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Mechanistic Insights on Epoxidation of Alkene by High-Valent Non-Heme Fe(IV) and Fe(V) Oxidants: A Comparative Theoretical Study

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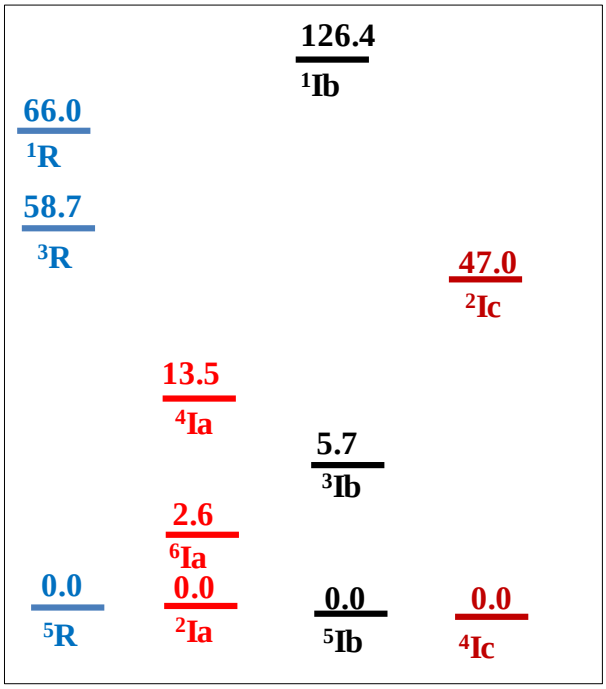


Fig. S1 B3LYP-D2 computed energies of **R**, $\mathbf{I_a}$, $\mathbf{I_b}$ and $\mathbf{I_c}$ (energy in kJ/mol).

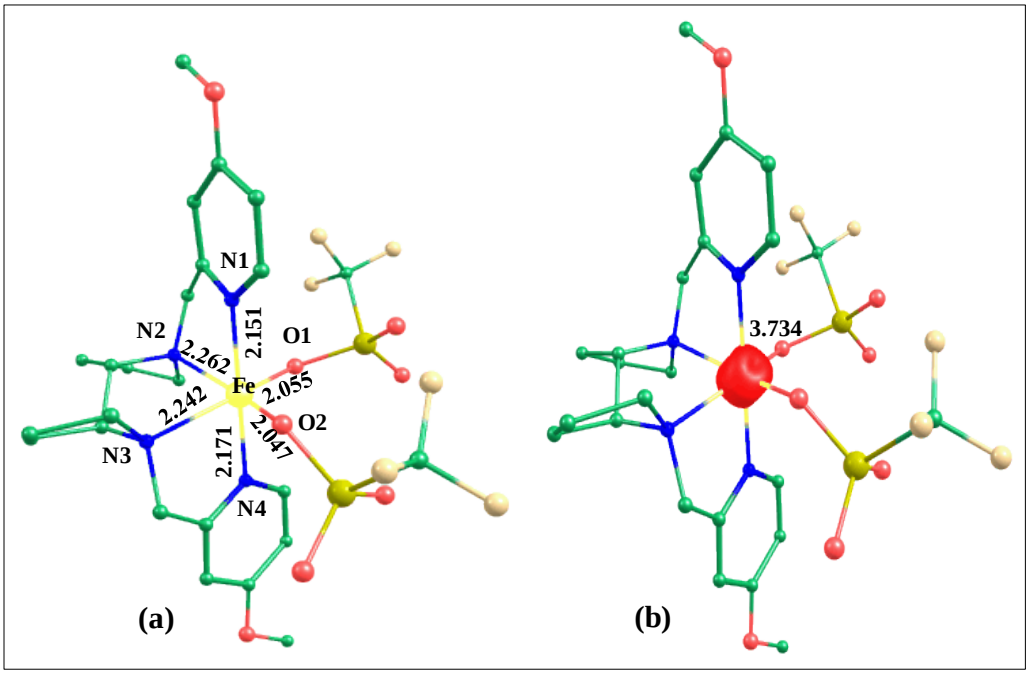


Fig. S2 B3LYP-D2 optimized structures of a) ^{5}**R** b) its spin density plot.

Table S1 B3LYP-D2 computed relative energy of isomers $\mathbf{I_a}$ and $\mathbf{I_a'}$ (ΔG in kJ/ mol).

Species	Relative Energy	Overall Relative Energy
$\mathbf{I}_a$		
$^6\mathbf{I}_a$	2.6	2.6
$^4\mathbf{I}_a$	13.5	13.5
$^2\mathbf{I}_a$	0	0
$\mathbf{I}_a'$		
$^6\mathbf{I}_a'$	2.4	2.7
$^4\mathbf{I}_a'$	21.0	21.4
$^2\mathbf{I}_a'$	0	0.3

[There are two possible isomers of $\mathbf{I_a}$ species. In one isomer, the -OOH group is *trans* to the alkylated amine ($\mathbf{I_a}$), and in the other, the -OOH group is *trans* to the pyridine ring ($\mathbf{I_a'}$). Our computed data reveals that both the isomers show a minor difference in relative energy (0.3 kJ/mol) $\mathbf{I_a}$ (see above table). Here, we have restricted our calculations on the -OOH group *trans* to the alkylated ammonia group ($\mathbf{I_a}$)].

Table S2 B3LYP-D2 computed structural parameters of main Fe species.

Spin states	Bond lengths (Å)										Bond angle (°)					
	Fe-N1	**Fe-N2**	**Fe-N3**	**Fe-N4**	**Fe-N_{avg}**	**Fe-O1**	**Fe-O2**	**O2-O3**	**O3-H2**	**O4-H2**	**∠Fe-N1-N4**	**∠N1-Fe-N2**	**∠N2-Fe-N3**	**∠N3-Fe-N4**	**∠Fe-O1-C1**	**∠Fe-O2-O3**
^{5}**R**	2.151	2.262	2.242	2.171	2.206	2.055	2.047	--	--	--	178.3	77.4	78.7	76.3	--	--
^{3}**R**	1.985	2.199	2.221	1.991	2.099	2.093	2.014	--	--	--	179.0	79.9	79.7	79.4	--	--
^{1}**R**	1.988	2.052	2.048	1.987	2.018	1.985	1.976	--	--	--	178.6	81.5	85.2	81.5	--	--
^{6}**I_a**	2.123	2.163	2.197	2.120	2.150	2.067	1.934	1.497	1.568	1.021	171.5	77.2	81.8	77.4	140.1	119.4
^{4}**I_a**	2.029	2.195	2.059	1.984	2.066	2.155	1.844	1.522	1.609	1.017	176.1	81.7	83.3	78.1	134.8	114.5
^{2}**I_a**	1.999	2.052	2.022	1.981	2.013	1.995	1.840	1.520	1.512	1.029	176.3	80.5	85.0	81.1	137.8	118.3
$^{6}TS_{hom}$	2.085	2.154	2.118	2.057	2.103	2.132	1.678	1.996	--	0.980	174.3	78.9	82.8	78.3	131.5	152.2
$^{4}TS_{hom}$	2.040	2.164	2.085	2.005	2.073	2.205	1.663	2.135	--	0.980	174.8	80.6	82.9	79.2	130.6	118.4
$^{2}TS_{hom}$	2.006	2.135	2.017	1.983	2.035	2.037	1.655	3.217	--	0.996	175.5	79.9	84.5	84.9	134.0	110.9
^{5}**I_b**	1.989	2.050	2.069	1.950	2.014	2.197	1.654	--	--	--	176.6	81.3	84.4	80.1	121.5	--
^{3}**I_b**	1.989	2.002	2.028	1.989	2.002	2.029	1.656	--	--	--	176.6	81.0	86.6	82.5	111.0	--
^{1}**I_b**	1.955	2.002	2.028	1.989	1.993	2.058	1.656	--	--	--	176.6	81.0	86.6	82.5	111.0	--
$^{6}TS_{het}$	2.086	2.152	2.116	2.072	2.106	2.101	1.691	1.934	1.028	1.575	174.2	78.6	83.0	78.2		142.9
$^{4}TS_{het}$	1.967	2.009	2.095	2.004	2.018	1.976	1.672	2.179	1.042	1.510	174.3	78.5	84.3	174.3		137.5
$^{2}TS_{het}$	1.970	2.052	2.098	1.984	2.026	1.900	1.668	2.476	0.987	1.748	173.2	79.6	83.4	81.6		134.9
^{4}**I_c**	1.949	2.090	2.064	1.995	2.024	1.829	1.647	--	--	--	175.6	80.9	83.5	79.6	123.9	—
^{2}**I_c**	1.971	2.010	1.950	2.006	1.984	1.990	1.655	--	--	--	175.9	80.0	84.6	81.6	125.1	--

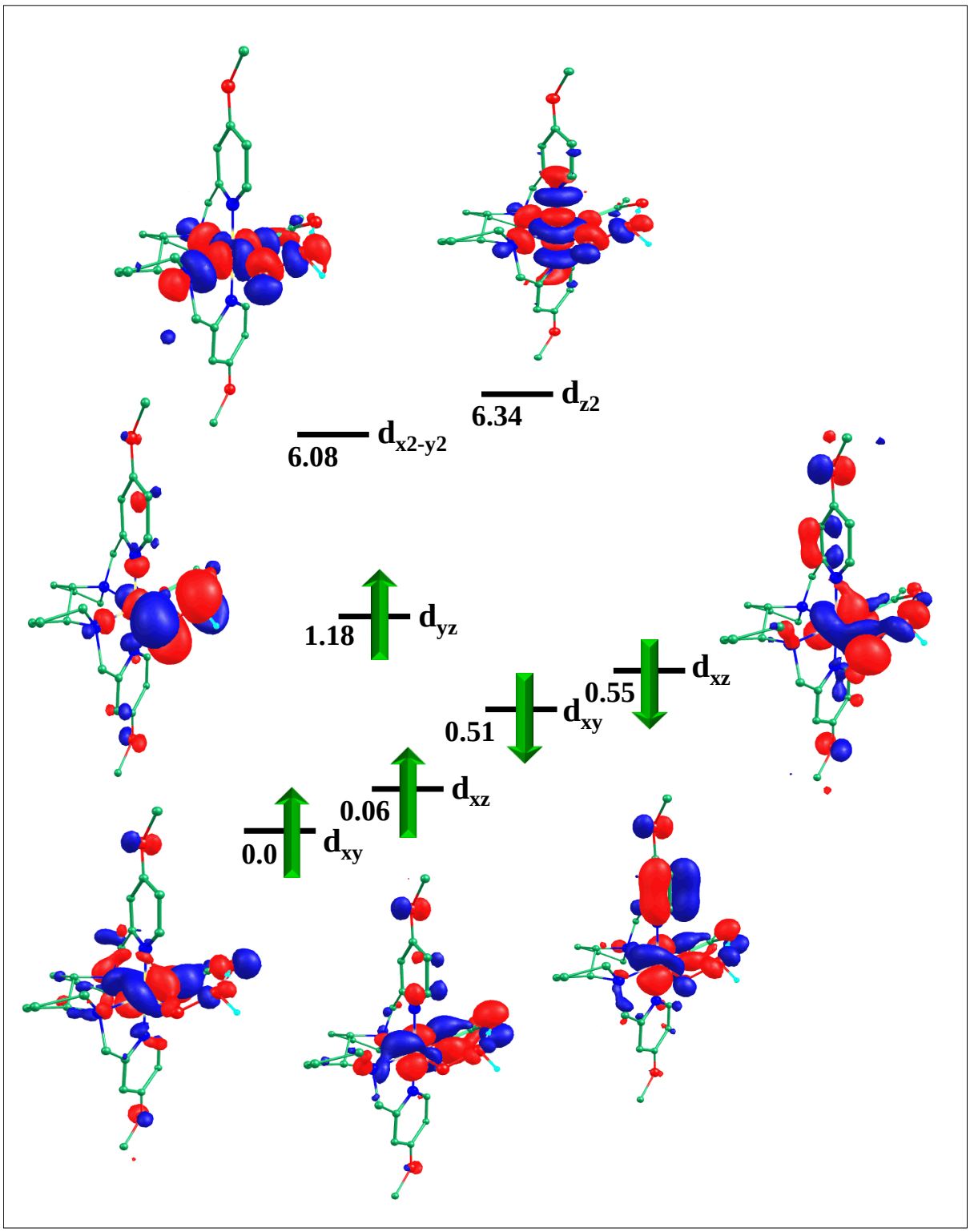


Fig. S3 B3LYP-D2 computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin of $^{2}\mathbf{I}_{a}$ species (energies are given in eV).

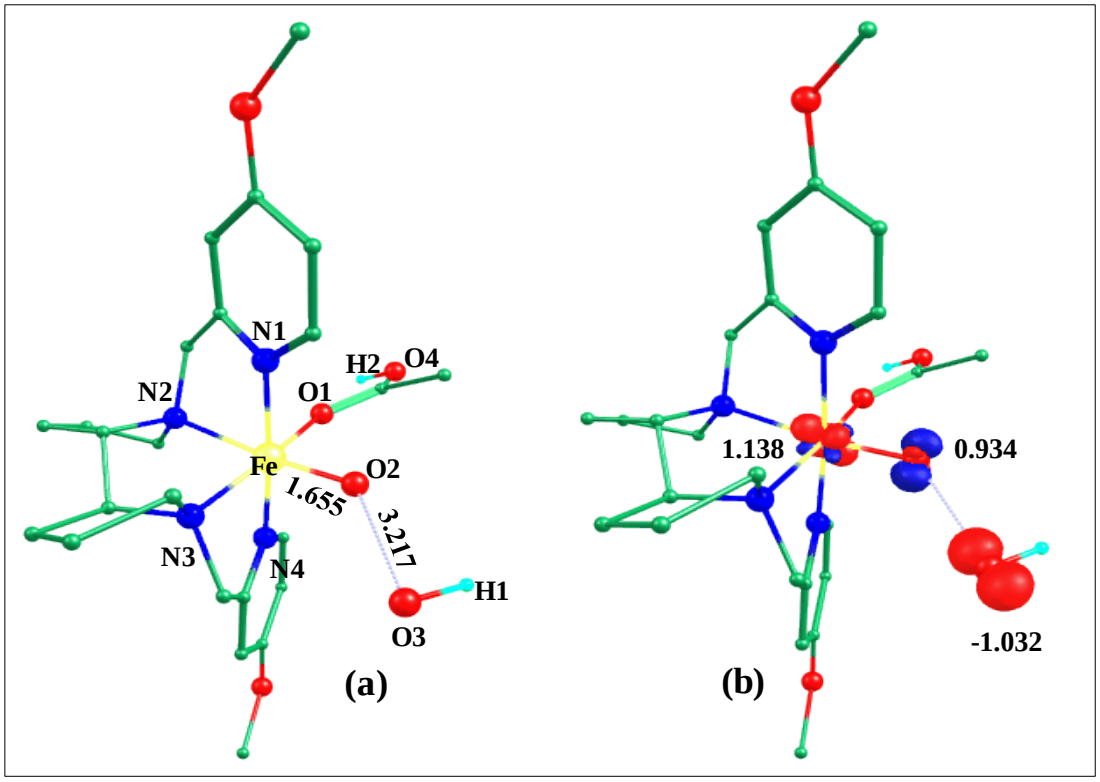


Fig. S4 B3LYP-D2 optimized structures of a) $^{2}TS_{hom}$ b) its spin density plot.

Table S3. B3LYP-D2 computed spin density values of main Fe species.

Spin states	Fe	O1	O2	O3
		R		
^{5}**R**	3.734	0.045	0.038	--
^{3}**R**	1.955	0.026	0.009	--
^{1}**R**	0.000	--	--	--
		I_a		
$^{6}I_a$	4.051	0.071	0.313	0.034
$^{4}I_a$	2.778	0.054	0.082	-0.004
$^{2}I_a$	0.968	-0.005	0.119	-0.002
		TS_{hom}		
$^{6}TS_{hom}$	3.303	0.039	0.559	0.848
$^{4}TS_{hom}$	2.625	0.043	-0.574	0.804
$^{2}TS_{hom}$	1.138	-0.005	0.934	-1.032
		I_b		
$^{5}I_b$	1.630	0.061	1.208	--
$^{3}I_b$	0.973	-0.006	0.102	--
$^{1}I_b$	0.973	-0.006	0.102	--
		TS_{het}		
$^{6}TS_{het}$	3.381	0.066	0.534	0.758
$^{4}TS_{het}$	2.100	-0.007	0.432	0.548
$^{2}TS_{het}$	1.663	-0.049	-0.186	-0.164
		I_c		
$^{4}I_c$	1.779	0.075	1.114	--
$^{2}I_c$	1.084	-0.028	0.971	--

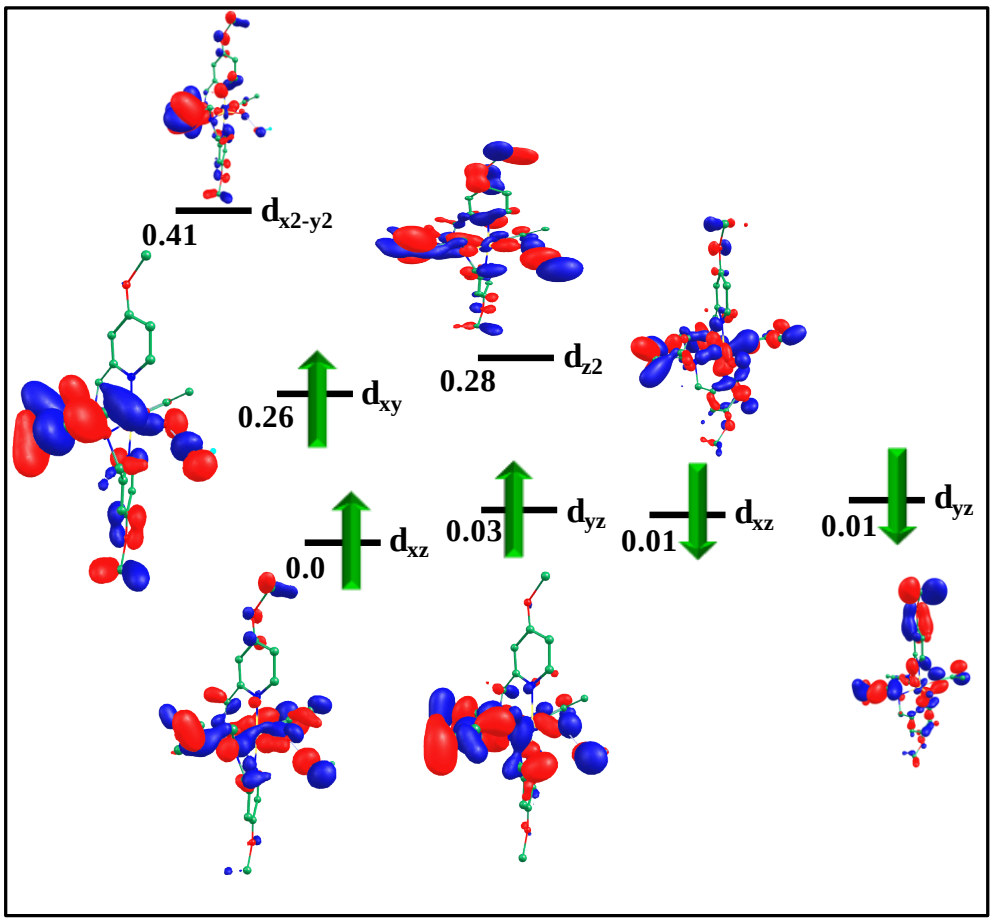


Fig. S5 Eigenvalue plot incorporating energies of d-based orbitals for alpha spin for $^{2}TS_{hom}$ (energies are given in eV).

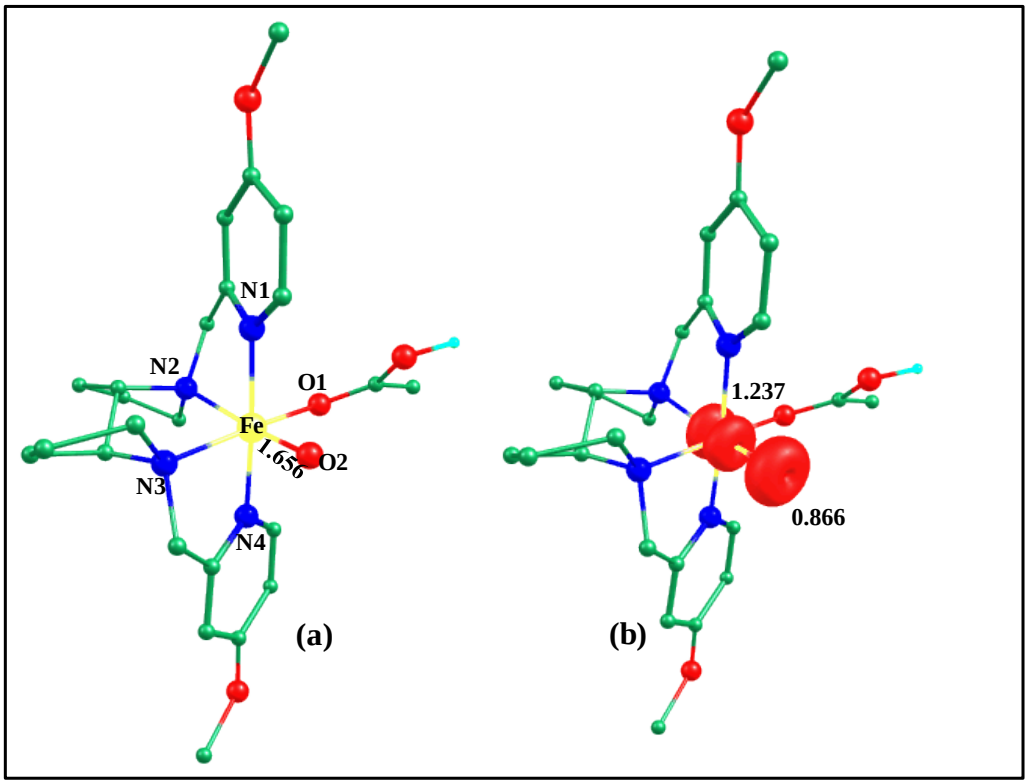


Fig. S6 B3LYP-D2 a) optimized structure and b) spin density plot of $^{3}\mathbf{I_b}$.

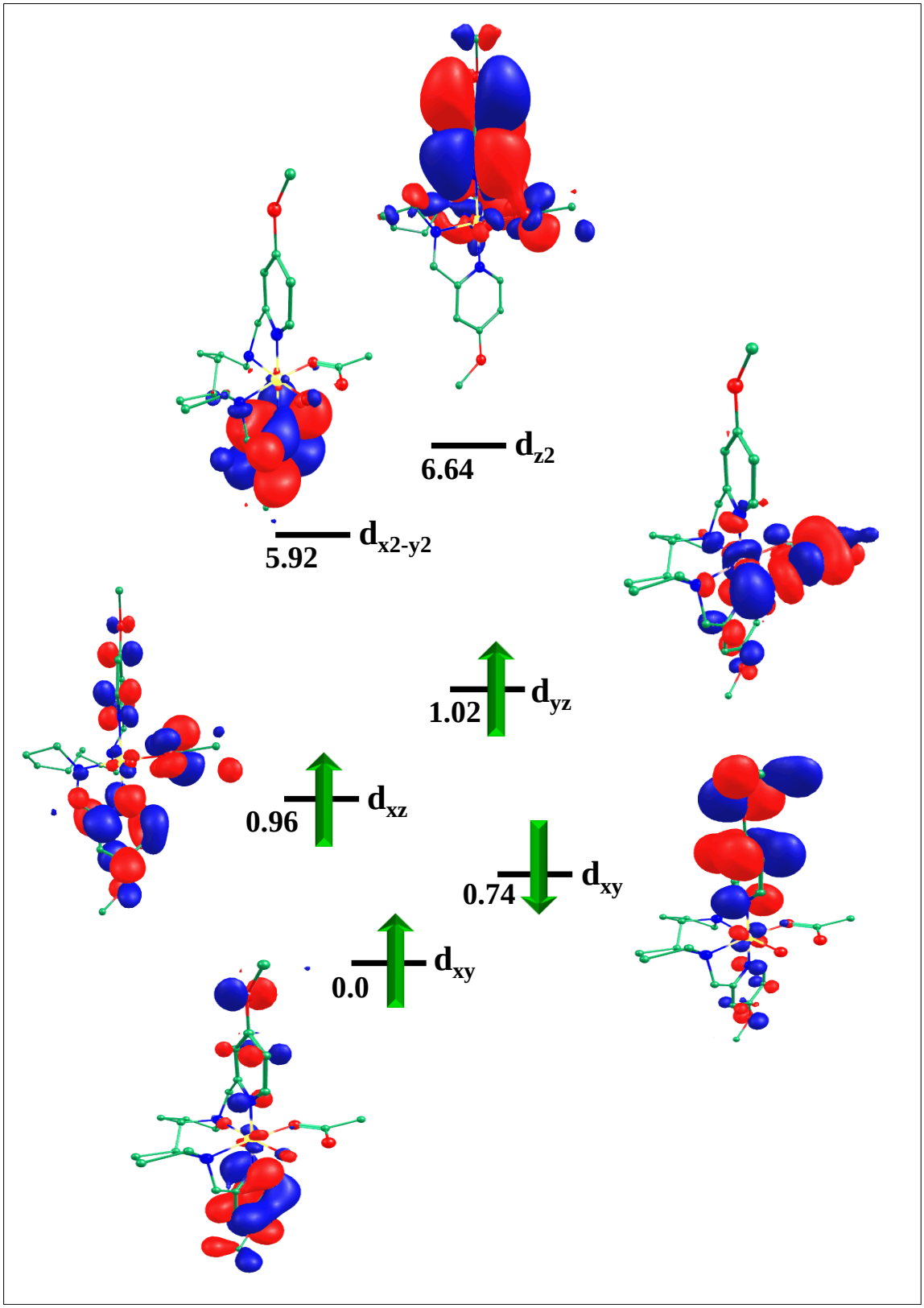


Fig. S7 B3LYP-D2 computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin of $^{3}\mathbf{I_b}$ species (energies are given in eV).

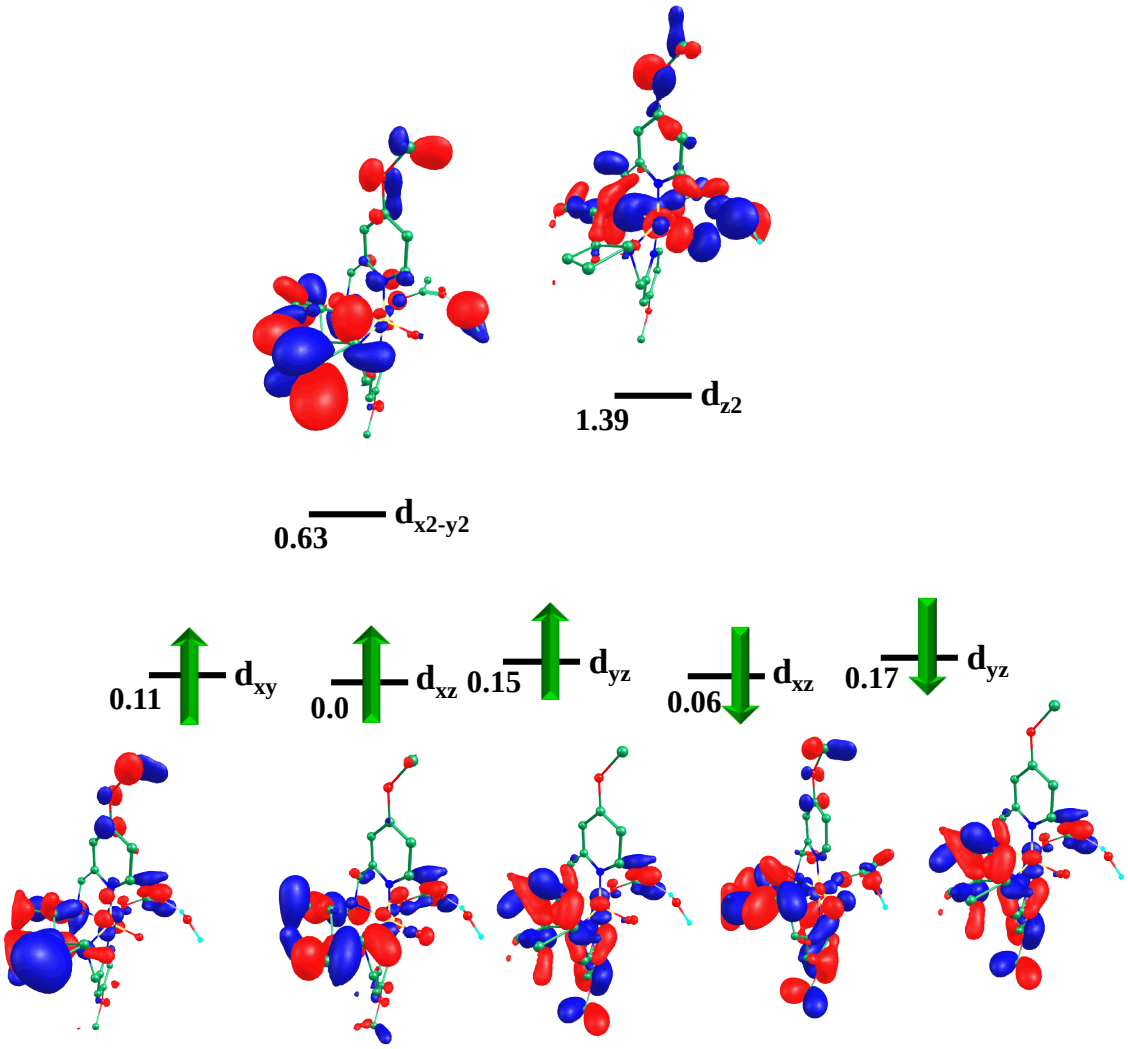


Fig. S8 B3LYP-D2 computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin of $^{2}TS_{het}$ species (energies are given in eV).

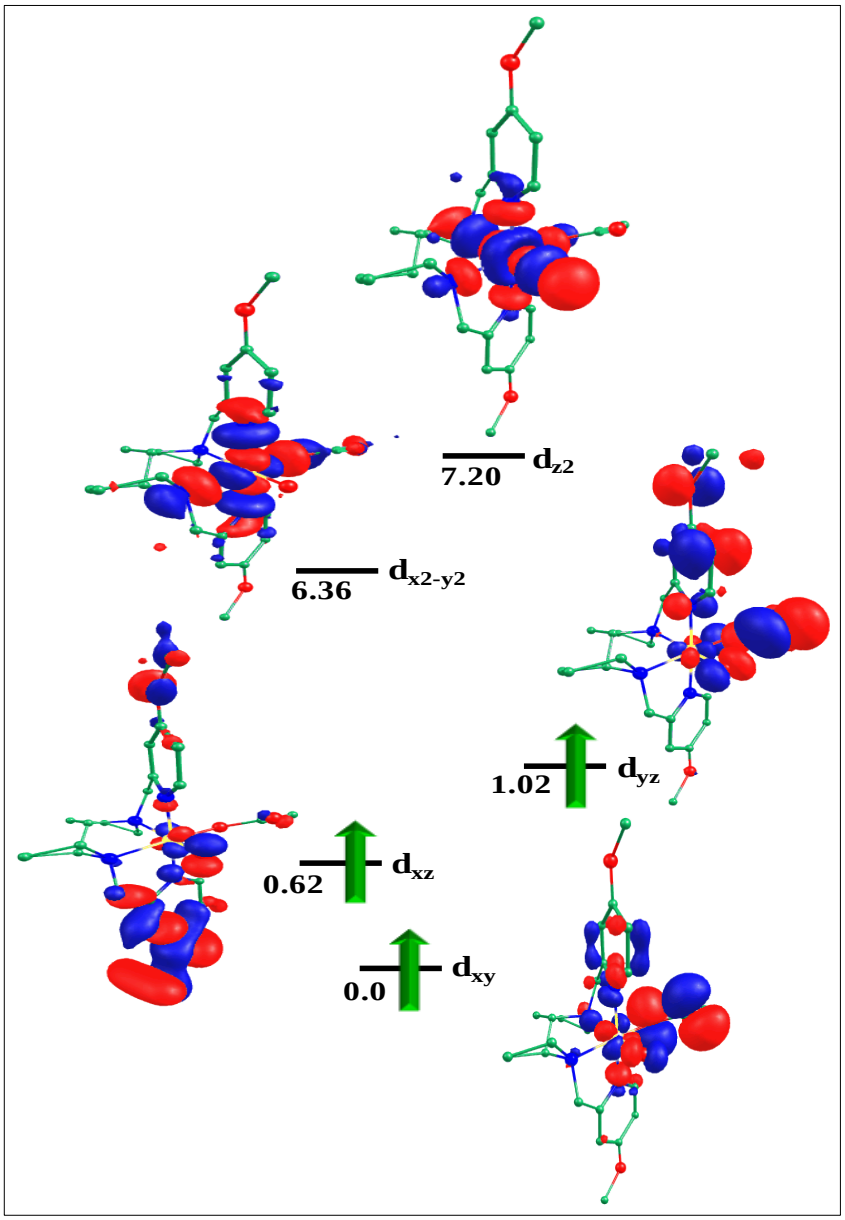


Fig. S9 B3LYP-D2 computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha spin of $^4\mathbf{I}_c$ species (energies are given in eV).

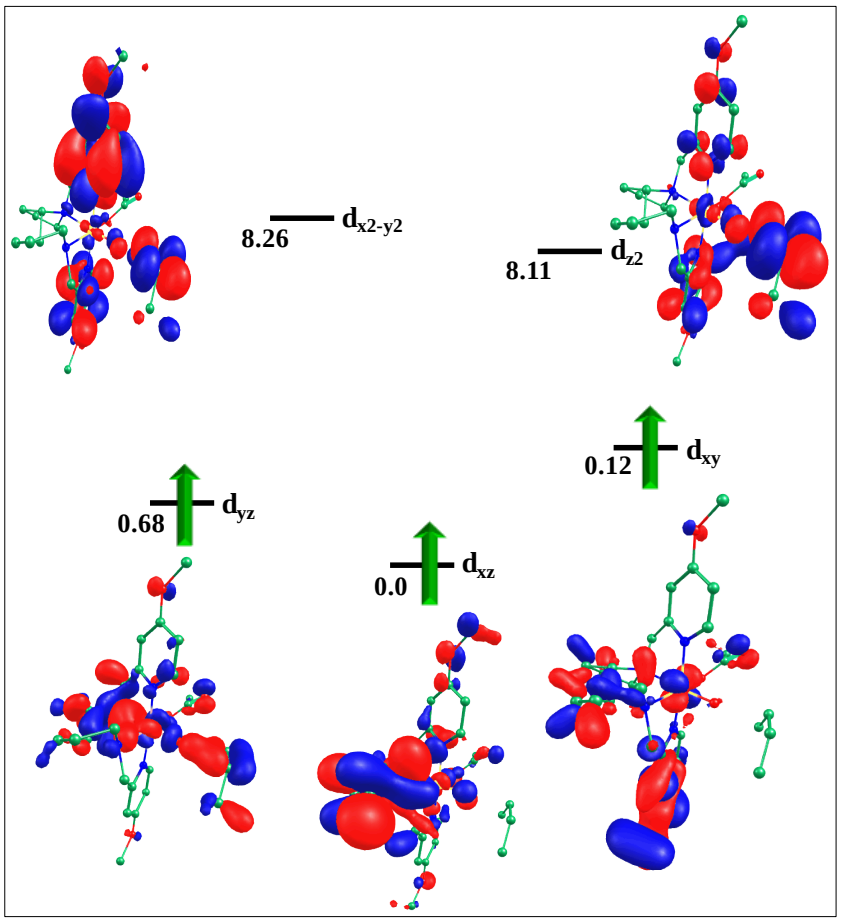
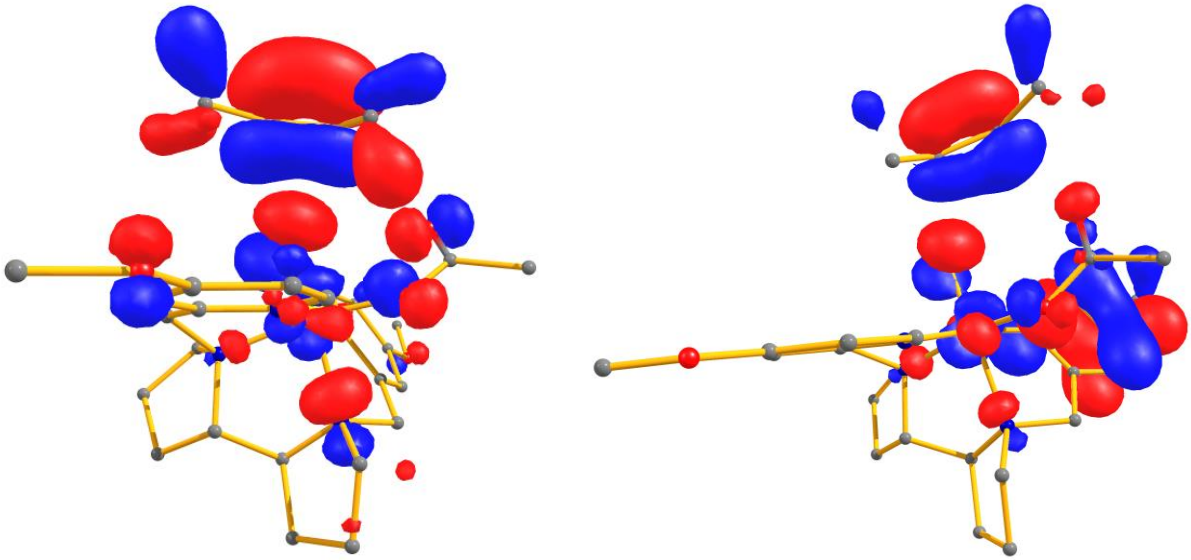


Fig. S10 B3LYP-D2 computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha spin of ^{4}tsI species (energies are given in eV).



(a) **(b)**

Fig. S11 HOMO-2 and HOMO-1 of transition state for (a) ^{4}tsI and (b) ^{4}tsII.

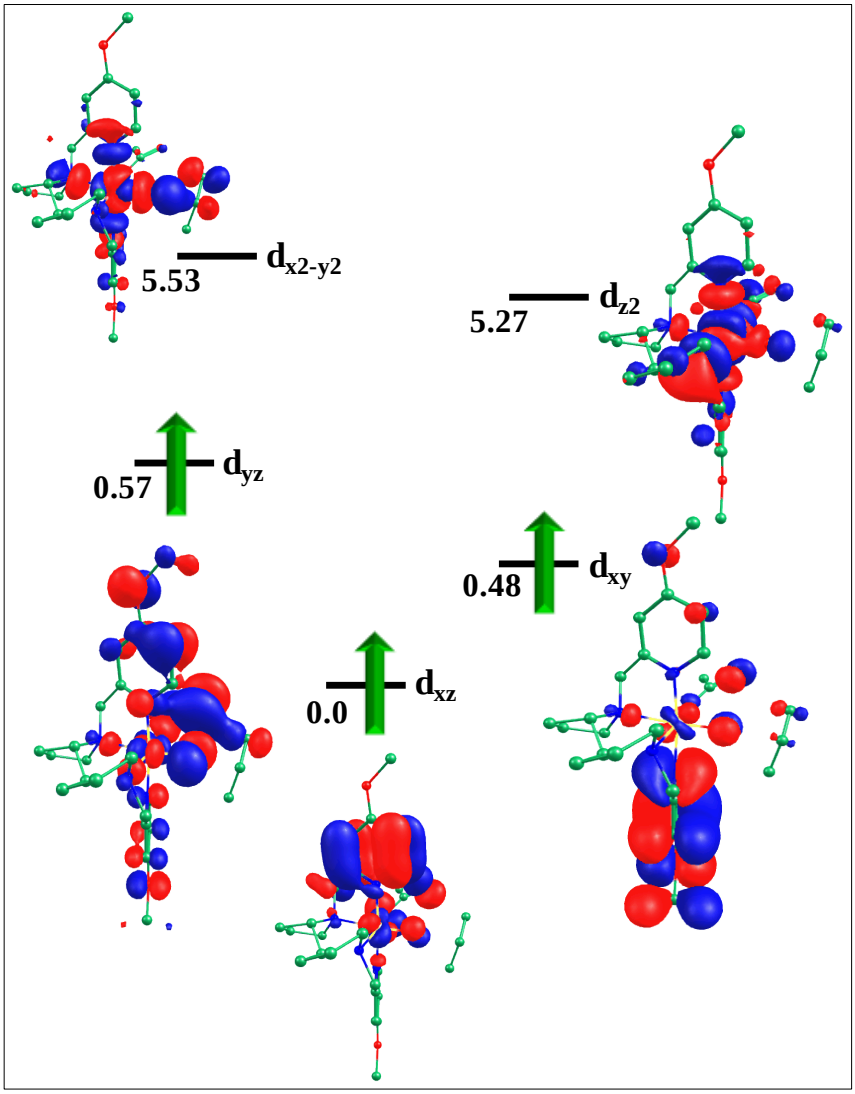


Fig. S12 B3LYP-D2 computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha spin of ^{4}tsII species (energies are given in eV).

Table S4 B3LYP-D2 computed structural parameters of Fe species generated during the epoxidation reaction.

Spin States	Bond Lengths (Å)				Bond Angles (º)				Spin Density Values		
	Fe-O2	O2-C1	O2-C2	C1-C2	∠Fe-O2-C1	∠Fe-O2-C2	∠O2-C1-C2	∠O2-C2-C1	Fe	O2	C1
^{4}tsI	1.690	2.397	2.340	1.403	129.1	159.8	70.5	74.9	1.435	0.836	0.337
^{2}tsI	1.732	2.556	2.515	1.370	127.2	144.2	72.6	75.9	1.041	0.097	0.138
^{6}intI	2.093	1.543	1.548	1.483	132.8	132.5	61.4	61.1	4.086	0.055	0.011
^{4}intI	2.175	1.535	1.542	1.482	132.8	135.0	61.4	60.9	2.842	0.038	0.007
^{2}intI	1.998	1.538	1.546	1.485	136.1	135.8	61.4	60.9	1.054	-0.002	-0.0002
^{4}tsII	1.677	2.968	2.242	1.412	141.5	141.5	106.4	46.4	1.329	0.837	0.444
^{2}tsII	1.661	3.151	2.380	1.416	133.1	121.7	109.5	45.3	1.231	0.763	-0.491

Computational details for EPR parameter calculations:

All calculations in this work were performed using the Orca 5.0 suite of programs.[1-3] The EPR calculations were optimized using the B3LYP[4-6] functional with D3BJ dispersion[7] corrections, and the ZORA-def2-TZVP[8] basis set for all atoms, incorporating the conductor-like polarizable continuum model (CPCM) using CH_3CN used as solvents.[9-10] This study was carried out using tight convergence (TightSCF with NoTrah). The RIJCOSX approximation was used to speed up the calculations.[11]

Table S5 Calculated EPR parameters for the **R**, **Ia**, **Ib** and **Ic**.

Species	g_{xx}	g_{yy}	g_{zz}	g_{iso}	D	E/D
^{5}**R**	2.020	2.043	2.067	2.043	-3.65	0.05
^{2}**Ia**	2.022	2.116	2.137	2.092	-	-
^{3}**Ib**	2.007	2.018	2.025	2.017	4.47	0.04
^{4}**Ic**	2.006	2.019	2.020	2.015	-0.89	0.15
^{2}**Ic**	2.004	2.027	2.044	2.025	-	-

Table S6 DFT computed of the ^{57}Fe and ^{17}O ferryl anisotropic hyperfine values for the **R**, **Ia**, **Ib** and **Ic**.

Species	^{57}Fe hyperfine (MHz)			^{17}O hyperfine (MHz)		
	$^{57Fe}A_{xx}$	$^{57Fe}A_{yy}$	$^{57Fe}A_{zz}$	$^{7O}A_{xx}$	$^{7O}A_{yy}$	$^{7O}A_{zz}$
^{5}**R**	-4.45	-21.52	-22.44	-15.35	-13.91	-18.85
^{2}**Ia**	-2.09	-10.08	-37.38	-51.34	20.30	5.52
^{3}**Ib**	5.30	-21.71	-20.33	46.62	-42.06	-56.08
^{4}**Ic**	-8.00	-12.03	-19.23	-32.43	-49.45	41.42
^{2}**Ic**	14.27	-43.27	-39.78	92.40	-109.11	-84.49

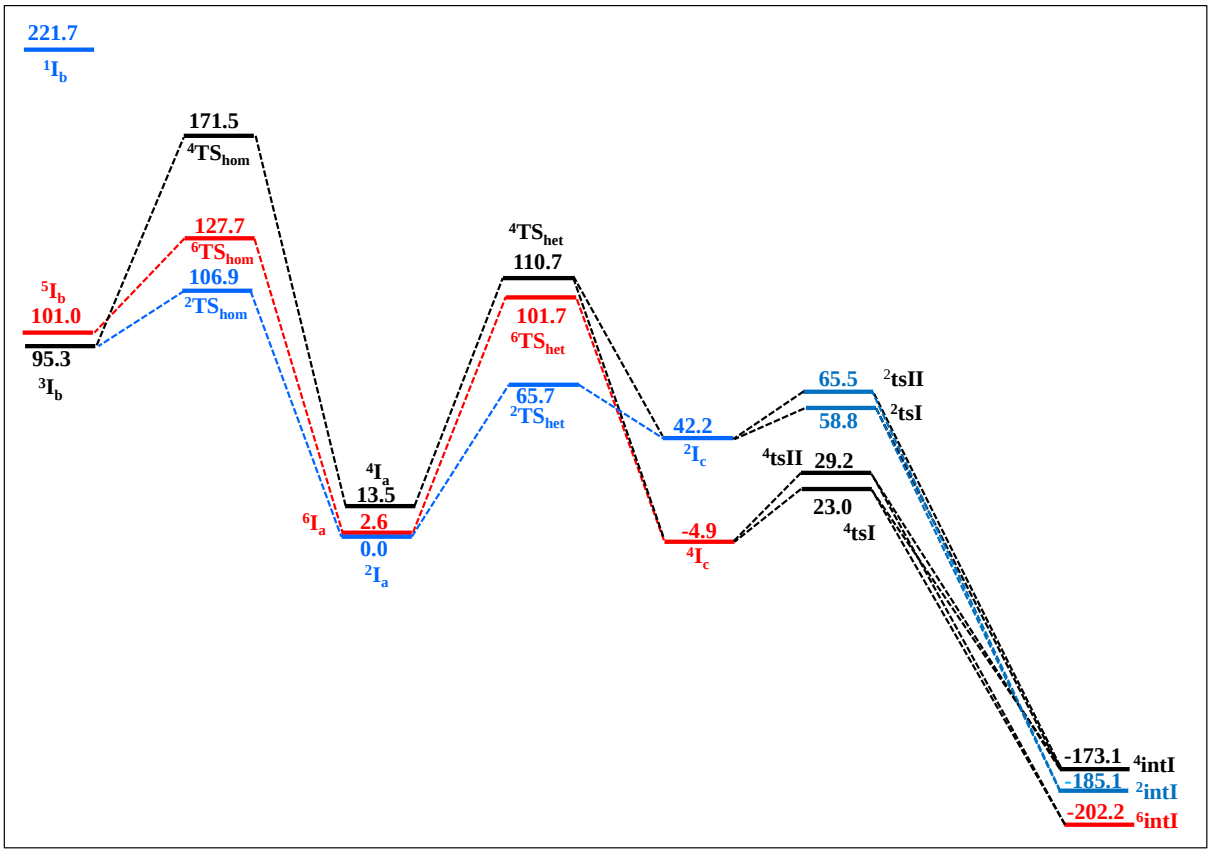


Fig. S13 B3LYP-D2 computed potential energy surface (ΔG in kJ/mol) for the homolytic and heterolytic O•••O bond cleavage for $\mathbf{I_a}$ species.

References:

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---------- *XYZ coordinates* ----------

$^{2}I_{a}$

Fe	-0.065664000	0.384227000	-0.255380000
O	0.712949000	2.031409000	-2.500134000
O	-6.150601000	0.944498000	-0.059364000
N	-2.028853000	0.584521000	-0.072779000
H	0.702338000	3.717764000	2.643014000
C	-2.663554000	1.545253000	0.659413000
H	-2.026950000	2.201481000	1.234299000
C	0.877248000	3.178914000	0.580422000
O	6.018859000	-0.305219000	0.092292000
N	-0.627533000	-1.433229000	-0.942091000
H	0.563320000	5.075123000	1.486424000
C	-4.039065000	1.666695000	0.664789000
H	-4.536426000	2.430875000	1.247698000
O	-0.243148000	0.963577000	-1.993319000
H	2.145388000	4.374664000	1.798900000
C	-4.813848000	0.774379000	-0.110597000
N	0.214424000	-0.576598000	1.537038000
N	1.918995000	0.151092000	-0.315150000
C	-4.155351000	-0.217842000	-0.867428000
H	-4.706030000	-0.922314000	-1.476742000
H	0.222414000	2.378725000	-3.276766000
C	-2.767697000	-0.270578000	-0.830409000
O	0.232887000	2.086491000	0.741644000
C	-7.044482000	0.078223000	-0.850524000
H	-8.045295000	0.442166000	-0.628262000
H	-6.933907000	-0.963078000	-0.530959000
H	-6.822549000	0.188505000	-1.916827000
C	-1.948500000	-1.228491000	-1.645441000
H	-2.456971000	-2.187120000	-1.790127000
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C	-0.815629000	-2.392852000	0.231387000
H	-1.806521000	-2.210533000	0.655082000
C	0.245997000	-2.078027000	1.278678000
H	1.232980000	-2.333807000	0.884322000
C	-0.045049000	-2.748075000	2.650884000

H	-0.783966000	-3.547306000	2.533173000
H	0.856548000	-3.203740000	3.068008000
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H	-1.816117000	-0.517604000	2.138819000
H	-0.756922000	0.563452000	3.064762000
C	1.553334000	-0.116125000	2.057230000
H	1.912310000	-0.785673000	2.845593000
H	1.404448000	0.878715000	2.484219000
C	2.510498000	-0.064503000	0.903284000
C	3.875998000	-0.225043000	1.037457000
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C	6.958456000	-0.242003000	-1.045172000
H	7.939043000	-0.389035000	-0.597673000
H	6.895758000	0.739825000	-1.524566000
H	6.734925000	-1.042624000	-1.757232000
C	1.080238000	4.132844000	1.707991000
O	1.393664000	3.538243000	-0.572641000
H	1.162941000	2.939435000	-1.377383000

$^{2}TS_{hom}$

Fe	-0.028449000	0.447131000	-0.173381000
O	-6.106797000	0.852443000	0.105142000
N	-1.979852000	0.610357000	0.054749000
H	0.794323000	3.348160000	-1.546409000
C	-2.635485000	1.501712000	0.851395000
H	-2.015704000	2.136287000	1.466900000
C	0.815138000	3.266856000	0.568134000
O	6.063593000	-0.223214000	0.041275000
N	-0.548439000	-1.346208000	-0.896460000
H	2.361501000	2.959845000	-0.845091000
C	-4.013377000	1.583042000	0.870317000
H	-4.529742000	2.292010000	1.504164000
O	-0.018351000	1.188880000	-1.700870000
H	1.761971000	4.642634000	-0.753206000
C	-4.766883000	0.722780000	0.038027000
N	0.290510000	-0.587185000	1.618859000
N	1.958417000	0.214203000	-0.237064000
C	-4.086125000	-0.197973000	-0.786466000
H	-4.618788000	-0.872184000	-1.443787000

C	-2.698067000	-0.215722000	-0.757313000
O	0.275183000	2.161718000	0.876636000
C	-6.980869000	0.020046000	-0.743760000
H	-7.990215000	0.336920000	-0.490358000
H	-6.837004000	-1.037979000	-0.502193000
H	-6.768760000	0.215298000	-1.799713000
C	-1.839846000	-1.064458000	-1.637948000
H	-2.321944000	-1.985306000	-1.973573000
H	-1.487080000	-0.456345000	-2.476640000
C	0.430848000	-2.036059000	-1.824878000
H	1.420937000	-1.954730000	-1.376307000
H	0.424507000	-1.525759000	-2.789566000
C	-0.047589000	-3.498656000	-1.847589000
H	0.770821000	-4.181804000	-2.087789000
H	-0.823624000	-3.638707000	-2.606312000
C	-0.621262000	-3.747746000	-0.416970000
H	0.050523000	-4.376204000	0.177007000
H	-1.586460000	-4.258450000	-0.459441000
C	-0.753169000	-2.343004000	0.236046000
H	-1.743077000	-2.166742000	0.664564000
C	0.313079000	-2.077610000	1.294281000
H	1.296245000	-2.320396000	0.882526000
C	0.029298000	-2.810245000	2.635958000
H	-0.725502000	-3.589666000	2.489339000
H	0.927819000	-3.301884000	3.017313000
C	-0.472507000	-1.708113000	3.619546000
H	0.293805000	-1.479829000	4.366905000
H	-1.373324000	-2.012684000	4.158141000
C	-0.740908000	-0.484896000	2.721811000
H	-1.726235000	-0.548082000	2.259983000
H	-0.645481000	0.481161000	3.220706000
C	1.640798000	-0.152734000	2.125058000
H	2.018140000	-0.847419000	2.883093000
H	1.507582000	0.828593000	2.589604000
C	2.575283000	-0.055950000	0.953840000
C	3.946347000	-0.209171000	1.045195000
H	4.430050000	-0.435640000	1.987270000
C	4.734859000	-0.066530000	-0.118756000
C	4.092570000	0.216616000	-1.344486000
H	4.651105000	0.328872000	-2.263810000
C	2.710377000	0.345610000	-1.361041000
H	2.160225000	0.559830000	-2.268053000
C	6.974558000	-0.097981000	-1.114791000
H	7.965860000	-0.267894000	-0.700274000
H	6.900592000	0.908269000	-1.538779000
H	6.732746000	-0.859450000	-1.862794000
C	1.473919000	3.591770000	-0.723172000

O	0.827844000	4.267466000	1.457113000
H	0.390170000	4.067069000	2.314995000
O	-0.879949000	0.589634000	-3.919801000
H	-0.748875000	1.563687000	-4.041681000

$^{2}TS_{het}$

Fe	0.058615000	-0.458015000	-0.126219000
O	6.121301000	-0.981963000	0.139001000
N	2.012131000	-0.634426000	0.066096000
H	-1.124687000	-3.457576000	2.908387000
C	2.640475000	-1.437066000	0.972424000
H	1.996383000	-1.966452000	1.659368000
C	-0.824978000	-2.993207000	0.826368000
O	-5.971055000	0.381235000	0.343313000
N	0.613956000	1.206037000	-1.191442000
H	-0.029967000	-4.555671000	2.041606000
C	4.015420000	-1.552269000	0.995686000
H	4.515739000	-2.187386000	1.715037000
O	0.102438000	-1.379894000	-1.516586000
H	-1.777903000	-4.670375000	1.753864000
C	4.787631000	-0.829129000	0.056054000
N	-0.107066000	0.906686000	1.458982000
N	-1.899812000	-0.136491000	-0.136582000
C	4.126815000	-0.009264000	-0.886826000
H	4.676826000	0.553535000	-1.629390000
C	2.740929000	0.050146000	-0.859377000
O	-0.225250000	-1.839944000	1.147985000
C	7.020834000	-0.295697000	-0.810617000
H	8.019595000	-0.607037000	-0.512622000
H	6.909068000	0.788664000	-0.710684000
H	6.802732000	-0.624518000	-1.831483000
C	1.912181000	0.810158000	-1.856418000
H	2.432465000	1.695504000	-2.234892000
H	1.655190000	0.159751000	-2.699586000
C	-0.380822000	1.724672000	-2.207837000
H	-1.360558000	1.726824000	-1.729791000
H	-0.406365000	1.050354000	-3.065285000
C	0.100698000	3.155337000	-2.502582000
H	-0.715998000	3.784649000	-2.864572000
H	0.877001000	3.151484000	-3.274379000
C	0.674686000	3.660082000	-1.142967000
H	-0.015473000	4.357548000	-0.657004000
H	1.621858000	4.187226000	-1.280896000
C	0.854349000	2.391502000	-0.258990000
H	1.866741000	2.299697000	0.143174000
C	-0.150676000	2.317044000	0.883943000
H	-1.156065000	2.494351000	0.493493000

C	0.212756000	3.261397000	2.064344000
H	0.945115000	4.008114000	1.740648000
H	-0.666109000	3.805838000	2.418353000
C	0.792695000	2.336851000	3.181219000
H	0.088472000	2.249570000	4.014166000
H	1.732369000	2.718809000	3.587835000
C	0.995444000	0.972380000	2.492954000
H	1.948668000	0.938550000	1.965744000
H	0.924490000	0.106904000	3.153401000
C	-1.424977000	0.581171000	2.118703000
H	-1.733166000	1.397232000	2.780297000
H	-1.268362000	-0.323289000	2.711779000
C	-2.432203000	0.327977000	1.038658000
C	-3.791009000	0.514881000	1.190870000
H	-4.209025000	0.895630000	2.114403000
C	-4.656908000	0.187850000	0.121343000
C	-4.099494000	-0.306746000	-1.075401000
H	-4.716505000	-0.587227000	-1.917878000
C	-2.722514000	-0.457995000	-1.170695000
H	-2.261042000	-0.884630000	-2.055166000
C	-6.959660000	0.043886000	-0.702082000
H	-7.921827000	0.282841000	-0.254389000
H	-6.897303000	-1.022336000	-0.940423000
H	-6.783552000	0.656727000	-1.591516000
C	-0.960119000	-3.977306000	1.961325000
O	-1.212992000	-3.259750000	-0.333502000
O	-1.591469000	-2.531983000	-2.906868000
H	-0.970063000	-2.877415000	-3.575344000
H	-1.470264000	-2.991672000	-2.041283000

$^3\mathbf{I}_\mathbf{b}$

Fe	-0.042110000	0.442182000	-0.346786000
O	-6.134133000	0.872711000	-0.202575000
N	-2.005974000	0.617017000	-0.159303000
H	0.041711000	4.485220000	1.758594000
C	-2.672199000	1.569680000	0.552144000
H	-2.059470000	2.250214000	1.124614000
C	0.793512000	3.292155000	0.155825000
O	6.036473000	-0.220250000	0.012940000
N	-0.554519000	-1.402514000	-0.939952000
H	0.007493000	5.276718000	0.165242000
C	-4.050609000	1.655545000	0.539655000
H	-4.575355000	2.413293000	1.106702000
O	-0.057526000	1.014824000	-1.901553000
H	1.548091000	5.107014000	1.030064000
C	-4.792419000	0.734613000	-0.234354000
N	0.238939000	-0.446933000	1.542870000

N	1.937275000	0.210543000	-0.356139000
C	-4.100419000	-0.251788000	-0.967937000
H	-4.625322000	-0.979159000	-1.572934000
C	-2.712399000	-0.268476000	-0.912651000
O	0.213208000	2.247458000	0.544960000
C	-6.994398000	-0.023799000	-0.996865000
H	-8.007140000	0.317564000	-0.793538000
H	-6.863217000	-1.058592000	-0.664066000
H	-6.759292000	0.080009000	-2.060995000
C	-1.853542000	-1.220917000	-1.692259000
H	-2.343339000	-2.187225000	-1.848640000
H	-1.596898000	-0.781990000	-2.661717000
C	0.443365000	-2.165963000	-1.783563000
H	1.424223000	-2.028756000	-1.328716000
H	0.456594000	-1.746667000	-2.790634000
C	-0.018811000	-3.631102000	-1.687989000
H	0.814234000	-4.321289000	-1.842587000
H	-0.770491000	-3.851030000	-2.452481000
C	-0.631139000	-3.758770000	-0.258253000
H	0.021347000	-4.336591000	0.404273000
H	-1.596694000	-4.270126000	-0.284724000
C	-0.776306000	-2.305316000	0.273616000
H	-1.774699000	-2.097152000	0.666297000
C	0.263885000	-1.955117000	1.332366000
H	1.256641000	-2.231509000	0.966727000
C	-0.058381000	-2.586409000	2.718018000
H	-0.827373000	-3.358960000	2.613612000
H	0.823193000	-3.067431000	3.149175000
C	-0.554927000	-1.407990000	3.611132000
H	0.209600000	-1.129882000	4.343386000
H	-1.461218000	-1.662811000	4.166239000
C	-0.803810000	-0.255319000	2.619498000
H	-1.783850000	-0.346697000	2.150065000
H	-0.708808000	0.745464000	3.045178000
C	1.586044000	0.020122000	2.024806000
H	1.953379000	-0.611110000	2.841418000
H	1.453418000	1.037253000	2.406590000
C	2.534399000	0.020189000	0.859452000
C	3.903721000	-0.128508000	0.982240000
H	4.372156000	-0.295644000	1.944194000
C	4.709060000	-0.060384000	-0.176035000
C	4.089225000	0.163904000	-1.423396000
H	4.663506000	0.233986000	-2.337144000
C	2.707767000	0.297689000	-1.469037000
H	2.177405000	0.489038000	-2.391984000
C	6.958792000	-0.179064000	-1.137851000
H	7.943577000	-0.343170000	-0.705600000

H	6.908581000	0.801500000	-1.621691000
H	6.709497000	-0.977212000	-1.844241000
C	0.588996000	4.616467000	0.824563000
O	1.616496000	3.211540000	-0.903113000
H	2.000747000	4.063285000	-1.200593000

^4I_c

Fe	0.000392000	0.485800000	-0.278906000
N	-1.983809000	0.633498000	-0.127306000
H	1.266786000	5.209502000	0.622294000
C	-2.627110000	1.579497000	0.615694000
H	-1.994410000	2.228798000	1.203494000
C	0.857188000	3.179301000	0.122194000
N	-0.563106000	-1.374201000	-0.976806000
H	0.745487000	4.202201000	2.011894000
C	-4.002210000	1.693395000	0.595594000
H	-4.512711000	2.445294000	1.183294000
O	-0.025509000	1.084600000	-1.813006000
H	-0.440714000	4.730899000	0.806194000
C	-4.759409000	0.819394000	-0.219206000
N	0.251693000	-0.531000000	1.530294000
N	1.930592000	0.219202000	-0.344306000
C	-4.083408000	-0.155405000	-0.987406000
H	-4.620707000	-0.845706000	-1.624106000
C	-2.698407000	-0.207403000	-0.925006000
O	0.209090000	2.055100000	0.637094000
C	-1.849306000	-1.142502000	-1.734706000
H	-2.349905000	-2.096203000	-1.929806000
H	-1.582507000	-0.677402000	-2.689706000
C	0.443995000	-2.107299000	-1.841706000
H	1.420795000	-1.992898000	-1.371406000
H	0.468694000	-1.651599000	-2.832806000
C	-0.028203000	-3.573200000	-1.806606000
H	0.806898000	-4.259599000	-1.966006000
H	-0.761103000	-3.762701000	-2.596806000
C	-0.676203000	-3.751101000	-0.397106000
H	-0.055502000	-4.375400000	0.253294000
H	-1.653303000	-4.235202000	-0.469806000
C	-0.800505000	-2.320401000	0.197694000
H	-1.795105000	-2.112002000	0.599594000
C	0.247795000	-2.030600000	1.266694000
H	1.235595000	-2.313598000	0.892294000
C	-0.088404000	-2.699200000	2.631294000
H	-0.875103000	-3.449801000	2.501394000
H	0.781596000	-3.214599000	3.045494000
C	-0.558306000	-1.539201000	3.563294000
H	0.214094000	-1.298100000	4.300094000

H	-1.466606000	-1.794302000	4.114794000
C	-0.792107000	-0.351601000	2.610994000
H	-1.772507000	-0.416302000	2.138194000
H	-0.679609000	0.635599000	3.061294000
C	1.604392000	-0.098398000	2.028094000
H	1.968793000	-0.769698000	2.812194000
H	1.481391000	0.905402000	2.445794000
C	2.540392000	-0.042597000	0.858694000
C	3.909692000	-0.166095000	0.954794000
H	4.392893000	-0.381695000	1.899594000
C	4.705092000	0.022206000	-0.202306000
C	4.068992000	0.332905000	-1.425706000
H	4.634192000	0.513906000	-2.329406000
C	2.689692000	0.433903000	-1.456206000
H	2.157491000	0.707503000	-2.356006000
C	0.599287000	4.409101000	0.946994000
O	1.556588000	3.115102000	-0.887906000
C	6.961392000	0.111209000	-1.164206000
H	6.857491000	1.135308000	-1.534506000
H	7.948292000	-0.046590000	-0.735206000
H	6.759493000	-0.619492000	-1.953206000
C	-6.975708000	0.155791000	-1.037206000
H	-7.978308000	0.519590000	-0.823106000
H	-6.727808000	0.305892000	-2.092606000
H	-6.878407000	-0.896508000	-0.752006000
O	-6.093209000	0.987492000	-0.193306000
O	6.029892000	-0.105293000	-0.033406000

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Fe	-0.047500000	0.197392000	-0.024908000
O	6.017526000	0.130272000	-0.753976000
N	1.903464000	0.161530000	-0.366273000
H	-0.413742000	2.753011000	-3.742581000
C	2.515869000	0.633617000	-1.487518000
H	1.852694000	1.006190000	-2.255377000
C	-1.213672000	2.200429000	-1.819434000
O	-6.148576000	-0.124620000	0.109042000
N	0.489240000	-1.200558000	1.377230000
H	-2.036204000	3.419300000	-3.377788000
C	3.891984000	0.625959000	-1.616648000
H	4.378059000	0.997194000	-2.509542000
O	0.108061000	1.442202000	1.108142000
H	-1.831227000	1.702517000	-3.816989000
C	4.681264000	0.113781000	-0.561983000
N	-0.451985000	-1.509334000	-1.204477000
N	-2.017303000	0.057080000	0.194149000
C	4.039908000	-0.375294000	0.596570000

H	4.603609000	-0.782560000	1.425736000
C	2.651859000	-0.324646000	0.658900000
O	-0.304448000	1.216042000	-1.611228000
C	6.926521000	-0.388854000	0.283775000
H	7.923146000	-0.247555000	-0.128980000
H	6.729007000	-1.451908000	0.455791000
H	6.807577000	0.186868000	1.207457000
C	1.848658000	-0.754872000	1.853774000
H	2.344521000	-1.554336000	2.414345000
H	1.684471000	0.101305000	2.515106000
C	-0.451045000	-1.397662000	2.544230000
H	-1.463149000	-1.443158000	2.140339000
H	-0.377403000	-0.541118000	3.216026000
C	-0.028670000	-2.747972000	3.150670000
H	-0.852635000	-3.219832000	3.691730000
H	0.793942000	-2.612390000	3.860453000
C	0.434419000	-3.594898000	1.925941000
H	-0.307139000	-4.357937000	1.667707000
H	1.372752000	-4.115306000	2.133861000
C	0.590306000	-2.588121000	0.749995000
H	1.563729000	-2.663734000	0.258104000
C	-0.511537000	-2.725257000	-0.295033000
H	-1.484344000	-2.731734000	0.203587000
C	-0.303281000	-3.957539000	-1.222610000
H	0.424671000	-4.646439000	-0.781395000
H	-1.233911000	-4.515275000	-1.354507000
C	0.206740000	-3.377859000	-2.579617000
H	-0.573947000	-3.443062000	-3.343865000
H	1.079638000	-3.915990000	-2.957588000
C	0.542567000	-1.905448000	-2.268743000
H	1.541093000	-1.816417000	-1.839844000
H	0.458855000	-1.220844000	-3.113860000
C	-1.803200000	-1.258493000	-1.815592000
H	-2.230777000	-2.185299000	-2.213333000
H	-1.650133000	-0.556225000	-2.639810000
C	-2.686483000	-0.641169000	-0.771894000
C	-4.066419000	-0.713379000	-0.792186000
H	-4.593468000	-1.275619000	-1.552839000
C	-4.804637000	-0.021201000	0.192037000
C	-4.108167000	0.715950000	1.171757000
H	-4.629298000	1.276020000	1.935638000
C	-2.721588000	0.736515000	1.130932000
H	-2.133824000	1.310860000	1.831655000
C	-7.005757000	0.592326000	1.071046000
H	-8.021607000	0.344229000	0.770836000
H	-6.832533000	1.670282000	0.992526000
H	-6.806525000	0.236440000	2.087021000

C	-1.385245000	2.548881000	-3.278613000
O	-1.828631000	2.768909000	-0.898537000
C	0.407942000	3.792485000	0.742039000
C	0.764557000	3.476264000	2.062311000
H	-0.641043000	3.972025000	0.529236000
H	-0.028555000	3.487974000	2.805301000
C	1.345812000	3.897089000	-0.397303000
H	2.398455000	3.884381000	-0.106440000
H	1.157681000	3.051884000	-1.078135000
H	1.137512000	4.808193000	-0.974776000
C	2.141750000	3.192783000	2.539900000
H	2.579985000	4.107583000	2.975260000
H	2.123761000	2.451389000	3.346603000
H	2.803228000	2.852974000	1.738754000

^{6}intI

Fe	-0.008131000	0.361762000	0.061445000
O	-6.260335000	0.337650000	0.270911000
N	-2.124739000	0.344505000	0.193508000
H	-0.301156000	3.292570000	3.555135000
C	-2.828077000	1.001109000	1.164286000
H	-2.229400000	1.526810000	1.895288000
C	1.001559000	2.429014000	2.090248000
O	6.171502000	-0.495974000	-0.199357000
N	-0.612133000	-1.362206000	-1.207539000
H	-0.100579000	4.273445000	2.099886000
C	-4.208045000	1.002462000	1.192267000
H	-4.760992000	1.521857000	1.964224000
O	-0.051633000	1.501004000	-1.693993000
H	1.226955000	4.180089000	3.297349000
C	-4.915480000	0.302599000	0.186458000
N	0.430586000	-1.262713000	1.438018000
N	2.065005000	0.044029000	-0.250395000
C	-4.187739000	-0.376675000	-0.814957000
H	-4.688365000	-0.930951000	-1.598143000
C	-2.798566000	-0.328288000	-0.777212000
O	0.080359000	1.705413000	1.379673000
C	-7.092998000	-0.364726000	-0.723795000
H	-8.116329000	-0.165213000	-0.413203000
H	-6.883741000	-1.438794000	-0.692916000
H	-6.906659000	0.044104000	-1.722072000
C	-1.927406000	-0.981969000	-1.819148000
H	-2.427966000	-1.852534000	-2.259890000
H	-1.707432000	-0.269708000	-2.621856000
C	0.360259000	-1.816569000	-2.267418000
H	1.359585000	-1.780378000	-1.832307000
H	0.322859000	-1.129282000	-3.114884000

C	-0.059508000	-3.267180000	-2.592560000
H	0.795871000	-3.866479000	-2.914961000
H	-0.793900000	-3.284585000	-3.404058000
C	-0.691865000	-3.804807000	-1.269946000
H	-0.085323000	-4.600103000	-0.825802000
H	-1.685645000	-4.223363000	-1.450548000
C	-0.766133000	-2.578523000	-0.313651000
H	-1.726652000	-2.505506000	0.204204000
C	0.361922000	-2.599195000	0.723642000
H	1.315612000	-2.759093000	0.213560000
C	0.102730000	-3.651606000	1.842937000
H	-0.676094000	-4.354475000	1.530304000
H	1.001856000	-4.238229000	2.048364000
C	-0.334844000	-2.834546000	3.098897000
H	0.451205000	-2.850029000	3.860211000
H	-1.242614000	-3.234811000	3.557618000
C	-0.549934000	-1.399421000	2.577139000
H	-1.552853000	-1.269692000	2.163907000
H	-0.366669000	-0.613025000	3.311278000
C	1.822403000	-0.995333000	1.937513000
H	2.227202000	-1.880662000	2.441213000
H	1.770082000	-0.173787000	2.656397000
C	2.701626000	-0.575790000	0.791879000
C	4.069763000	-0.769106000	0.799630000
H	4.565919000	-1.264135000	1.624915000
C	4.841139000	-0.291157000	-0.280223000
C	4.183603000	0.338711000	-1.360295000
H	4.728867000	0.702433000	-2.220611000
C	2.805035000	0.476666000	-1.304404000
H	2.255223000	0.926065000	-2.118806000
C	7.065137000	-0.015505000	-1.270084000
H	8.063008000	-0.295983000	-0.939849000
H	6.981686000	1.071789000	-1.364176000
H	6.817861000	-0.511960000	-2.213943000
C	0.429103000	3.621522000	2.805099000
O	2.193514000	2.093266000	2.118616000
C	-0.928875000	2.683826000	-2.157226000
H	-1.324601000	2.475579000	-3.148777000
C	0.536897000	2.886300000	-2.056844000
H	1.101614000	2.795599000	-2.982417000
C	1.205519000	3.668458000	-0.964051000
H	1.539115000	4.627577000	-1.379776000
H	0.533649000	3.867683000	-0.129355000
H	2.087213000	3.140803000	-0.585343000
C	-1.906428000	3.239192000	-1.162812000
H	-2.140702000	4.276203000	-1.437519000
H	-2.839743000	2.668846000	-1.174707000

H	-1.499639000	3.222572000	-0.149631000

^{4}tsII

Fe	-0.001014000	0.117499000	-0.055070000
O	-6.074995000	0.349976000	0.479703000
N	-1.953930000	0.173859000	0.234187000
H	0.460684000	3.290214000	3.282221000
C	-2.578389000	0.792909000	1.274001000
H	-1.924198000	1.227680000	2.016536000
C	1.108971000	2.336397000	1.472797000
O	6.092666000	-0.438564000	-0.045772000
N	-0.541654000	-1.408421000	-1.305184000
H	2.158682000	3.616955000	2.839112000
C	-3.956681000	0.852976000	1.356258000
H	-4.453172000	1.340524000	2.185179000
O	-0.078006000	1.239674000	-1.299230000
H	1.679949000	2.036465000	3.529318000
C	-4.735444000	0.259033000	0.337237000
N	0.332540000	-1.456722000	1.315533000
N	1.973757000	-0.080506000	-0.204785000
C	-4.081604000	-0.379362000	-0.738463000
H	-4.636945000	-0.851005000	-1.538493000
C	-2.691438000	-0.391843000	-0.757449000
O	0.272928000	1.299856000	1.424624000
C	-6.973324000	-0.242349000	-0.527845000
H	-7.975115000	-0.022073000	-0.165240000
H	-6.813208000	-1.324112000	-0.581449000
H	-6.804681000	0.227954000	-1.502087000
C	-1.871109000	-0.978325000	-1.871967000
H	-2.378435000	-1.819161000	-2.356697000
H	-1.657060000	-0.208682000	-2.620197000
C	0.426733000	-1.759443000	-2.409818000
H	1.424440000	-1.779990000	-1.970162000
H	0.395370000	-0.983328000	-3.175917000
C	-0.012529000	-3.159538000	-2.875695000
H	0.819053000	-3.713287000	-3.318603000
H	-0.797400000	-3.085845000	-3.635402000
C	-0.557665000	-3.847650000	-1.585402000
H	0.135916000	-4.611187000	-1.218300000
H	-1.512885000	-4.344434000	-1.773728000
C	-0.705418000	-2.713407000	-0.531390000
H	-1.691741000	-2.702327000	-0.059751000
C	0.367089000	-2.768523000	0.551083000
H	1.350053000	-2.865397000	0.082056000
C	0.095066000	-3.881729000	1.604639000
H	-0.653537000	-4.586865000	1.228413000
H	1.000216000	-4.456626000	1.816192000

C	-0.412903000	-3.136372000	2.878882000
H	0.354314000	-3.141333000	3.659414000
H	-1.309257000	-3.599227000	3.299447000
C	-0.691782000	-1.698726000	2.398149000
H	-1.679816000	-1.624943000	1.942652000
H	-0.598200000	-0.926221000	3.162743000
C	1.681275000	-1.181982000	1.922124000
H	2.074614000	-2.072340000	2.424528000
H	1.538249000	-0.390308000	2.662635000
C	2.601571000	-0.705577000	0.836717000
C	3.977232000	-0.834406000	0.884153000
H	4.470964000	-1.340442000	1.704321000
C	4.755391000	-0.280851000	-0.155519000
C	4.102599000	0.385010000	-1.213246000
H	4.655747000	0.837731000	-2.024505000
C	2.717063000	0.468884000	-1.195633000
H	2.161188000	0.988148000	-1.962751000
C	6.988978000	0.122148000	-1.073136000
H	7.989645000	-0.143102000	-0.738528000
H	6.872523000	1.209753000	-1.116383000
H	6.774541000	-0.333093000	-2.045436000
C	1.378228000	2.854567000	2.865936000
O	1.627115000	2.870460000	0.457404000
C	0.328761000	4.176334000	-1.142414000
C	-0.671691000	3.360995000	-1.716999000
H	1.301761000	4.193751000	-1.620713000
H	-0.483899000	2.975816000	-2.713340000
C	0.077142000	5.175032000	-0.071998000
H	-0.773112000	4.912537000	0.564553000
H	0.975343000	5.308348000	0.536783000
H	-0.146588000	6.153027000	-0.533799000
C	-2.062478000	3.273084000	-1.190710000
H	-2.633158000	4.161634000	-1.510876000
H	-2.574316000	2.391370000	-1.582299000
H	-2.084690000	3.246026000	-0.097481000

---------- End of the Coordinates ----------