.102859000	1.614332000	-0.605340000
H	-2.362659000	4.772279000	-1.170994000
H	0.032426000	5.346053000	-1.080497000
H	3.855143000	3.858125000	-0.173370000
H	-4.113143000	3.377701000	0.600061000
H	-3.211757000	2.843306000	2.040758000
H	1.369653000	4.020437000	2.267452000
H	2.041465000	4.940845000	0.896795000
C	-2.023084000	1.514568000	5.024246000
H	-2.926807000	0.923737000	4.878391000
H	-1.718072000	1.624288000	6.064915000
H	-1.933942000	2.407805000	4.409641000
H	-1.089491000	0.773647000	4.529848000

Imaginary Frequency: $i1105\text{ cm}^{-1}$

⁵P_{Me}

Fe	0.129862000	-0.286659000	2.359964000
C	-0.011076000	3.633228000	1.528065000
N	-1.171362000	3.890037000	0.820241000
C	-0.927731000	4.222609000	-0.579614000
C	0.640465000	4.247935000	-0.670882000
N	1.052631000	3.930684000	0.691622000
N	0.939958000	3.207161000	-1.621242000
C	-0.192061000	2.455975000	-1.932297000
N	-1.300934000	3.175396000	-1.495156000
C	-2.612195000	3.048657000	-2.124369000
N	-3.450153000	2.020526000	-1.569972000
C	-3.609796000	0.802478000	-2.234126000
N	-4.247132000	-0.063819000	-1.336968000
C	-4.409578000	0.521594000	-0.034092000
C	-3.964688000	2.016497000	-0.227008000
N	-2.953607000	2.204042000	0.811332000
C	-2.603770000	1.020417000	1.385918000
N	-3.466058000	0.038574000	0.975236000
C	-4.327489000	-1.479936000	-1.623925000
N	-3.196235000	-2.278754000	-1.154366000
C	-2.100099000	-2.524870000	-1.981437000
N	-1.332111000	-3.518269000	-1.361060000
C	-1.863394000	-3.941260000	-0.095266000
C	-3.170061000	-3.069721000	0.047107000
N	-1.064509000	-3.539945000	1.068677000
C	-1.661404000	-2.531921000	1.762349000
N	-2.906949000	-2.311262000	1.274855000
C	-0.062514000	-3.910264000	-1.911263000
N	1.077050000	-3.191785000	-1.318039000

C	1.887883000	-2.406043000	-2.187683000
N	3.094993000	-2.189598000	-1.532526000
C	3.208070000	-2.940281000	-0.310026000
C	1.903581000	-3.805931000	-0.285995000
N	3.074693000	-2.171473000	0.927651000
C	1.981104000	-2.525891000	1.658838000
N	1.387934000	-3.610669000	1.058942000
C	4.125149000	-1.330293000	-2.115844000
N	3.993542000	0.077156000	-1.806059000
C	3.221279000	0.912951000	-2.623328000
N	3.107375000	2.133200000	-1.956372000
C	3.768580000	2.156443000	-0.680691000
C	4.316082000	0.688748000	-0.544085000
N	2.867692000	2.292922000	0.465340000
C	2.682264000	1.101250000	1.093063000
N	3.557486000	0.178905000	0.597338000
C	-3.675547000	-1.178835000	1.734562000
C	0.149996000	-4.182978000	1.546877000
C	3.885941000	-1.043856000	1.301850000
O	-1.862468000	-2.010429000	-3.045702000
O	1.563668000	-2.008277000	-3.275370000
O	2.779733000	0.647484000	-3.713056000
O	-1.149944000	-1.912032000	2.715254000
O	-1.664995000	0.877707000	2.185552000
O	1.596111000	-1.956345000	2.689618000
O	1.865821000	0.904580000	2.012653000
C	2.166286000	3.125560000	-2.406231000
C	-2.462389000	3.489607000	1.312636000
C	2.397898000	3.562149000	1.032758000
O	-3.302811000	0.564196000	-3.375017000
O	-0.206446000	1.368311000	-2.480202000
O	0.068273000	3.260676000	2.690406000
O	0.196052000	0.764334000	4.161276000
O	0.051835000	-0.686320000	0.114957000
H	0.279877000	-1.523875000	-0.341972000
H	-0.099924000	-0.037810000	-0.601565000
H	-0.082844000	-3.659044000	-2.974558000
H	0.079466000	-4.990169000	-1.786538000
H	5.103998000	-1.693749000	-1.788676000
H	4.045349000	-1.415391000	-3.201548000
H	-4.364961000	-1.568033000	-2.711656000
H	-5.244361000	-1.891212000	-1.189568000
H	-4.085191000	-3.658644000	0.166439000
H	-2.043370000	-5.021160000	-0.064446000
H	2.078462000	-4.869098000	-0.483518000
H	4.132498000	-3.527258000	-0.286401000
H	5.389206000	0.632264000	-0.331432000
H	0.118037000	-5.237685000	1.260870000
H	0.166111000	-4.102626000	2.634705000
H	3.742040000	-0.887373000	2.372105000

H	4.938779000	-1.271930000	1.108899000
H	-3.392076000	-1.002496000	2.773380000
H	-4.738920000	-1.431610000	1.689681000
H	-2.481957000	2.790381000	-3.177750000
H	-3.101986000	4.026079000	-2.050166000
H	2.626851000	4.119682000	-2.394900000
H	1.918447000	2.854794000	-3.435004000
H	-5.435761000	0.409318000	0.333117000
H	-4.773690000	2.743098000	-0.094167000
H	-1.406007000	5.173019000	-0.836517000
H	1.054588000	5.211742000	-0.983532000
H	4.545591000	2.927200000	-0.633994000
H	-3.211576000	4.241579000	1.047593000
H	-2.380086000	3.431586000	2.399206000
H	2.437508000	3.492039000	2.120910000
H	3.094346000	4.335602000	0.694917000
H	0.052974000	1.699507000	3.896577000
C	1.315060000	0.672034000	5.067490000
H	1.446949000	-0.388115000	5.285863000
H	2.219748000	1.068407000	4.596202000
H	1.091619000	1.215533000	5.989003000

³P_{Me}

Fe	0.122390000	-0.309727000	2.232873000
C	-0.031560000	3.590852000	1.631911000
N	-1.189196000	3.871120000	0.924359000
C	-0.939012000	4.231227000	-0.466258000
C	0.628918000	4.271114000	-0.546777000
N	1.035127000	3.923063000	0.809606000
N	0.941532000	3.252676000	-1.517268000
C	-0.178618000	2.483285000	-1.825204000
N	-1.298243000	3.192591000	-1.398619000
C	-2.598402000	3.082471000	-2.055216000
N	-3.453238000	2.051561000	-1.533771000
C	-3.615237000	0.850743000	-2.228420000
N	-4.264505000	-0.033851000	-1.357917000
C	-4.414864000	0.516343000	-0.038117000
C	-3.978148000	2.017989000	-0.194433000
N	-2.972743000	2.184869000	0.851952000
C	-2.596786000	0.984322000	1.369918000
N	-3.455049000	0.007505000	0.943797000
C	-4.322047000	-1.446818000	-1.670869000
N	-3.180932000	-2.237543000	-1.210702000
C	-2.083329000	-2.458774000	-2.042317000
N	-1.310608000	-3.462407000	-1.445480000
C	-1.843020000	-3.923827000	-0.192552000
C	-3.157033000	-3.067059000	-0.032870000
N	-1.051780000	-3.550015000	0.983765000
C	-1.664609000	-2.573476000	1.716792000

N	-2.911072000	-2.349530000	1.219987000
C	-0.036921000	-3.829131000	-2.000044000
N	1.095755000	-3.121751000	-1.375609000
C	1.913489000	-2.316600000	-2.223455000
N	3.122125000	-2.127815000	-1.563367000
C	3.227585000	-2.908721000	-0.358901000
C	1.922063000	-3.773651000	-0.364313000
N	3.082898000	-2.169487000	0.895013000
C	1.979859000	-2.539224000	1.604637000
N	1.401962000	-3.619897000	0.983845000
C	4.152663000	-1.247667000	-2.115279000
N	4.012395000	0.150822000	-1.768908000
C	3.243985000	1.004691000	-2.570443000
N	3.119437000	2.206660000	-1.872889000
C	3.774588000	2.201937000	-0.593591000
C	4.323666000	0.731943000	-0.489654000
N	2.868367000	2.309272000	0.551213000
C	2.679338000	1.102453000	1.147079000
N	3.556099000	0.191783000	0.631288000
C	-3.672323000	-1.220433000	1.690897000
C	0.158722000	-4.204127000	1.450931000
C	3.884654000	-1.047919000	1.305457000
O	-1.846100000	-1.917403000	-3.093569000
O	1.591131000	-1.884783000	-3.298486000
O	2.811784000	0.766926000	-3.670308000
O	-1.172126000	-1.980810000	2.689887000
O	-1.635469000	0.828942000	2.142069000
O	1.574328000	-1.977211000	2.631286000
O	1.856196000	0.884171000	2.056256000
C	2.170560000	3.200480000	-2.300726000
C	-2.483548000	3.456019000	1.393384000
C	2.382998000	3.560807000	1.146016000
O	-3.299682000	0.639823000	-3.372433000
O	-0.176196000	1.386304000	-2.357651000
O	0.041838000	3.173502000	2.778372000
O	0.110740000	0.439169000	4.080500000
O	0.036018000	-0.699978000	0.135473000
H	0.276986000	-1.531073000	-0.331898000
H	-0.089801000	-0.026393000	-0.565648000
H	-0.051973000	-3.543948000	-3.054795000
H	0.112540000	-4.911317000	-1.908660000
H	5.130573000	-1.616032000	-1.791115000
H	4.081239000	-1.303627000	-3.203451000
H	-4.354889000	-1.514734000	-2.760158000
H	-5.234594000	-1.878559000	-1.247709000
H	-4.067995000	-3.667827000	0.056281000
H	-2.015894000	-5.005471000	-0.194510000
H	2.095398000	-4.829492000	-0.597894000
H	4.151847000	-3.495973000	-0.343553000
H	5.395123000	0.672006000	-0.269655000

H	0.132422000	-5.252087000	1.140439000
H	0.170161000	-4.148233000	2.540312000
H	3.729709000	-0.920246000	2.377883000
H	4.940333000	-1.265606000	1.116329000
H	-3.387214000	-1.057992000	2.731536000
H	-4.738239000	-1.461412000	1.641925000
H	-2.451132000	2.840361000	-3.110233000
H	-3.082207000	4.062423000	-1.974796000
H	2.620320000	4.198813000	-2.262875000
H	1.929414000	2.954069000	-3.337211000
H	-5.435775000	0.389207000	0.338227000
H	-4.790927000	2.738019000	-0.050898000
H	-1.424496000	5.180693000	-0.712450000
H	1.038677000	5.244003000	-0.835598000
H	4.550063000	2.972584000	-0.525561000
H	-3.231470000	4.214251000	1.143268000
H	-2.411000000	3.367059000	2.478566000
H	2.420951000	3.465482000	2.232291000
H	3.072170000	4.348957000	0.827908000
H	0.039453000	1.407960000	3.932405000
C	1.199029000	0.149916000	4.989407000
H	1.244648000	-0.935064000	5.069410000
H	2.139779000	0.537269000	4.589407000
H	0.975672000	0.593293000	5.962599000