

Electronic Supporting Information

**DFT mechanistic study on the formation of 8-oxoguanine and spiroiminodihydantoin mediated by iron Fenton reactions**

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Table S1. Energy differences (kcal mol<sup>-1</sup>) between singlet-quintet and triplet-quintet states<sup>a</sup>

	PBE0		PW6B95	
	$\Delta E_{\text{singlet-quintet}}$	$\Delta E_{\text{triplet-quintet}}$	$\Delta E_{\text{singlet-quintet}}$	$\Delta E_{\text{triplet-quintet}}$
<b>I<sub>OH</sub></b>	n.a. <sup>b</sup>	22.5	n.a. <sup>b</sup>	17.0
<b>I1</b>	31.4	24.2	22.5	19.1
<b>I2</b>	27.0	19.7	19.5	19.2
<b>I3</b>	n.a. <sup>c</sup>	24.0	n.a. <sup>c</sup>	20.8
<b>I4</b>	39.2	8.2	33.9	5.6
<b>I5</b>	35.3	19.8	26.2	17.1
<b>I6</b>	n.a. <sup>d</sup>	21.5	n.a. <sup>d</sup>	16.4
<b>I7</b>	31.9	25.0	23.4	22.0
<b>I8</b>	32.4	21.7	24.9	19.1

<sup>a</sup> Calculations at PBE0-D3/Def2-QZVP//PBE0-D3/6-31+G(d) and PW6B95-D3/Def2-QZVP//PBE0-D3/6-31+G(d) levels. <sup>b</sup> **I<sub>OH</sub>** singlet state does not exist and the corresponding geometry optimization converges to **I2**. <sup>c</sup> **I3** singlet state does not exist and the corresponding geometry optimization converges to **I7**. <sup>d</sup> **I6** singlet state does not exist and the corresponding geometry optimization converges to **I7**.

Table S2. Activation energies (kcal mol<sup>-1</sup>) of aqueous Fenton reactions

	<b>RC</b>	<b>TS<sub>oo</sub></b>
B3LYP-D3/Def2-QZVP//B3LYP-D3/6-31+G(d)	7.2	21.5
M06-D3/Def2-QZVP//M06-D3/6-31+G(d)	7.6	20.8
$\omega$ B97XD/Def2-QZVP// $\omega$ B97XD/6-31+G(d)	6.6	29.0
PW6B95-D3/Def2-QZVP//PW6B95-D3/6-31+G(d)	5.9	26.5

Table S3. Natural population analyses of charge (q) and spin density ( $\rho$ )

	q(Fe) <sup>a</sup>	q(G)	q(C)	$\rho$ (Fe) <sup>a</sup>	$\rho$ (G)	$\rho$ (C)
<b>RC</b>	-0.217	0.130	0.090	3.932	0.068	0.000
<b>I<sub>OH</sub></b>	-0.259	0.226	0.099	4.846	0.128	0.000
<b>I1</b>	-0.356	0.242	0.111	4.737	-0.737	0.000
<b>I2</b>	-0.011	-0.116	0.127	4.217	-0.217	0.000
<b>I3</b>	0.554	-0.635	0.081	3.919	0.083	0.000
<b>I4</b>	-0.358	0.263	0.098	3.882	0.116	0.000
<b>I5<sup>b</sup></b>	0.141	-0.230	0.107	4.379	-0.378	0.000
<b>I6</b>	-0.273	0.032	0.094	4.820	-0.642	0.000
<b>I7</b>	-0.158	0.068	0.087	3.927	0.072	0.000
<b>I8</b>	-0.159	0.065	0.095	3.968	0.032	0.000
<b>I9</b>	-1.043	0.886	0.150	3.951	0.046	0.000
<b>I10</b>	-0.249	0.123	0.131	3.938	0.060	0.000
<b>I11</b>	-0.206	0.079	0.127	3.935	0.065	0.000
<b>I12</b>	-0.205	0.080	0.127	3.929	0.071	0.000
<b>I13</b>	-0.245	0.158	0.134	4.850	0.135	0.000
<b>I14</b>	-0.278	0.109	0.171	4.798	-0.797	0.000
<b>I15</b>	-0.219	0.102	0.116	3.940	0.060	0.000
<b>I16</b>	-0.317	0.192	0.133	3.879	0.118	0.000
<b>I17<sup>b</sup></b>	0.249	-0.390	0.162	4.491	-0.490	0.000
<b>I18<sup>b</sup></b>	-0.225	0.102	0.166	3.907	0.092	0.000
<b>I19</b>	-0.254	-0.047	0.127	4.834	-0.702	0.000
<b>I20</b>	-0.190	0.077	0.115	3.940	0.060	0.000

<sup>a</sup> Including coordinated ligands except guanine. <sup>b</sup> Oxo atom is included to guanine moiety.

PBE0-D3/6-31+G(d) optimized coordinates  
 H<sub>2</sub>O  
 E(6-31+G\*) = -76.345928; E(Def2-QZVP) = -76.392978;  
 G<sub>corr</sub> = 0.010501

0 1  
 O 0.00000000 0.00000000 0.11829700  
 H 0.00000000 0.76476400 -0.47318800  
 H 0.00000000 -0.76476400 -0.47318800

H<sub>2</sub>O<sub>2</sub>  
 E(6-31+G\*) = -151.393934; E(Def2-QZVP) = -  
 151.474151; G<sub>corr</sub> = 0.007571

0 1  
 O -0.70667300 -0.10709700 -0.06619100  
 H -1.01445900 0.59683500 0.52952500  
 O 0.70667300 0.10709600 -0.06619200  
 H 1.01445800 -0.59682500 0.52953700

Fe<sup>II</sup>(H<sub>2</sub>O)<sub>6</sub>  
 E(6-31+G\*) = -1721.284737; E(Def2-QZVP) = -  
 1721.718915; G<sub>corr</sub> = 0.105357

2 5  
 Fe -0.00001500 0.00000700 0.00001300  
 O 1.71000200 0.49427600 -1.17356100  
 H 2.27093500 1.25180100 -0.94453400  
 H 1.55371200 0.55372600 -2.12948700  
 O 1.06384400 0.31193700 1.79264000  
 H 1.27174100 1.19594400 2.13264500  
 H 1.83972600 -0.24280100 1.96957000  
 O -1.71003500 -0.49427500 1.17356800  
 H -2.27094700 -1.25181800 0.94454700  
 H -1.55375600 -0.55370500 2.12949800  
 O -1.06386600 -0.31193700 -1.79261700  
 H -1.83976400 0.24277600 -1.96955200  
 H -1.27173600 -1.19595200 -2.13262000  
 O -0.80785100 1.97384500 -0.13067200  
 H -0.40339500 2.65521900 -0.68888700  
 H -1.14621800 2.42994200 0.65482300

O 0.80786400 -1.97382200 0.13068600  
 H 0.40338000 -2.65524300 0.68882300  
 H 1.14630100 -2.42985800 -0.65481400

**RC** Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(H<sub>2</sub>O<sub>2</sub>)  
 E(6-31+G\*) = -1796.330047; E(Def2-QZVP) = -  
 1796.796686; G<sub>corr</sub> = 0.112751

2 5  
 Fe 0.30319600 0.00339700 -0.07360000  
 O -0.19282600 -0.84203200 -1.93298600  
 H -0.53238900 -1.75057200 -1.96505200  
 H -0.72990100 -0.33131100 -2.55928500  
 O 1.21093300 -1.81367900 0.46939600  
 H 1.96801400 -2.17142900 -0.01968300  
 H 0.75664100 -2.57096000 0.86906000  
 O 0.53727000 0.70261700 1.90536000  
 H 0.58074000 1.66219900 2.04400200  
 H 1.21838400 0.31021400 2.47428100  
 O -0.70646600 1.80936000 -0.45111000  
 H -0.52313000 2.39849900 -1.19803400  
 H -1.67395000 1.68459400 -0.40453900  
 O 2.24398000 0.60761000 -0.68993500  
 H 2.36283600 1.37249400 -1.27375400  
 H 2.97283600 0.64486000 -0.05127600  
 O -1.69775900 -0.66967100 0.64258300  
 H -1.78461700 -0.75668300 1.60963800  
 O -2.76438300 0.22435600 0.32419000  
 H -3.33882000 -0.34489500 -0.21896900

**TS<sub>00</sub>** for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>6</sub> system  
 E(6-31+G\*) = -1796.304998; E(Def2-QZVP) = -  
 1796.769056; G<sub>corr</sub> = 0.113141

2 5  
 Fe -0.20080400 0.01035500 -0.02692000  
 O -0.32235400 -2.02647400 0.40335200  
 H -0.61721200 -2.59939900 -0.32397900  
 H 0.40472600 -2.49266400 0.84765000  
 O -1.53422200 -0.42628700 -1.55871100

H -2.48029400 -0.25768000 -1.41758000  
H -1.35386300 -0.32708300 -2.50660200  
O -0.40131300 2.05716600 -0.31190400  
H -0.13458200 2.66903100 0.39343400  
H -1.13805300 2.46917300 -0.79103200  
O 0.99683000 0.44095400 1.58209600  
H 0.87441200 0.12344600 2.48995800  
H 1.92465500 0.25510400 1.29177200  
O -2.03269400 0.07762100 1.07572200  
H -2.20319100 -0.67267900 1.66818800  
H -2.27779800 0.87674700 1.56873800  
O 1.37229200 -0.11835200 -1.07397700  
H 1.61146000 0.59650500 -1.69141600  
O 2.90286500 -0.00431400 -0.19310700  
H 3.13821000 -0.93736000 -0.35156500

**I<sub>OH</sub>** for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>6</sub> system

E(6-31+G\*) = -1796.316772; E(Def2-QZVP) = -  
1796.781864; G<sub>corr</sub> = 0.108407

2 5

Fe -0.11926000 0.03818100 -0.09882800  
O 0.08142100 -1.96292200 0.31016500  
H -0.62803000 -2.54813200 -0.00564500  
H 0.93209900 -2.32245300 -0.06786800  
O -1.63434800 -0.35871800 -1.41323800  
H -2.57207800 -0.26702300 -1.17664500  
H -1.54805700 -0.26108600 -2.37557000  
O -0.68943500 2.04363900 -0.10537600  
H -0.06993400 2.67836100 0.29344000  
H -1.02220400 2.44991600 -0.92338800  
O 1.06543400 0.58692200 1.49831800  
H 0.83240000 0.34697900 2.41044800  
H 2.02957000 0.49792100 1.41355000  
O -1.69279200 -0.04589700 1.30602900  
H -1.83366300 -0.74808100 1.96118900  
H -2.09419100 0.76772900 1.65197100  
O 1.24633200 0.07703900 -1.28981900  
H 1.56226500 0.87042500 -1.75039400

O 2.41628100 -2.34233800 -1.00874000  
H 2.23456500 -1.40899900 -1.31536800

**TS<sub>oxo</sub>** for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>6</sub> system

E(6-31+G\*) = -11796.299007; E(Def2-QZVP) = -  
1796.765623; G<sub>corr</sub> = 0.108582

2 5

Fe -0.20411700 0.00888400 -0.10349800  
O -0.31658300 -1.97110700 0.55169700  
H -0.82148000 -2.56874000 -0.02651300  
H 0.51857800 -2.42769500 0.74993200  
O -1.66960600 -0.47087600 -1.44382400  
H -2.60006100 -0.26460000 -1.25075900  
H -1.54764000 -0.44304400 -2.40771100  
O -0.62872000 2.05471200 -0.24189100  
H 0.02269200 2.62410300 0.20312400  
H -0.76305900 2.43709600 -1.12588800  
O 1.01969300 0.50268500 1.44682100  
H 0.86815800 0.26974900 2.37721500  
H 1.96619500 0.32947000 1.21107800  
O -1.83360700 0.14988400 1.21716600  
H -1.99997700 -0.51302700 1.90676300  
H -2.14284000 1.00961700 1.54543100  
O 1.17288100 -0.11179700 -1.25794500  
H 2.25971700 0.11030400 -1.04540000  
O 3.08180500 -0.03054800 -0.15920900  
H 3.31802200 -0.97850200 -0.17206200

**I<sub>oxo</sub>** for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>6</sub> system

E(6-31+G\*) = -1796.337288; E(Def2-QZVP) = -  
1796.800496; G<sub>corr</sub> = 0.114724

2 5

Fe -0.34548700 -0.03237600 -0.10730600  
O -0.36576000 -2.05067400 0.44211900  
H -0.92500600 -2.60389600 -0.13055400  
H 0.49959400 -2.49260800 0.47495900  
O -2.05720800 -0.42950900 -1.09740000  
H -2.91164000 -0.17943900 -0.70555800

H -2.12139200 -0.33403000 -2.06232100  
 O -0.72996900 2.01989700 -0.20265600  
 H 0.06109900 2.56505500 -0.04971100  
 H -1.12761900 2.35225400 -1.02518700  
 O 1.18654500 0.37571300 1.03812100  
 H 1.15697600 0.25002200 2.00039000  
 H 2.13150500 0.19134000 0.69675900  
 O -1.60436100 0.10228100 1.48834600  
 H -1.61404200 -0.60209100 2.15785000  
 H -1.73836700 0.95223000 1.93990100  
 O 0.55274900 -0.15918500 -1.41231500  
 H 3.80747000 0.59954900 -0.50210500  
 O 3.54821500 -0.07503200 0.14364000  
 H 3.59051600 -0.91761800 -0.33337200

Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(SO<sub>4</sub>)

E(6-31+G\*) = -2343.897910; E(Def2-QZVP) = -  
 2344.515055; G<sub>corr</sub> = 0.101383

0 5

Fe -0.16513300 -0.14019400 -0.31454900  
 O -0.20068900 -0.84965100 -2.32525700  
 H 0.76135900 -1.09814000 -2.44717300  
 H -0.70283500 -1.67089500 -2.43735100  
 O 0.81520200 0.13901100 1.65437500  
 H 0.93734200 1.07396400 1.87824900  
 H 1.71023100 -0.18982500 1.39060000  
 O -0.64378300 1.93797000 -0.46146500  
 H 0.08390100 2.36959700 -0.93857500  
 H -1.46460900 2.24386900 -0.87546800  
 O -1.86293800 -0.51999300 0.98453900  
 H -1.60920800 -0.42527000 1.91640600  
 S 2.81750800 -0.34564800 -1.08061800  
 O 2.44298100 -1.30590200 -2.18066400  
 O 2.84853800 -1.09115800 0.24822200  
 O 4.09862400 0.34083000 -1.34198200  
 O 1.67578600 0.67479600 -0.97345300  
 H -2.66348900 0.01505300 0.87523700  
 O 0.40484400 -2.20953300 0.11845700

H 1.38295400 -2.12251700 0.24633900  
 H 0.04859500 -2.58967500 0.93434700

*cis*-**RC** Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(SO<sub>4</sub>)(H<sub>2</sub>O<sub>2</sub>)

E(6-31+G\*) = -2418.946963; E(Def2-QZVP) = -  
 2419.597424; G<sub>corr</sub> = 0.102714

0 5

Fe -0.05957100 -0.03174900 -0.36052600  
 O -0.27360400 -0.82900900 -2.36112700  
 H 0.67696300 -0.96669600 -2.65213300  
 H -0.70182000 -1.69509200 -2.42588100  
 O 0.77556100 0.96551000 1.62709300  
 H 1.69705200 0.66572900 1.48741500  
 O -0.85564100 1.74002700 -1.26255000  
 H -0.50624800 2.60662400 -1.00572700  
 H -0.81328000 1.70644300 -2.23114400  
 O -1.79530100 0.01234700 0.88720700  
 H -1.49703100 0.06358000 1.81567200  
 S 2.86788300 -0.72272500 -1.34283700  
 O 2.33324000 -0.99485700 -2.72448900  
 O 2.82291700 -1.97587000 -0.50928300  
 O 4.21760700 -0.12731800 -1.37878600  
 O 1.89596400 0.29379900 -0.68138400  
 H -2.37410100 0.77708600 0.74389600  
 O 0.41672400 -1.91230800 0.59889800  
 H 1.34335200 -2.09488900 0.26867800  
 H 0.48403400 -1.85275100 1.56443200  
 O 0.31223900 0.15184400 2.70458600  
 H 0.37846800 0.75520900 3.46618300

*cis*-**TS<sub>00</sub>** for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(SO<sub>4</sub>) system

E(6-31+G\*) = -2418.928215; E(Def2-QZVP) = -  
 2419.577067; G<sub>corr</sub> = 0.102352

0 5

Fe 0.27954900 0.11739300 -0.16399700  
 O -0.37168400 -0.66605000 -2.03209300  
 H 0.46915500 -0.94840500 -2.50618000  
 H -0.94593300 -1.44519000 -1.98626300

O 0.55396100 1.04444400 1.52627300  
H 1.48264700 1.09439800 1.82149000  
O -0.54175900 1.88637600 -1.02192000  
H -0.11592600 2.73917600 -0.84461100  
H -0.63837500 1.81900500 -1.98554700  
O -1.70119300 -0.22784600 0.60566700  
H -1.56121300 -0.20595300 1.57606500  
S 2.86584800 -0.92940500 -1.61354800  
O 2.06396100 -1.18387600 -2.86164700  
O 2.86286900 -2.14491900 -0.72788100  
O 4.22758200 -0.45397300 -1.91187300  
O 2.11792200 0.19208400 -0.82674000  
H -2.33430300 0.48048500 0.40941500  
O 0.66407700 -1.79817000 0.68106100  
H 1.53069900 -2.08970800 0.26901700  
H 0.80379000 -1.76166100 1.64068000  
O -0.04601700 0.13194200 2.81310300  
H -0.32025100 0.88479000 3.36772000

*cis-I<sub>OH</sub>* for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(SO<sub>4</sub>) system

E(6-31+G\*) = -2418.951681; E(Def2-QZVP) = -  
2419.602225; G<sub>corr</sub> = 0.099096

0 5

Fe 0.44442500 0.07445700 0.01030900  
O -0.41309500 -0.72257900 -1.76040500  
H 0.33852600 -0.98756900 -2.37147200  
H -0.97678500 -1.50234700 -1.64083300  
O 0.83389500 0.89351600 1.62936500  
H 1.75617500 1.10906400 1.83292000  
O -0.34537200 1.85643500 -0.82841200  
H 0.06438300 2.68130800 -0.52173100  
H -0.34808200 1.89105600 -1.79883600  
O -1.55068400 -0.24767200 0.68798500  
H -1.63662100 -0.03953900 1.65341500  
S 2.81116800 -0.92331500 -1.81294800  
O 1.87915700 -1.16237900 -2.96203200  
O 2.92578200 -2.14382900 -0.94861100  
O 4.11170600 -0.38398500 -2.22499800

O 2.10520100 0.16756600 -0.91403100  
H -2.19208700 0.32277200 0.23465300  
O 0.82614700 -1.88927500 0.59289500  
H 1.66421100 -2.16254400 0.10428000  
H 1.01234500 -1.97189100 1.54187300  
O -1.15485900 0.54385400 3.28762700  
H -0.28093900 0.78285100 2.83797600

*cis-TS<sub>oxo</sub>* for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(SO<sub>4</sub>) system

E(6-31+G\*) = -2418.935385; E(Def2-QZVP) = -  
2419.587647; G<sub>corr</sub> = 0.097675

0 5

Fe 0.52456200 -0.13406600 0.13708500  
O -0.45516300 -0.72958800 -1.63118100  
H 0.24636700 -0.88348200 -2.33523900  
H -0.98383500 -1.54049700 -1.57139800  
O 1.04907000 0.50714000 1.79593200  
H 0.54070000 0.29657600 2.73947900  
O -0.26763800 1.76464300 -0.39497000  
H 0.14509700 2.50158000 0.08445800  
H -0.22207800 1.99247000 -1.33775300  
O -1.41240500 -0.55429200 0.89916800  
H -1.39566100 -0.23616000 1.84196900  
S 2.74813800 -0.82552000 -1.97995100  
O 1.72432200 -0.93447900 -3.06904800  
O 2.95432600 -2.14502300 -1.29845500  
O 3.99856200 -0.19947700 -2.42118700  
O 2.10402600 0.11867200 -0.88702400  
H -2.11815300 -0.05670900 0.45626700  
O 0.99646000 -2.13798900 0.43811600  
H 1.79287900 -2.32778100 -0.14957200  
H 1.25389800 -2.35822100 1.34759500  
O -0.61673300 0.37271100 3.26181100  
H -0.78822300 1.32721000 3.36001500

*cis-I<sub>oxo</sub>* for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(SO<sub>4</sub>) system

E(6-31+G\*) = -2418.971242; E(Def2-QZVP) = -  
2419.618226; G<sub>corr</sub> = 0.105486

0 5  
 Fe 0.50943500 0.29377900 -0.11144100  
 O -0.40476700 -0.62250200 -1.68423900  
 H 0.30810900 -1.06848200 -2.24822100  
 H -1.02707400 -1.30912100 -1.39559900  
 O 1.09846200 1.13982200 1.11582500  
 H 0.31556000 -0.01413600 3.45758000  
 O -0.38087300 1.97957800 -0.98886800  
 H 0.08584300 2.82069500 -0.85936600  
 H -0.54267700 1.88872000 -1.94244100  
 O -1.35343900 0.02274600 0.78793900  
 H -1.16880200 -0.20749100 1.73434200  
 S 2.76751800 -1.00933500 -1.82379700  
 O 1.74542600 -1.48112300 -2.82132800  
 O 2.98775900 -2.03474000 -0.75572500  
 O 4.01240300 -0.55804100 -2.45920400  
 O 2.13964000 0.24648100 -1.10531400  
 H -1.86120000 0.85066800 0.79841900  
 O 0.80777200 -1.61292600 0.68109500  
 H 1.69346700 -1.92911700 0.34613500  
 H 0.81326500 -1.57541000 1.65975000  
 O -0.17026500 -0.76145500 3.07659200  
 H -0.55704400 -1.24088900 3.82398300

*trans*-**RC** Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(SO<sub>4</sub>)(H<sub>2</sub>O<sub>2</sub>)

E(6-31+G\*) = -2418.944832; E(Def2-QZVP) = -  
 2419.595957; G<sub>corr</sub> = 0.102494

0 5  
 Fe 0.37691300 0.03114700 -0.77149600  
 O -1.11428100 -0.03336400 -2.34816600  
 H -1.69363300 -0.79562700 -2.19095700  
 H -1.68491200 0.75397500 -2.24047500  
 O 1.02095100 0.82315500 1.16352400  
 H 1.61545900 1.58786900 1.14925300  
 H 1.58296000 0.06073600 1.49833100  
 O -1.34150900 1.43011200 0.04843300  
 H -0.94893900 2.15327100 0.56988500  
 O -0.88949800 -1.47218800 0.14345800

H -0.25397300 -2.21286700 0.36829300  
 O 1.95305800 -1.17305000 -0.76985300  
 O 1.14848700 -3.11492800 0.51048100  
 O 2.44323400 -1.33734400 1.63236200  
 O 3.55952300 -2.85504900 0.02878900  
 H -1.29872300 -1.19928300 0.97754300  
 O 1.05624700 1.70204400 -1.91799200  
 H 1.75977300 2.28076200 -1.58822300  
 H 1.27468700 1.52291100 -2.84529400  
 O -2.10009100 2.11892400 -0.94385000  
 H -3.00731000 2.02548900 -0.60139600  
 S 2.30482600 -2.15916700 0.37555700

*trans*-**TS<sub>00</sub>** for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(SO<sub>4</sub>) system

E(6-31+G\*) = -2418.926758; E(Def2-QZVP) = -  
 2419.576627; G<sub>corr</sub> = 0.101182

0 5  
 Fe 0.08215200 0.24884800 -0.50801900  
 O -1.03734300 -0.13283300 -2.27562000  
 H -1.45075100 -1.00695300 -2.34155500  
 H -1.76728400 0.52721900 -2.22784600  
 O 1.13937200 0.68768700 1.27862500  
 H 1.48238500 1.57722500 1.44661100  
 H 1.91595900 0.04965000 1.31730300  
 O -1.29320500 1.55096000 -0.09045500  
 H -1.09980400 2.45155500 0.22414800  
 O -0.94850800 -1.27812600 0.47651900  
 H -0.26934900 -2.00851300 0.63701100  
 O 1.48747400 -1.10018500 -0.99258500  
 O 1.08908500 -2.90776900 0.61124700  
 O 2.87646900 -1.25110200 1.02897900  
 O 3.13648300 -2.91769300 -0.77939200  
 H -1.33159100 -1.04756700 1.33635000  
 O 1.29376600 1.56378000 -1.65953900  
 H 1.43759800 2.49193500 -1.41792200  
 H 2.17440200 1.16614000 -1.76261700  
 O -2.36692600 2.00505700 -1.30752200  
 H -3.17517300 1.76411700 -0.81909400



S 2.18643600 -2.08590700 -0.01881900

*trans-I<sub>OH</sub>* for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(SO<sub>4</sub>) system

E(6-31+G\*) = -2418.949594; E(Def2-QZVP) = -  
2419.600888; G<sub>corr</sub> = 0.099577

0 5

Fe 0.05991900 0.34316100 -0.40960600

O -1.08664000 -0.08736400 -2.09449400

H -1.18742900 -1.02747500 -2.31155800

H -1.99219700 0.31678800 -2.06497900

O 1.25251300 0.68869600 1.27893300

H 1.67731000 1.55441200 1.37893300

H 1.98154900 -0.00906300 1.28047900

O -1.12001600 1.71388300 0.02048800

H -1.03271900 2.25343500 0.81896600

O -0.91900100 -1.12786900 0.67724200

H -0.30719500 -1.92510300 0.76351500

O 1.31218800 -1.03191000 -0.97402700

O 0.96567300 -2.92647700 0.54003300

O 2.83573900 -1.35319300 0.91615100

O 2.90019500 -2.91276400 -1.00553600

H -1.20490500 -0.87474800 1.56868100

O 1.26047700 1.60964700 -1.59376600

H 1.27233700 2.55911400 -1.39449300

H 2.18360400 1.32286500 -1.68578200

O -3.23757100 1.46933000 -1.49443000

H -2.54522800 1.73897600 -0.80716200

S 2.05008800 -2.11662500 -0.11169100

*trans-TS<sub>oxo</sub>* for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(SO<sub>4</sub>) system

E(6-31+G\*) = -2418.933496; E(Def2-QZVP) = -  
2419.586237; G<sub>corr</sub> = 0.096809

0 5

Fe -0.00979000 0.26306100 -0.38497300

O -1.25521500 -0.19611600 -1.98049500

H -1.49561200 -1.13071400 -2.08036300

H -2.09563400 0.32359900 -1.83660500

O 1.21096400 0.67232800 1.25617200

H 1.54835000 1.57281200 1.38016100

H 1.99807300 0.04369600 1.21964800

O -1.17919200 1.62520800 0.16222300

H -2.25329400 1.59628200 -0.04517800

O -0.88428600 -1.24141100 0.74095700

H -0.22536200 -2.00249900 0.81091700

O 1.26524700 -1.04288100 -1.00238700

O 1.10044500 -2.92599500 0.55350100

O 2.91010000 -1.25740400 0.80085300

O 2.94249000 -2.84266500 -1.10016900

H -1.14872700 -0.99617000 1.64151000

O 1.02778600 1.61795600 -1.61297700

H 0.96325000 2.56371400 -1.40423000

H 1.96661400 1.41924800 -1.76161100

O -3.03902500 1.50182900 -1.04381500

H -2.96408100 2.35618100 -1.50609800

S 2.10807600 -2.07753000 -0.16685300

*trans-I<sub>oxo</sub>* for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(SO<sub>4</sub>) system

E(6-31+G\*) = -2418.972682; E(Def2-QZVP) = -  
2419.621093; G<sub>corr</sub> = 0.105931

0 5

Fe 0.09493200 0.44566500 -0.31301600

O -1.09683000 0.06801500 -1.90063600

H -1.07154800 -0.86900000 -2.15386900

H -2.04710700 0.32315400 -1.70039200

O 1.37427500 0.61617500 1.26951000

H 1.72541000 1.49770000 1.46802700

H 2.14093700 -0.03148200 1.16134900

O -0.82178300 1.68065100 0.17590300

H -2.84870800 1.56692800 -0.35457000

O -0.91256200 -0.97784200 0.77693700

H -0.31297000 -1.78553400 0.83897400

O 1.18526300 -0.96538500 -1.03983100

O 0.92528800 -2.81626400 0.55162300

O 2.92392800 -1.36179000 0.65075500

O 2.63303500 -2.93238500 -1.23945100

H -1.11970900 -0.69483900 1.68135000

O 1.30147300 1.64940200 -1.51090600  
H 1.44953200 2.57054200 -1.24389600  
H 2.17288100 1.25268300 -1.67700300  
O -3.35422800 1.02843300 -0.98959400  
H -3.81214600 1.66069400 -1.56214500  
S 1.96181700 -2.08299500 -0.24893200

Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(HPO<sub>4</sub>)

E(6-31+G\*) = -2287.809476; E(Def2-QZVP) = -  
2288.406831; G<sub>corr</sub> = 0.111333

0 5

Fe 0.30171900 0.62184300 -0.64493700  
O -0.51819100 -0.65368600 -2.21104200  
H -0.20168600 -1.52362400 -1.83428700  
H -1.48507900 -0.70740000 -2.23454300  
O 0.97165600 0.83487300 1.39327300  
H 1.66094000 1.50638000 1.50394700  
H 1.42245000 -0.06523000 1.51795500  
O -1.36339800 1.93021500 -0.51107400  
H -1.57326900 2.55970300 -1.21681500  
H -2.19429700 1.48582700 -0.28107800  
O -1.17155600 -0.72240100 0.48419900  
H -0.73842100 -1.59241600 0.27247000  
P 1.76667600 -1.89393200 -0.17125500  
O 1.95230800 -0.57498200 -0.98528700  
O 0.45099100 -2.58635800 -0.59332500  
O 1.90838600 -1.62453200 1.33396600  
O 2.94468000 -2.93616200 -0.63481600  
H 3.80014500 -2.67520400 -0.26216100  
H -1.07542000 -0.60781000 1.44109400  
O 1.76515800 2.13088800 -1.17193900  
H 2.52038100 1.57562700 -1.43184300  
H 1.61067400 2.74771300 -1.90260500

*cis*-**RC** Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(HPO<sub>4</sub>)(H<sub>2</sub>O<sub>2</sub>)

E(6-31+G\*) = -2362.858611; E(Def2-QZVP) = -  
2363.489340; G<sub>corr</sub> = 0.111347

0 5

Fe -0.06081400 -0.02063700 -0.38144500  
O -0.23629500 -0.79381100 -2.39723200  
H 0.73376600 -0.93958100 -2.66632600  
H -0.66790800 -1.65664600 -2.47818900  
O 0.76535700 1.02675900 1.67185300  
H 1.63312200 0.68248300 1.35949700  
O -0.91400500 1.73219200 -1.30038900  
H -0.55419700 2.60282000 -1.07351900  
H -0.86726300 1.66335800 -2.26712900  
O -1.79010200 0.02653200 0.87489900  
H -1.48658000 0.06315200 1.80177900  
O 2.34262200 -1.02965700 -2.71435500  
O 2.79905300 -2.07460700 -0.39398500  
O 4.24621500 -0.09928900 -1.22570200  
O 1.87984800 0.30651400 -0.58807500  
H -2.34453100 0.81093600 0.74156100  
O 0.37994100 -1.90695200 0.62495500  
H 1.32027000 -2.10918100 0.31422200  
H 0.44343600 -1.78395600 1.58517000  
O 0.36888200 0.11025400 2.69281200  
H 0.53351300 0.61769800 3.50672900  
P 2.76688800 -0.80836100 -1.25680900  
H 4.93034800 -0.70963800 -1.53881800

*cis*-**TS<sub>00</sub>** for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(HPO<sub>4</sub>)(H<sub>2</sub>O<sub>2</sub>)

E(6-31+G\*) = -2362.842429; E(Def2-QZVP) = -  
2363.471413; G<sub>corr</sub> = 0.111516

0 5

Fe 0.33988100 0.11320500 -0.14086200  
O -0.24711500 -0.66419600 -2.05918800  
H 0.62487000 -0.98472900 -2.47897300  
H -0.84283900 -1.42728200 -2.03151100  
O 0.47150400 1.06665000 1.57318200  
H 1.38687800 1.16246600 1.89785600  
O -0.52673500 1.85693800 -1.05734100  
H -0.10827800 2.72007500 -0.91852400  
H -0.58514100 1.72830100 -2.01801500  
O -1.69643900 -0.24992500 0.52856000

H -1.60370800 -0.24475900 1.50348300  
 O 2.16127300 -1.33940800 -2.76672200  
 O 2.91740400 -2.26821900 -0.44846900  
 O 4.39941400 -0.65365000 -1.69148300  
 O 2.17073400 0.15325100 -0.71097600  
 H -2.29692400 0.48148200 0.31558200  
 O 0.66463500 -1.79620100 0.79792000  
 H 1.56252900 -2.10508600 0.44441900  
 H 0.75192800 -1.70599300 1.75970600  
 O -0.13381000 0.15232400 2.83103000  
 H -0.46383900 0.89434300 3.36907300  
 P 2.84789100 -1.09071400 -1.41840100  
 H 4.45808800 -0.04597400 -2.44416700

*cis-I<sub>OH</sub>* for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(HPO<sub>4</sub>)(H<sub>2</sub>O<sub>2</sub>)

E(6-31+G\*) = -2362.869219; E(Def2-QZVP) = -  
 2363.500150; G<sub>corr</sub> = 0.109443

0 5

Fe 0.46316000 0.09622000 0.01194000  
 O -0.27835000 -0.77642600 -1.78465200  
 H 0.52101900 -1.07043200 -2.34114600  
 H -0.85405800 -1.54705900 -1.66773600  
 O 0.67713300 1.03692700 1.61363200  
 H 1.57830700 1.26809300 1.88251100  
 O -0.35392200 1.82818600 -0.93973800  
 H 0.02760800 2.66933500 -0.64200800  
 H -0.29235700 1.82170200 -1.90849700  
 O -1.59078500 -0.25872600 0.55700400  
 H -1.73450800 -0.06005400 1.51591800  
 O 2.03206200 -1.33176200 -2.84264300  
 O 2.99716500 -2.23329700 -0.58887700  
 O 4.32718600 -0.57121200 -1.94132600  
 O 2.15204400 0.15056200 -0.79160300  
 H -2.18452300 0.33713100 0.07285800  
 O 0.83649800 -1.81505900 0.77043700  
 H 1.72091700 -2.11361100 0.35108200  
 H 0.96105700 -1.81522200 1.73243800  
 O -1.33772900 0.54123800 3.18145300

H -0.46781500 0.83520600 2.74870200  
 P 2.82939900 -1.07533800 -1.56602800  
 H 4.31769200 0.01649800 -2.71254100

*cis-TS<sub>oxo</sub>* for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(HPO<sub>4</sub>)(H<sub>2</sub>O<sub>2</sub>)

E(6-31+G\*) = -2362.853020; E(Def2-QZVP) = -  
 2636.486031; G<sub>corr</sub> = 0.106771

0 5

Fe 0.50423000 -0.04855000 0.12278500  
 O -0.30830000 -0.75881700 -1.69440200  
 H 0.46934000 -0.98516500 -2.31487500  
 H -0.86126600 -1.55200900 -1.62484100  
 O 0.83735100 0.74871600 1.78202200  
 H 0.24737200 0.57269000 2.67463100  
 O -0.26646000 1.80807300 -0.61239500  
 H 0.11689800 2.58321000 -0.17110900  
 H -0.15004100 1.95056500 -1.56554100  
 O -1.52141500 -0.41322700 0.72081600  
 H -1.58495000 -0.03071200 1.63818900  
 O 1.94241300 -1.19462600 -2.90736500  
 O 3.02245000 -2.28686700 -0.79317400  
 O 4.27610700 -0.49821600 -2.05297600  
 O 2.15511100 0.09565200 -0.74006300  
 H -2.15691100 0.08156800 0.17993300  
 O 0.91436200 -2.01592300 0.67488200  
 H 1.78799700 -2.26740900 0.20337400  
 H 1.05373700 -2.13541400 1.62741800  
 O -0.96954500 0.66765700 3.08285700  
 H -1.15695400 1.62322500 3.10629200  
 P 2.80268600 -1.04904800 -1.65425900  
 H 4.22809200 0.15180000 -2.77091500

*cis-I<sub>oxo</sub>* for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(HPO<sub>4</sub>)(H<sub>2</sub>O<sub>2</sub>)

E(6-31+G\*) = -2362.887681; E(Def2-QZVP) = -  
 2363.514943; G<sub>corr</sub> = 0.115903

0 5

Fe 0.49734000 0.33633700 -0.12596000  
 O -0.23089200 -0.64194800 -1.76294700

H 0.55529600 -1.10832900 -2.24236500  
H -0.87589300 -1.32371100 -1.51740600  
O 0.91589300 1.24639300 1.13296600  
H 0.01410200 0.39263700 3.15689300  
O -0.34416900 1.98359500 -1.17448600  
H 0.11093100 2.83177100 -1.05309000  
H -0.39966300 1.82830300 -2.13154800  
O -1.46830600 0.08811100 0.54448200  
H -1.39733300 -0.06171000 1.52159000  
O 1.95953100 -1.59386700 -2.64769500  
O 2.99858400 -2.12393700 -0.30971100  
O 4.29335000 -0.73336100 -1.97180500  
O 2.19599500 0.22523700 -0.88891200  
H -1.96799100 0.91258600 0.42709000  
O 0.67990200 -1.55373200 0.80615700  
H 1.60370400 -1.89099700 0.59010200  
H 0.57992200 -1.45635800 1.77333700  
O -0.50845200 -0.41116000 3.00522700  
H -0.92461600 -0.63491500 3.85024900  
P 2.80756600 -1.14210600 -1.45413200  
H 4.25302400 -0.26883900 -2.82197200

*trans*-**RC** Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(HPO<sub>4</sub>)(H<sub>2</sub>O<sub>2</sub>)

E(6-31+G\*) = -2362.857269; E(Def2-QZVP) = -  
2363.488607; G<sub>corr</sub> = 0.112122

0 5

Fe 0.41713100 0.01888500 -0.80793200  
O -1.10255400 -0.02518000 -2.37981800  
H -1.65948900 -0.79570100 -2.18386400  
H -1.67923800 0.75132200 -2.23503400  
O 1.08621900 0.87691600 1.11425500  
H 1.68250700 1.63798200 1.06516800  
H 1.66121100 0.10989300 1.46384900  
O -1.31984600 1.36472500 0.07302700  
H -0.89024500 2.06552400 0.59648400  
O -0.90295200 -1.52746900 0.03614100  
H -0.26456600 -2.25983100 0.31633700  
P 2.19111600 -2.10912000 0.46481100

O 1.93551700 -1.19655900 -0.79353800  
O 1.08111000 -3.14891500 0.62326100  
O 2.47824800 -1.23062000 1.69201800  
O 3.54085100 -2.97532100 0.12235400  
H 4.32734000 -2.41081800 0.16263200  
H -1.36698900 -1.24792900 0.83836600  
O 1.02101000 1.77369900 -1.89409900  
H 1.76885300 2.31244800 -1.59597600  
H 1.15341100 1.64664700 -2.84594200  
O -2.08296200 2.09010900 -0.88940900  
H -2.98509600 2.00602300 -0.53225100

*trans*-**TS<sub>OO</sub>** for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(HPO<sub>4</sub>)(H<sub>2</sub>O<sub>2</sub>)

E(6-31+G\*) = -2362.839604; E(Def2-QZVP) = -  
2363.469897; G<sub>corr</sub> = 0.109447

0 5

Fe 0.13599700 0.22823500 -0.43774100  
O -0.80434800 0.01321300 -2.34799200  
H -1.05510400 -0.87551700 -2.64038000  
H -1.62842300 0.54572400 -2.27609200  
O 1.14069800 0.79665200 1.36916900  
H 1.52512400 1.68513200 1.38501600  
H 1.90579700 0.13314200 1.48024400  
O -1.32895600 1.47120400 -0.04281100  
H -1.14711100 2.37703500 0.26333400  
O -0.93594800 -1.33134800 0.43629300  
H -0.25283300 -2.07259500 0.64075900  
P 2.15100700 -1.99492800 0.29818200  
O 1.59952700 -1.04688800 -0.82963100  
O 1.04207200 -2.94502400 0.76684700  
O 2.84058700 -1.16294300 1.38786400  
O 3.27014500 -2.95940500 -0.40703500  
H 4.09805000 -2.47582200 -0.54736700  
H -1.40702600 -1.12914500 1.25813000  
O 1.35560600 1.73251000 -1.39979900  
H 2.18486900 1.26906700 -1.60796900  
H 1.01134400 2.04087200 -2.25324100  
O -2.38867500 1.88752000 -1.25150300

H -3.19121000 1.57061800 -0.79943700

*trans-I<sub>OH</sub>* for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(HPO<sub>4</sub>)(H<sub>2</sub>O<sub>2</sub>)

E(6-31+G\*) = -2362.866716; E(Def2-QZVP) = -  
2363.498566; G<sub>corr</sub> = 0.108110

0 5

Fe 0.15590500 0.34134500 -0.37552000

O -0.77165100 -0.03128300 -2.22610300

H -0.77673600 -0.96279100 -2.49572000

H -1.70461800 0.30100300 -2.26580600

O 1.18754200 0.80554100 1.38835100

H 1.63805900 1.66376900 1.35323300

H 1.91402000 0.08825500 1.49548500

O -1.12968800 1.67531600 -0.08670600

H -1.10532600 2.24426500 0.69498300

O -0.93213200 -1.16453400 0.54591900

H -0.32266100 -1.97172500 0.70654100

P 2.04998600 -2.01209300 0.27262800

O 1.47179300 -0.97660500 -0.78971000

O 0.92727600 -2.94741700 0.71220100

O 2.77636900 -1.22269100 1.36401500

O 3.11841300 -2.93283500 -0.53562700

H 3.95842500 -2.46552300 -0.66207400

H -1.37225500 -0.94056100 1.37986200

O 1.45531800 1.71395700 -1.36708000

H 2.10772600 1.23828400 -1.90707900

H 1.02807500 2.35994200 -1.95178200

O -3.07745500 1.34848800 -1.76508800

H -2.45179600 1.62860400 -1.01408600

*trans-TS<sub>oxo</sub>* for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(HPO<sub>4</sub>)(H<sub>2</sub>O<sub>2</sub>)

E(6-31+G\*) = -2362.850896; E(Def2-QZVP) = -  
2363.484279; G<sub>corr</sub> = 0.105656

0 5

Fe 0.11651600 0.34991200 -0.38640300

O -0.82427300 0.02990900 -2.22534400

H -0.97010100 -0.89944300 -2.46093300

H -1.71393100 0.48048200 -2.16672200

O 1.11794400 0.77389000 1.39770000

H 1.53787500 1.64788500 1.41636600

H 1.85891900 0.07244400 1.49284100

O -1.12224800 1.73141000 -0.01266900

H -1.87610300 2.09294400 -0.70054300

O -0.99831800 -1.13955600 0.51313100

H -0.39369100 -1.95398000 0.66896700

P 1.98412700 -2.01709400 0.24349200

O 1.41575600 -0.96371900 -0.81168400

O 0.84411000 -2.93404300 0.67627900

O 2.72520000 -1.24433800 1.33498900

O 3.03245700 -2.94692900 -0.57736700

H 3.88352000 -2.49739200 -0.69459300

H -1.42870500 -0.91285800 1.35185200

O 1.43078700 1.74138100 -1.32846500

H 2.09643000 1.27566100 -1.86110900

H 1.03229100 2.41150000 -1.90633000

O -2.77162100 1.63398600 -1.51338500

H -3.44067000 1.21348800 -0.94466000

*trans-I<sub>oxo</sub>* for Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(HPO<sub>4</sub>)(H<sub>2</sub>O<sub>2</sub>)

E(6-31+G\*) = -2362.889693; E(Def2-QZVP) = -  
2363.518720; G<sub>corr</sub> = 0.115059

0 5

Fe 0.19310500 0.53710800 -0.28770200

O -0.66831900 0.25753600 -2.12419800

H -0.58281800 -0.67079000 -2.39557900

H -1.64010900 0.49765000 -2.09225600

O 1.25866500 0.73021500 1.45726100

H 1.66315600 1.60544900 1.56132600

H 1.99917000 0.01987500 1.47392600

O -0.78932900 1.77929100 0.05431300

H -2.58045500 1.66239300 -0.80184600

O -1.01569900 -0.89147600 0.55164600

H -0.45644800 -1.74220100 0.69587300

P 1.88395000 -1.99298600 0.17646400

O 1.35341100 -0.86952800 -0.82433500

O 0.69317800 -2.80498300 0.67920400

O 2.77722100 -1.32576900 1.22369400  
O 2.77029200 -2.99781600 -0.74034700  
H 3.65432900 -2.63553500 -0.90600800  
H -1.40983400 -0.63578900 1.39980700  
O 1.64946000 1.77677500 -1.20438600  
H 2.21440600 1.20083700 -1.74742900  
H 1.29307900 2.45632300 -1.79873100  
O -3.02124500 1.29372200 -1.59164000  
H -3.70289700 0.69523700 -1.25364700

GC base pair

$E(6-31+G^*) = -936.586427$ ;  $E(\text{Def2-QZVP}) = -936.967994$ ;  $G_{\text{corr}} = 0.178439$

0 1

N 1.91097100 3.32035000 -0.04095100  
C 2.82878200 2.29905400 -0.02115800  
H 3.89250700 2.49711500 -0.01903200  
N 2.27209600 1.11516800 -0.00598700  
C 0.91625700 1.37573300 -0.01642100  
C -0.20442700 0.49888200 -0.00833200  
O -0.20444800 -0.74452200 0.01072900  
N -1.41045500 1.19659700 -0.02475400  
H -2.27024500 0.61172900 -0.02036100  
C -1.54147400 2.56257400 -0.04585400  
N -2.79201800 3.04606400 -0.05774000  
H -3.62388000 2.44287700 -0.05868900  
H -2.90680200 4.04791400 -0.07816100  
N -0.50818000 3.39274100 -0.05356600  
C 0.67188900 2.75004100 -0.03826200  
N -6.14942600 -0.60662800 -0.02019400  
C -6.12031200 -1.96194900 0.00867100  
C -4.99516800 0.16474100 -0.03044000  
H -7.08087800 -2.46477200 0.01480700  
C -4.93394400 -2.61786700 0.02835000  
N -3.80329400 -0.47190600 -0.01116300  
O -5.10683600 1.40315600 -0.05679700  
H -4.88732100 -3.69951500 0.05154200  
C -3.74867300 -1.81147200 0.01706700

N -2.54230500 -2.37836400 0.03458800  
H -1.69241800 -1.80036800 0.02622300  
H -2.44942300 -3.38285400 0.05609700  
H 2.11368700 4.31095200 -0.05450600  
H -7.03185100 -0.11053700 -0.03475400

*cis*-[Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(GC)]<sup>2+</sup>

$E(6-31+G^*) = -2581.557638$ ;  $E(\text{Def2-QZVP}) = -2582.324659$ ;  $G_{\text{corr}} = 0.288692$

2 5

N 1.90484300 3.32770500 -0.03978800  
C 2.82612700 2.33065300 -0.02421300  
H 3.89022200 2.52090700 -0.02215000  
N 2.26660100 1.14007300 -0.01050100  
C 0.90136800 1.38116000 -0.01865600  
C -0.21559300 0.51774100 -0.01259100  
O -0.19751300 -0.74508600 0.00488600  
N -1.41575300 1.18543900 -0.02615500  
H -2.27575900 0.58724200 -0.02124300  
C -1.55082300 2.55568700 -0.04496200  
N -2.79211500 3.03827800 -0.05658000  
H -3.62750700 2.43376900 -0.05750200  
H -2.90419400 4.04124900 -0.07281000  
N -0.51134900 3.38587900 -0.05147200  
C 0.66209100 2.75518300 -0.03768900  
N -6.12807600 -0.58788800 -0.02292200  
C -6.11964900 -1.94298900 0.00657100  
C -4.96430200 0.16597300 -0.03119700  
H -7.08736700 -2.43169000 0.01072400  
C -4.94272600 -2.61533500 0.02926600  
N -3.77934200 -0.48610200 -0.00931100  
O -5.06042300 1.40561300 -0.05832100  
H -4.91089500 -3.69741300 0.05307400  
C -3.74687300 -1.82704200 0.01993500  
N -2.55136900 -2.41670700 0.04081600  
H -1.69671900 -1.85686100 0.03184300  
H -2.47359400 -3.42239800 0.06152600  
H 2.10597000 4.31999700 -0.05016100

H -7.00287100 -0.07810300 -0.03946400  
 Fe 3.25645300 -0.73597100 0.01735800  
 O 4.31183800 -2.62281400 -0.14421500  
 H 4.83819500 -2.88309100 0.62754800  
 O 1.93840500 -1.41120300 1.56250100  
 H 1.01563200 -1.35429500 1.22698800  
 O 4.70327700 -0.05141000 -1.40941400  
 H 4.43228900 0.37742800 -2.23556500  
 O 4.65106600 -0.31508500 1.56824700  
 H 4.31958300 -0.00721200 2.42596000  
 O 1.93793400 -1.68795200 -1.36712800  
 H 2.00924600 -1.48860000 -2.31232800  
 H 5.36104500 -0.71980700 -1.65789700  
 H 3.77314400 -3.39468000 -0.37777600  
 H 2.04473200 -2.28703400 1.96171300  
 H 5.44288500 0.21116900 1.37801200  
 H 1.02383900 -1.44260600 -1.08747500

**RC** for *cis*-[Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(GC)]<sup>2+</sup> system

E(6-31+G\*) = -2656.599472; E(Def2-QZVP) = -  
 2657.400099; G<sub>corr</sub> = 0.289153

2 5

N -1.82725600 3.19212400 0.12623000  
 C -2.71515200 2.16582400 0.14160200  
 H -3.78626100 2.30974300 0.15953500  
 N -2.11336500 0.99561300 0.12186400  
 C -0.75796800 1.28119300 0.09316500  
 C 0.38390100 0.45263000 0.06708800  
 O 0.40120400 -0.81041600 0.05874800  
 N 1.56202100 1.15772400 0.04614200  
 H 2.44062300 0.58735600 0.01922900  
 C 1.65264100 2.53212200 0.05035700  
 N 2.87767900 3.05409100 0.02672600  
 H 3.73159100 2.47638800 0.00807400  
 H 2.95793000 4.06024400 0.02907900  
 N 0.58754500 3.32928600 0.07666300  
 C -0.56522100 2.66181400 0.09651300  
 N 6.32256900 -0.46821800 -0.10152500

C 6.35502600 -1.82290000 -0.13476200  
 C 5.13687200 0.24921200 -0.05414600  
 H 7.33667800 -2.28153800 -0.17073000  
 C 5.19932900 -2.53134600 -0.12235900  
 N 3.97257100 -0.43934700 -0.04058200  
 O 5.19513100 1.49116400 -0.02629000  
 H 5.20013900 -3.61386700 -0.14806900  
 C 3.98060700 -1.78055700 -0.07321900  
 N 2.80395800 -2.40713100 -0.05874000  
 H 1.93294600 -1.87443300 -0.02039000  
 H 2.75711600 -3.41469900 -0.08069800  
 H -2.06153300 4.17716600 0.13432200  
 H 7.18131700 0.06835600 -0.11138500  
 Fe -3.03549000 -0.89708400 0.17671000  
 O -4.09225600 -2.76231100 0.21908100  
 H -4.69435700 -2.96455200 -0.51373900  
 O -1.75631900 -1.55510400 -1.43021400  
 H -0.82738600 -1.45242800 -1.12114600  
 O -4.43342300 -0.17874700 1.61408200  
 H -4.13706900 0.11147200 2.49015100  
 O -4.36964900 -0.43944600 -1.49995600  
 H -3.90536900 -0.25697600 -2.33756500  
 O -1.66639000 -1.84188600 1.49233800  
 H -1.71198300 -1.70052900 2.44949500  
 H -5.22736500 -0.71499000 1.76257100  
 H -3.58388400 -3.57139300 0.38465100  
 H -1.83774300 -2.45425200 -1.78116900  
 H -0.76569000 -1.56777900 1.19829100  
 O -5.19324500 0.71142400 -1.33013300  
 H -6.07764900 0.33652200 -1.48908000

**TS<sub>00</sub>** for *cis*-[Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(GC)]<sup>2+</sup> system

E(6-31+G\*) = -2656.574031; E(Def2-QZVP) = -  
 2657.372479; G<sub>corr</sub> = 0.289447

2 5

N -1.84687700 3.14326800 0.03025500  
 C -2.72494400 2.11381200 -0.01277100  
 H -3.79884600 2.23523700 -0.07364400

N -2.10982600 0.94698700 0.00182200  
 C -0.75513400 1.24268100 0.04704000  
 C 0.39668300 0.43084100 0.00689700  
 O 0.42461600 -0.83251200 -0.06375900  
 N 1.56640600 1.14449100 0.04162200  
 H 2.45231000 0.58285500 0.01631800  
 C 1.64106500 2.51955400 0.08715500  
 N 2.85791700 3.05564600 0.12356500  
 H 3.71945800 2.48802400 0.11286800  
 H 2.92536200 4.06256800 0.14857200  
 N 0.56496400 3.30394400 0.09092000  
 C -0.57858900 2.62531400 0.06389200  
 N 6.34286500 -0.41827100 -0.02882800  
 C 6.39571900 -1.77023900 -0.10904800  
 C 5.14644000 0.28105100 0.00961900  
 H 7.38442600 -2.21420000 -0.13285600  
 C 5.25033000 -2.49382100 -0.15561700  
 N 3.99173600 -0.42259800 -0.03541100  
 O 5.18658500 1.52181800 0.08387800  
 H 5.26741400 -3.57451700 -0.22071100  
 C 4.02008400 -1.76175500 -0.11536900  
 N 2.85295500 -2.40465600 -0.15744900  
 H 1.97402800 -1.88610500 -0.12901500  
 H 2.82086900 -3.41135600 -0.21557300  
 H -2.09064400 4.12630700 0.02449100  
 H 7.19353700 0.12999300 0.00618100  
 Fe -3.09574800 -0.89364200 0.02508500  
 O -3.93149900 -2.80743600 0.35513400  
 H -4.50354000 -3.22334200 -0.30839800  
 O -1.76849100 -1.53209400 -1.46784100  
 H -0.83194100 -1.42278900 -1.16467600  
 O -4.27781100 -0.37348600 1.69374700  
 H -3.98208800 0.25444300 2.37149900  
 O -4.51135900 -0.52509700 -1.16194600  
 H -4.35936200 -0.45413900 -2.12002100  
 O -1.65044600 -1.76469100 1.36835000  
 H -1.67881400 -1.49557000 2.29931600  
 H -4.72866700 -1.09750000 2.15769300

H -3.32910000 -3.49106700 0.69015100  
 H -1.85498100 -2.43258800 -1.81817600  
 H -0.74085500 -1.55454100 1.04420300  
 O -5.40953800 0.99506400 -1.07850500  
 H -6.13648200 0.59414500 -0.56915000

**I<sub>OH</sub>** for *cis*-[Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(GC)]<sup>2+</sup> system

E(6-31+G\*) = -2565.588387; E(Def2-QZVP) = -2657.387508; G<sub>corr</sub> = 0.289001

2 5

N -1.89375500 3.06596600 -0.03399200  
 C -2.75067900 2.02309900 -0.07016200  
 H -3.82869500 2.13503100 -0.10905000  
 N -2.10978200 0.86697300 -0.04740400  
 C -0.76052400 1.18822400 -0.00152700  
 C 0.40853700 0.40142600 -0.02126100  
 O 0.45998800 -0.86352900 -0.06902600  
 N 1.56198400 1.13747400 0.01139600  
 H 2.46057300 0.59302700 0.00419000  
 C 1.60739000 2.51476900 0.04010500  
 N 2.81030500 3.07773800 0.07513500  
 H 3.68503200 2.52910600 0.07380300  
 H 2.85493100 4.08630400 0.08893000  
 N 0.51337300 3.27586300 0.02998200  
 C -0.61372000 2.57417100 0.00510100  
 N 6.36734900 -0.31633400 0.01846400  
 C 6.45255900 -1.66845300 -0.01941900  
 C 5.15493100 0.35534000 0.02539600  
 H 7.45138800 -2.08972700 -0.02101100  
 C 5.32470700 -2.41968900 -0.05339300  
 N 4.01698800 -0.37599800 -0.00815800  
 O 5.16595400 1.59841900 0.06229500  
 H 5.36719100 -3.50119500 -0.08475500  
 C 4.07753400 -1.71606900 -0.04652100  
 N 2.92666500 -2.38811000 -0.07863000  
 H 2.03573200 -1.89103400 -0.07702700  
 H 2.91914700 -3.39658200 -0.10688900  
 H -2.15785300 4.04415800 -0.04229400



H 7.20448200 0.25285500 0.04487600  
 Fe -3.06687800 -0.97405500 -0.08918000  
 O -3.83918400 -2.87531000 0.29197900  
 H -4.42510800 -3.29711300 -0.35690100  
 O -1.67812300 -1.61618900 -1.46554600  
 H -0.74726600 -1.47807600 -1.14089600  
 O -4.24534100 -0.39397700 1.53974700  
 H -3.96714600 0.22750900 2.23181500  
 O -4.42390900 -0.58226900 -1.24109500  
 H -4.29776800 -0.59089600 -2.20264800  
 O -1.65007200 -1.74524400 1.32096200  
 H -1.72331100 -1.50090900 2.25667400  
 H -4.78581500 -1.07860100 1.96836600  
 H -3.24890200 -3.55775100 0.65181800  
 H -1.74016300 -2.52003700 -1.81531500  
 H -0.72288000 -1.54583600 1.03989900  
 O -6.01375300 1.39935000 -0.23428400  
 H -5.55553500 0.61329400 -0.64264600

**TS<sub>oxo</sub>** for *cis*-[Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(GC)]<sup>2+</sup> system

E(6-31+G\*) = -2656.571777; E(Def2-QZVP) = -  
 2657.372134; G<sub>corr</sub> = 0.285179

2 5

N -1.74369100 3.20495300 -0.10586900  
 C -2.63965800 2.19627000 -0.14597200  
 H -3.70656500 2.35426100 -0.21562200  
 N -2.04855200 1.01610400 -0.09111900  
 C -0.68889400 1.28288400 -0.02515500  
 C 0.44739500 0.44830400 -0.03174400  
 O 0.44721400 -0.81719300 -0.07906600  
 N 1.62917800 1.13738500 0.01009200  
 H 2.50524500 0.55706500 0.01053500  
 C 1.73008300 2.51191100 0.03228500  
 N 2.95376400 3.02579700 0.08298600  
 H 3.80522700 2.44183600 0.10500700  
 H 3.03916800 4.03182600 0.09246800  
 N 0.66818200 3.31717700 -0.00046100  
 C -0.48559600 2.66174200 -0.03497000

N 6.37127200 -0.50654200 0.05583200  
 C 6.40381400 -1.85963200 -0.01421700  
 C 5.18618500 0.21203000 0.06498000  
 H 7.38550200 -2.31952600 -0.01557200  
 C 5.24795400 -2.56491800 -0.07860200  
 N 4.02097000 -0.47289500 0.00189400  
 O 5.24549600 1.45260400 0.13066400  
 H 5.24900200 -3.64613800 -0.13606600  
 C 4.02919200 -1.81312400 -0.06752800  
 N 2.85306600 -2.43793800 -0.12731300  
 H 1.98239400 -1.90634500 -0.11634700  
 H 2.80540800 -3.44440500 -0.17867100  
 H -1.96745900 4.19288300 -0.13460900  
 H 7.22984900 0.02832600 0.10363600  
 Fe -3.08224900 -0.77655100 -0.11031200  
 O -3.89559600 -2.67193300 0.24373900  
 H -4.51855400 -3.06004300 -0.39162300  
 O -1.72717500 -1.46028800 -1.49675200  
 H -0.79130300 -1.38377300 -1.17110300  
 O -4.22864700 -0.28372800 1.64795200  
 H -3.95434700 0.40613900 2.27504500  
 O -4.40201900 -0.27071900 -1.19842000  
 H -5.45536500 0.11880500 -0.97783900  
 O -1.69905500 -1.58505800 1.30889200  
 H -1.74515600 -1.31664500 2.23921700  
 H -4.52453200 -1.04186100 2.18042000  
 H -3.31226800 -3.38092900 0.56113700  
 H -1.84090400 -2.34642600 -1.87694500  
 H -0.76608400 -1.43663800 1.01313600  
 O -6.42705400 -0.01819200 -0.31550900  
 H -6.09828800 0.13688200 0.59315200

**I<sub>oxo</sub>** for *cis*-[Fe<sup>II</sup>(H<sub>2</sub>O)<sub>5</sub>(GC)]<sup>2+</sup> system

E(6-31+G\*) = -2656.605026; E(Def2-QZVP) = -  
 2657.402458; G<sub>corr</sub> = 0.293861

2 5

N -1.96659200 2.98212800 -0.11520900  
 C -2.81016600 1.93213100 -0.14178000

H -3.89365500 2.01879000 -0.19059800  
 N -2.14780200 0.78819900 -0.07848800  
 C -0.79954400 1.12191400 -0.02029100  
 C 0.38706200 0.35991300 0.00057200  
 O 0.47084800 -0.90422400 0.00164900  
 N 1.52445800 1.12030900 0.01440200  
 H 2.43386500 0.59305400 0.02792400  
 C 1.54305700 2.49762500 0.00672200  
 N 2.73249000 3.08671600 0.03439100  
 H 3.61868100 2.55694800 0.06730500  
 H 2.75552900 4.09615300 0.02580000  
 N 0.43242300 3.23434300 -0.02935500  
 C -0.67888700 2.51089300 -0.04930000  
 N 6.35990300 -0.22656500 0.06253300  
 C 6.47645700 -1.57600200 0.01423000  
 C 5.13243800 0.41699900 0.07141500  
 H 7.48453300 -1.97450900 0.01026700  
 C 5.36615400 -2.35259700 -0.02616500  
 N 4.01143100 -0.33985000 0.03263000  
 O 5.11518300 1.65985300 0.11491900  
 H 5.43303300 -3.43265600 -0.06494000  
 C 4.10319900 -1.67800200 -0.01356000  
 N 2.96853600 -2.37676000 -0.04847500  
 H 2.06657800 -1.90110500 -0.03263500  
 H 2.98472900 -3.38502600 -0.07956300  
 H -2.24334500 3.95664400 -0.14513200  
 H 7.18343400 0.36180200 0.09404400  
 Fe -3.01322900 -1.00845500 -0.11276800  
 O -3.79523900 -2.86114600 0.08000000  
 H -4.36472700 -3.21230900 -0.62475300  
 O -1.62667800 -1.60785300 -1.57320000  
 H -0.69708400 -1.60763100 -1.24948200  
 O -4.21939000 -0.54126700 1.59256300  
 H -3.89380900 -0.02131900 2.34470200  
 O -4.15117400 -0.57054400 -1.14900000  
 H -5.65561400 0.63054800 -0.50026400  
 O -1.66469700 -1.75575400 1.19487100  
 H -1.75355600 -1.52768400 2.13443000

H -4.72932600 -1.27982900 1.96426000  
 H -3.19443600 -3.57093800 0.36577400  
 H -1.77400000 -2.43554300 -2.05741100  
 H -0.72670700 -1.53590600 0.91595900  
 O -5.91844600 1.49338300 -0.14000900  
 H -6.09598300 1.31389200 0.79386400

*cis*-Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(SO<sub>4</sub>)(GC)

E(6-31+G\*) = -3204.168348; E(Def2-QZVP) = -3205.120542; G<sub>corr</sub> = 0.278208

0 5

N 2.21039900 3.00101100 -0.37326700  
 C 3.06108400 1.95033300 -0.21154200  
 H 4.13659500 2.05983600 -0.22427100  
 N 2.42198000 0.81401000 -0.05709700  
 C 1.07958600 1.14309800 -0.12782200  
 C -0.08991200 0.35534000 -0.06885500  
 O -0.15320700 -0.89753600 0.07207900  
 N -1.24455000 1.09161400 -0.19365100  
 H -2.14066900 0.55362500 -0.14418900  
 C -1.28870500 2.45591100 -0.37336800  
 N -2.49748700 3.01036800 -0.47425900  
 H -3.36878700 2.46258600 -0.42940300  
 H -2.54444300 4.00914100 -0.61085200  
 N -0.19884700 3.21326800 -0.44912400  
 C 0.93239700 2.51647800 -0.32492700  
 N -6.06113900 -0.38030100 -0.05397400  
 C -6.13588400 -1.71704900 0.15825100  
 C -4.85307900 0.29469800 -0.14805900  
 H -7.13145700 -2.14229300 0.21465000  
 C -5.00237100 -2.44954100 0.28708800  
 N -3.71097100 -0.41869800 -0.02321300  
 O -4.87255700 1.52283700 -0.34271500  
 H -5.03658700 -3.51861400 0.45633400  
 C -3.76030000 -1.74280400 0.18666400  
 N -2.60289000 -2.39409800 0.30107800  
 H -1.71519600 -1.89221900 0.22494100  
 H -2.58689300 -3.39066100 0.45699800

H 2.47858100 3.96745100 -0.50965600  
H -6.90229400 0.17442900 -0.15227700  
Fe 3.37808100 -1.10079200 0.16915100  
O 4.18830800 -3.10113400 0.39802000  
H 5.06545600 -3.01289900 -0.07705500  
O 1.92299500 -1.62029000 1.67570400  
H 1.03218500 -1.49853100 1.27248500  
O 4.70876100 -0.42456800 1.72388500  
H 4.46357200 0.39628200 2.17401100  
O 1.97521100 -2.07510900 -1.24655500  
H 2.13153800 -1.83689100 -2.17217400  
H 3.66102200 -3.71639000 -0.13332900  
H 1.96025300 -2.52873200 2.00897000  
H 5.55520700 -0.24028800 1.21965200  
H 1.08163200 -1.73718300 -1.01972200  
O 4.70198400 -0.67909700 -1.32104200  
O 6.38164400 -2.43438800 -0.92141100  
O 6.70297200 -0.17326800 0.01743400  
O 6.90059500 -0.53631100 -2.41856800  
S 6.21299300 -0.95614700 -1.17747200

**RC** for *cis*-Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(SO<sub>4</sub>)(GC) system

E(6-31+G\*) = -3279.216091; E(Def2-QZVP) = -  
3280.201538; G<sub>corr</sub> = 0.279600

0 5

N 2.16644600 3.03415900 -0.38384700  
C 3.02321200 1.98990800 -0.21459800  
H 4.09688700 2.10949200 -0.19932800  
N 2.39153400 0.84842700 -0.07440300  
C 1.04685900 1.16726800 -0.15815100  
C -0.11785800 0.37453800 -0.09008800  
O -0.17373300 -0.87703300 0.07060800  
N -1.27687700 1.10192500 -0.22403200  
H -2.16961200 0.55858800 -0.17203200  
C -1.32908900 2.46480400 -0.41137600  
N -2.54100700 3.01059900 -0.52353500  
H -3.40869100 2.45691500 -0.48303800  
H -2.59383500 4.00848400 -0.66427000

N -0.24383700 3.22916700 -0.48180100  
C 0.89146600 2.54008900 -0.35147100  
N -6.08364300 -0.40469100 -0.11702300  
C -6.15038700 -1.74020700 0.10541700  
C -4.87989600 0.27928900 -0.20126800  
H -7.14321100 -2.17294000 0.15265800  
C -5.01282800 -2.46244300 0.25472800  
N -3.73382400 -0.42387600 -0.05615800  
O -4.90662000 1.50561900 -0.40610500  
H -5.04072500 -3.53036100 0.43218800  
C -3.77523300 -1.74661500 0.16375200  
N -2.61415100 -2.38760000 0.29766000  
H -1.72956500 -1.87965100 0.22531000  
H -2.59197000 -3.38284300 0.46108900  
H 2.42898700 4.00338200 -0.51067800  
H -6.92792700 0.14237500 -0.23045600  
Fe 3.35017100 -1.05039200 0.14396400  
O 4.15171700 -3.05297800 0.41091500  
H 5.01037700 -3.00394600 -0.10010600  
O 1.92393100 -1.55086500 1.67220400  
H 1.02723500 -1.44027000 1.27738200  
O 4.77614000 -0.41445300 1.65378200  
O 1.94180100 -2.06030600 -1.23608300  
H 2.08873000 -1.84695100 -2.16926300  
H 3.58912400 -3.66818100 -0.08372700  
H 1.96849800 -2.45295600 2.02196800  
H 5.61936200 -0.27561500 1.09705500  
H 1.04630200 -1.72491400 -1.01118200  
O 4.66740300 -0.66217700 -1.34925100  
O 6.30670200 -2.46797000 -1.01868100  
O 6.70406800 -0.23556300 -0.04290500  
O 6.84810600 -0.55286600 -2.48827900  
S 6.17252200 -0.98472900 -1.24813800  
O 4.55268000 0.86740400 2.25074800  
H 4.85233700 0.70512000 3.16119400

**TS<sub>00</sub>** for *cis*-Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(SO<sub>4</sub>)(GC) system

E(6-31+G\*) = -3279.194059; E(Def2-QZVP) = -

3280.176887;  $G_{\text{corr}} = 0.278649$

0 5

N 2.16331200 3.04943400 -0.26286900  
C 3.02283100 2.01413200 -0.07852000  
H 4.09339100 2.14140400 -0.01186100  
N 2.39406300 0.86477400 0.02224900  
C 1.04886100 1.17173200 -0.09925600  
C -0.11264000 0.37478400 -0.04343700  
O -0.15999900 -0.87604600 0.13136300  
N -1.27216900 1.09331000 -0.20123200  
H -2.16339600 0.54419500 -0.16375400  
C -1.32768400 2.45655500 -0.38816300  
N -2.53825800 2.99554100 -0.52994200  
H -3.40375200 2.43642700 -0.51173600  
H -2.59332600 3.99386200 -0.66737700  
N -0.24465500 3.22766700 -0.42801500  
C 0.89056000 2.54538700 -0.27803100  
N -6.06498000 -0.44081300 -0.21436200  
C -6.13122000 -1.77557800 0.01240000  
C -4.86315200 0.24929900 -0.26572700  
H -7.12268400 -2.21350300 0.03215000  
C -4.99477200 -2.49082100 0.19898400  
N -3.71794000 -0.44674300 -0.08319600  
O -4.89043700 1.47456200 -0.47687700  
H -5.02224300 -3.55801700 0.38054100  
C -3.75885300 -1.76881900 0.14140500  
N -2.59904400 -2.40317800 0.31281800  
H -1.71549400 -1.89200100 0.26098500  
H -2.57609000 -3.39776900 0.48017500  
H 2.42198800 4.02303500 -0.36308000  
H -6.90844800 0.10123000 -0.35487900  
Fe 3.41994000 -0.97557700 0.25302400  
O 4.04288600 -3.02577800 0.45545100  
H 4.90187300 -3.03323500 -0.06196700  
O 1.95917600 -1.47394900 1.71956900  
H 1.05691800 -1.38512000 1.32567600  
O 4.76613800 -0.40032700 1.45117400  
O 2.00098900 -1.97183100 -1.12431100

H 2.18221900 -1.73244600 -2.04571500  
H 3.42404100 -3.55620300 -0.07206000  
H 2.02206300 -2.36926600 2.08594900  
H 5.62018100 -0.25191100 0.94328500  
H 1.08281100 -1.68244300 -0.92467000  
O 4.55531000 -0.77335500 -1.35659100  
O 6.17917200 -2.59198200 -1.04409800  
O 6.72760900 -0.29860900 -0.30997100  
O 6.59855600 -0.82375800 -2.72490000  
S 6.07256800 -1.12868500 -1.38165200  
O 4.78903800 1.13836600 2.28013200  
H 4.89521800 0.72673000 3.15436800

$I_{\text{OH}}$  for *cis*-Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(SO<sub>4</sub>)(GC) system

E(6-31+G\*) = -3279.212634; E(Def2-QZVP) = -  
3280.195758;  $G_{\text{corr}} = 0.278206$

0 5

N 2.21974400 2.98476400 -0.28649700  
C 3.07067400 1.94251500 -0.12571700  
H 4.14566800 2.05191500 -0.11477900  
N 2.42696900 0.79850200 -0.00828800  
C 1.08372700 1.11985400 -0.09715800  
C -0.08737400 0.33492200 -0.04385200  
O -0.14442000 -0.91938000 0.09923300  
N -1.23887300 1.06840000 -0.17361300  
H -2.13703000 0.52827000 -0.13442600  
C -1.28016900 2.43514600 -0.34236900  
N -2.48387400 2.99181000 -0.45361900  
H -3.35732800 2.44410600 -0.42589700  
H -2.52728100 3.99235800 -0.57990900  
N -0.18684000 3.19257600 -0.39600200  
C 0.94044200 2.49649400 -0.27073300  
N -6.04733600 -0.39585200 -0.12424500  
C -6.13035500 -1.73384700 0.07614800  
C -4.83616600 0.27607500 -0.18799600  
H -7.12799200 -2.15667400 0.10850100  
C -5.00176800 -2.47042500 0.22313800  
N -3.69833200 -0.44119100 -0.04489500

O -4.84863100 1.50574400 -0.37368800  
 H -5.04224900 -3.54066800 0.38316900  
 C -3.75600700 -1.76691400 0.15390700  
 N -2.60378100 -2.42363800 0.28754400  
 H -1.71350200 -1.92626200 0.23085000  
 H -2.59410400 -3.42155700 0.43511900  
 H 2.48823600 3.95520600 -0.39454800  
 H -6.88464300 0.16224200 -0.23580300  
 Fe 3.47369000 -1.02533200 0.24523000  
 O 4.04263700 -3.05849200 0.36598600  
 H 4.94139300 -3.05649400 -0.08831500  
 O 1.96783600 -1.55600100 1.63577000  
 H 1.06091500 -1.46201300 1.25026000  
 O 4.64475200 -0.41887900 1.53902400  
 O 2.05270900 -1.89081700 -1.18871600  
 H 2.21316000 -1.58929600 -2.09625100  
 H 3.46120700 -3.58443200 -0.20751100  
 H 2.03568000 -2.45238800 1.99974200  
 H 5.53260700 -0.24868900 1.14815800  
 H 1.12157600 -1.66164600 -0.96671900  
 O 4.62812000 -0.78412700 -1.27627100  
 O 6.27219900 -2.57449400 -0.93397600  
 O 6.79212800 -0.26548400 -0.22108700  
 O 6.67353800 -0.81912900 -2.63303700  
 S 6.17128100 -1.11330200 -1.28026400  
 O 3.65641500 1.77751600 2.70574200  
 H 4.06556000 0.93063300 2.35022200

**TS<sub>oxo</sub> (TS3)** for *cis*-Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(SO<sub>4</sub>)(GC) system

E(6-31+G\*) = -3279.199706; E(Def2-QZVP) = -3280.185392; G<sub>corr</sub> = 0.275437

0 5

N 2.16953900 3.06078800 -0.14777200  
 C 3.03517900 2.03575900 0.04596200  
 H 4.10876000 2.15662900 0.14231300  
 N 2.40952500 0.87929200 0.12561100  
 C 1.06258100 1.17312000 -0.01967100  
 C -0.09789900 0.37272900 0.01326600

O -0.14467800 -0.87954600 0.18093900  
 N -1.25673700 1.08661000 -0.16068500  
 H -2.14642100 0.53255800 -0.14306800  
 C -1.31498700 2.45055100 -0.34135100  
 N -2.52366500 2.98624900 -0.50070900  
 H -3.38754100 2.42346800 -0.50533700  
 H -2.57920200 3.98495000 -0.63586500  
 N -0.23344100 3.22534600 -0.35767700  
 C 0.90067600 2.54754400 -0.19211200  
 N -6.04034500 -0.46173700 -0.28871900  
 C -6.10890200 -1.79774000 -0.07042800  
 C -4.83940200 0.23115200 -0.30831900  
 H -7.09955500 -2.23787500 -0.07583700  
 C -4.97541700 -2.51137100 0.13878700  
 N -3.69684600 -0.46306200 -0.10287200  
 O -4.86497900 1.45750500 -0.51344400  
 H -5.00456400 -3.57947500 0.31436700  
 C -3.74019200 -1.78651300 0.11364600  
 N -2.58353200 -2.41976200 0.30872300  
 H -1.70033500 -1.90731100 0.27793900  
 H -2.56213400 -3.41540000 0.47002200  
 H 2.42183200 4.03750400 -0.23537900  
 H -6.88151900 0.07938400 -0.44566200  
 Fe 3.50017300 -0.91273600 0.38342100  
 O 4.07825200 -2.93027600 0.53834500  
 H 4.94665000 -2.92966000 0.02558200  
 O 1.96854800 -1.45993900 1.76227300  
 H 1.07020100 -1.38704100 1.35374200  
 O 4.64635400 -0.34878800 1.68165600  
 O 2.07287900 -1.85130100 -1.02163700  
 H 2.26840700 -1.56152900 -1.92611000  
 H 3.46744500 -3.47189300 0.01160100  
 H 2.04031400 -2.35002200 2.14015300  
 H 5.44729900 0.43893300 1.61182800  
 H 1.13587100 -1.61751200 -0.83140500  
 O 4.52699200 -0.69665300 -1.23543300  
 O 6.18735400 -2.49130100 -0.92010200  
 O 6.92096300 -0.14227200 -1.12457500

O 6.00156500 -1.31849700 -3.08998700  
 S 5.96943600 -1.17998900 -1.62338600  
 O 5.96794000 1.30372200 0.94908100  
 H 6.35697100 0.79772800 0.18125500

**I<sub>Oxo</sub> (I4)** for *cis*-Fe<sup>II</sup>(H<sub>2</sub>O)<sub>4</sub>(SO<sub>4</sub>)(GC) system  
 E(6-31+G\*) = -3279.231160; E(Def2-QZVP) = -  
 3280.212758; G<sub>corr</sub> = 0.282490

0 5

N 2.16953900 3.06078800 -0.14777200  
 C 3.03517900 2.03575900 0.04596200  
 H 4.10876000 2.15662900 0.14231300  
 N 2.40952500 0.87929200 0.12561100  
 C 1.06258100 1.17312000 -0.01967100  
 C -0.09789900 0.37272900 0.01326600  
 O -0.14467800 -0.87954600 0.18093900  
 N -1.25673700 1.08661000 -0.16068500  
 H -2.14642100 0.53255800 -0.14306800  
 C -1.31498700 2.45055100 -0.34135100  
 N -2.52366500 2.98624900 -0.50070900  
 H -3.38754100 2.42346800 -0.50533700  
 H -2.57920200 3.98495000 -0.63586500  
 N -0.23344100 3.22534600 -0.35767700  
 C 0.90067600 2.54754400 -0.19211200  
 N -6.04034500 -0.46173700 -0.28871900  
 C -6.10890200 -1.79774000 -0.07042800  
 C -4.83940200 0.23115200 -0.30831900  
 H -7.09955500 -2.23787500 -0.07583700  
 C -4.97541700 -2.51137100 0.13878700  
 N -3.69684600 -0.46306200 -0.10287200  
 O -4.86497900 1.45750500 -0.51344400  
 H -5.00456400 -3.57947500 0.31436700  
 C -3.74019200 -1.78651300 0.11364600  
 N -2.58353200 -2.41976200 0.30872300  
 H -1.70033500 -1.90731100 0.27793900  
 H -2.56213400 -3.41540000 0.47002200  
 H 2.42183200 4.03750400 -0.23537900  
 H -6.88151900 0.07938400 -0.44566200

Fe 3.50017300 -0.91273600 0.38342100  
 O 4.07825200 -2.93027600 0.53834500  
 H 4.94665000 -2.92966000 0.02558200  
 O 1.96854800 -1.45993900 1.76227300  
 H 1.07020100 -1.38704100 1.35374200  
 O 4.64635400 -0.34878800 1.68165600  
 O 2.07287900 -1.85130100 -1.02163700  
 H 2.26840700 -1.56152900 -1.92611000  
 H 3.46744500 -3.47189300 0.01160100  
 H 2.04031400 -2.35002200 2.14015300  
 H 5.44729900 0.43893300 1.61182800  
 H 1.13587100 -1.61751200 -0.83140500  
 O 4.52699200 -0.69665300 -1.23543300  
 O 6.18735400 -2.49130100 -0.92010200  
 O 6.92096300 -0.14227200 -1.12457500  
 O 6.00156500 -1.31849700 -3.08998700  
 S 5.96943600 -1.17998900 -1.62338600  
 O 5.96794000 1.30372200 0.94908100  
 H 6.35697100 0.79772800 0.18125500

**TS1**

E(6-31+G\*) = -3279.211444; E(Def2-QZVP) = -  
 3280.194375; G<sub>corr</sub> = 0.280704

0 5

N 0.82648600 3.26474700 -0.15695300  
 C 1.75212200 2.29397800 0.06628600  
 H 2.81522400 2.46215500 -0.01672700  
 N 1.18113600 1.09091500 0.12958500  
 C -0.16473900 1.31370300 -0.00081800  
 C -1.27879700 0.43944000 0.01351900  
 O -1.24217800 -0.81261900 0.15373700  
 N -2.47569100 1.08441400 -0.15655000  
 H -3.33290300 0.47793500 -0.15144300  
 C -2.61307900 2.44562000 -0.32337800  
 N -3.84756900 2.91076000 -0.47457700  
 H -4.68002300 2.29932900 -0.47551100  
 H -3.96077600 3.90650400 -0.59865700  
 N -1.57853600 3.28687400 -0.33779700

C -0.40673100 2.68383800 -0.17891700  
 N -7.15542100 -0.72462400 -0.29039300  
 C -7.14809500 -2.06797700 -0.10980900  
 C -5.99497500 0.03335000 -0.30195400  
 H -8.11278700 -2.56227500 -0.11904600  
 C -5.97494000 -2.72328700 0.06939300  
 N -4.81375200 -0.60162500 -0.12586300  
 O -6.09014900 1.26166400 -0.47362200  
 H -5.94326600 -3.79589600 0.21483900  
 C -4.78196600 -1.93096200 0.05494100  
 N -3.59092000 -2.50500100 0.22357100  
 H -2.73801000 -1.94434400 0.20887100  
 H -3.51418800 -3.50160600 0.36002000  
 H 1.02252000 4.25442900 -0.24035200  
 H -8.02651700 -0.22684800 -0.42620900  
 Fe 2.36486900 -0.63636900 0.47176200  
 O 3.10148500 -2.61060800 0.63500200  
 H 4.01590000 -2.53276500 0.21963800  
 O 0.84220300 -1.28492200 1.79407700  
 H -0.05002800 -1.27239300 1.36915600  
 O 3.40478400 0.08723300 1.80957700  
 O 1.09071400 -1.63545800 -1.02235300  
 H 1.27976500 -1.33283800 -1.92399900  
 H 2.59329200 -3.18819800 0.04196100  
 H 0.96908000 -2.16835900 2.17360100  
 H 4.29733100 0.31723800 1.46395400  
 H 0.13485100 -1.47655200 -0.85827100  
 O 3.55991200 -0.30315200 -1.00339800  
 O 5.33491000 -1.94277600 -0.57088500  
 O 5.62077400 0.40606900 0.14378200  
 O 5.66036400 -0.16822100 -2.26610300  
 S 5.12367900 -0.49718100 -0.93442400  
 O 2.09336000 2.45441000 2.26727700  
 H 2.60272700 1.60057200 2.29367800

## II

$E(6-31+G^*) = -3279.268392$ ;  $E(\text{Def2-QZVP}) = -3280.251629$ ;  $G_{\text{corr}} = 0.285043$

O 5  
 N 0.81566300 3.31012700 0.01854700  
 C 1.85651300 2.35284500 0.33131400  
 H 2.62693800 2.33955600 -0.45220400  
 N 1.15859800 1.05064600 0.31922300  
 C -0.13589900 1.30602000 0.13542300  
 C -1.26733300 0.43831000 0.14141000  
 O -1.23393000 -0.80297000 0.34079200  
 N -2.46005700 1.07392800 -0.09371200  
 H -3.31947900 0.46769000 -0.10832500  
 C -2.58054100 2.42613300 -0.29659900  
 N -3.79389900 2.89679200 -0.52107000  
 H -4.63300600 2.28952600 -0.55551600  
 H -3.89068400 3.89182100 -0.66974400  
 N -1.54298900 3.27806600 -0.27287300  
 C -0.37251200 2.71168900 -0.05587300  
 N -7.11422300 -0.71138100 -0.44866400  
 C -7.12645800 -2.04906300 -0.22934100  
 C -5.95141300 0.04025700 -0.40523100  
 H -8.09132400 -2.53960600 -0.28730300  
 C -5.97163100 -2.70389800 0.04540400  
 N -4.78851200 -0.59428200 -0.13452800  
 O -6.02674400 1.26439600 -0.61663100  
 H -5.95594800 -3.77181900 0.22363300  
 C -4.77543600 -1.91801700 0.08580400  
 N -3.60125400 -2.49143000 0.34805900  
 H -2.74483600 -1.93690400 0.36552900  
 H -3.53887700 -3.48443200 0.51516300  
 H 0.97415300 4.30750200 -0.03148100  
 H -7.97195000 -0.21446000 -0.65499700  
 Fe 2.33949200 -0.58462500 0.57676300  
 O 3.11568400 -2.55732200 0.80978400  
 H 3.97535200 -2.51771000 0.28527900  
 O 0.90478700 -1.26644400 2.00631800  
 H 0.00128900 -1.25185700 1.61479000  
 O 3.52817300 0.24716700 1.74846700  
 O 1.04916400 -1.72759800 -0.82223200  
 H 1.24629800 -1.46823000 -1.73552300

H 2.54412300 -3.16210500 0.30873400  
H 1.04870000 -2.15922200 2.35670500  
H 4.40884500 0.33804500 1.31765900  
H 0.09830700 -1.54327800 -0.66557500  
O 3.43301600 -0.34862500 -1.02454700  
O 5.18358200 -2.04453900 -0.71646000  
O 5.61691300 0.30394500 -0.08979100  
O 5.40856500 -0.32125500 -2.47845800  
S 4.98128800 -0.59973700 -1.09493600  
O 2.39332100 2.63591100 1.57638500  
H 2.94943500 1.83727700 1.80855400

**I2**

E(6-31+G\*) = -3279.260855; E(Def2-QZVP) = -  
3280.244722; G<sub>corr</sub> = 0.281254

0 5

N 0.79459700 3.32258900 0.06153700  
C 1.90279100 2.34752500 0.29136200  
H 2.48505500 2.29109400 -0.65148500  
N 1.11748900 1.01990100 0.29322200  
C -0.13738300 1.30726300 0.13851900  
C -1.29835100 0.42224500 0.11566600  
O -1.24635900 -0.80953100 0.26034700  
N -2.47714600 1.07045400 -0.08222200  
H -3.34534400 0.46929000 -0.10918500  
C -2.59204000 2.44183900 -0.23886800  
N -3.80670100 2.90653700 -0.42748600  
H -4.64855100 2.29622100 -0.46422700  
H -3.91138500 3.90601500 -0.54417800  
N -1.56091100 3.29604400 -0.20726400  
C -0.37806200 2.73988500 -0.01921600  
N -7.14119800 -0.65568000 -0.39102000  
C -7.16683200 -1.99922100 -0.21341900  
C -5.96787600 0.07753700 -0.35557200  
H -8.13967300 -2.47482700 -0.26043500  
C -6.01442600 -2.67744500 0.00935000  
N -4.80637300 -0.57930600 -0.13659000  
O -6.03200800 1.30907800 -0.52665600

H -6.00886800 -3.75059500 0.15329200  
C -4.80676500 -1.90984100 0.04253100  
N -3.63583800 -2.50921000 0.25596500  
H -2.77223900 -1.96994000 0.27320200  
H -3.58437500 -3.50744000 0.39306400  
H 0.95203500 4.32210800 0.02997900  
H -7.99681000 -0.14075600 -0.55863500  
Fe 2.24603800 -0.64143900 0.48677800  
O 3.16371100 -2.59988500 0.72474000  
H 3.98813000 -2.53381400 0.15322700  
O 0.88860700 -1.40851200 1.95990100  
H -0.02999400 -1.42245200 1.62621700  
O 3.51874000 0.23128800 1.85812800  
O 1.05548300 -1.78592600 -0.95310400  
H 1.28386400 -1.53162900 -1.86058700  
H 2.60247900 -3.24831900 0.27107200  
H 1.08218100 -2.29866200 2.29143300  
H 4.41432900 0.21479000 1.42616500  
H 0.10133800 -1.60966800 -0.84267500  
O 3.51301700 -0.19605700 -0.99183400  
O 5.16198100 -2.02020100 -0.88449800  
O 5.63515100 0.14406100 0.19993400  
O 5.60423900 -0.02007500 -2.27065500  
S 5.03291600 -0.52225400 -1.00505200  
O 2.58021000 2.55699700 1.38859100  
H 3.22821900 1.21414700 1.79410100

**TS2**

E(6-31+G\*) = -3279.241599; E(Def2-QZVP) = -  
3280.225233; G<sub>corr</sub> = 0.280471

0 5

N -1.17689100 2.99893200 -0.60550300  
C -2.07122100 1.92359700 -0.96031400  
H -2.44619400 1.39285500 0.12031400  
N -1.21992700 0.77897400 -1.13198300  
C 0.00146100 1.15171900 -0.78066400  
C 1.18621600 0.35904500 -0.57114500  
O 1.26656900 -0.87689200 -0.72233900



N 2.26730200 1.09739600 -0.18423600  
 H 3.16597900 0.56935400 -0.04302100  
 C 2.23502900 2.45761300 0.06732900  
 N 3.37673700 3.01269300 0.43870800  
 H 4.25779200 2.47805300 0.53661700  
 H 3.37243200 4.00384100 0.63549600  
 N 1.13697300 3.20667300 -0.03736200  
 C 0.06616500 2.54514600 -0.46156000  
 N 6.99066500 -0.29124700 0.73264500  
 C 7.12955600 -1.63038300 0.57570500  
 C 5.78280300 0.36046300 0.54345900  
 H 8.11940800 -2.03717600 0.74819500  
 C 6.06270400 -2.38749600 0.22010300  
 N 4.70580300 -0.37659900 0.18849200  
 O 5.74067900 1.59306300 0.70795300  
 H 6.14858800 -3.45886900 0.08856200  
 C 4.81953200 -1.70398600 0.02668800  
 N 3.72669400 -2.38145500 -0.32430600  
 H 2.84114300 -1.89699700 -0.46926800  
 H 3.76093700 -3.38015900 -0.46286000  
 H -1.48710500 3.94972100 -0.44713400  
 H 7.78211700 0.28173200 0.99811100  
 Fe -2.27963100 -1.09226600 -0.79615800  
 O -3.50965500 -2.72574100 -0.13964300  
 H -3.85677600 -2.44256400 0.75206400  
 O -0.83157800 -2.15030100 -1.97455800  
 H 0.04808000 -1.79782100 -1.71052000  
 O -3.95766400 -0.30749100 -1.75205900  
 O -0.96248600 -1.70364500 0.83441900  
 H -1.19939400 -1.10838900 1.56558900  
 H -3.05887600 -3.57103100 -0.00081000  
 H -0.77057400 -3.11455800 -1.90486400  
 H -4.64206900 -0.26482200 -1.03365000  
 H -0.01279500 -1.57717700 0.65786000  
 O -2.92763800 0.16196600 0.90870400  
 O -4.30792100 -1.47082400 2.07977800  
 O -5.36145400 0.11358700 0.51142300  
 O -4.48085500 0.93001100 2.67820100

S -4.33225000 -0.05131800 1.58820600  
 O -3.12136500 2.15521500 -1.67584400  
 H -3.73429800 0.67052700 -1.88292900

**I3**

$E(6-31+G^*) = -3279.335503$ ;  $E(\text{Def2-QZVP}) = -3280.325956$ ;  $G_{\text{corr}} = 0.280234$

0 5

N 0.85189300 3.17228900 -0.00344300  
 C 1.78463400 2.14791100 -0.03721100  
 H 3.65997000 1.18417400 -0.43473100  
 N 1.16399700 0.95542100 -0.00880200  
 C -0.20095300 1.24526400 0.01223900  
 C -1.33865700 0.43454200 -0.03080100  
 O -1.37843600 -0.83892700 -0.08693800  
 N -2.52889100 1.13560000 -0.01591500  
 H -3.40135200 0.56348700 -0.03921300  
 C -2.62296300 2.49984000 0.01518000  
 N -3.85094700 3.03021400 0.03457500  
 H -4.70428100 2.45662200 0.00564900  
 H -3.92680800 4.03609400 0.03813600  
 N -1.55478100 3.29346700 0.02560600  
 C -0.39944500 2.62816600 0.01759800  
 N -7.30130000 -0.51715500 -0.08385300  
 C -7.32203700 -1.87246300 -0.10892200  
 C -6.12062700 0.21193500 -0.06355800  
 H -8.29968600 -2.34069000 -0.12233300  
 C -6.15990500 -2.57064000 -0.11657700  
 N -4.95119100 -0.46692700 -0.07229600  
 O -6.18919500 1.45326800 -0.03874500  
 H -6.15097000 -3.65337300 -0.13621500  
 C -4.94700800 -1.80796200 -0.09820700  
 N -3.76350300 -2.42115800 -0.10623200  
 H -2.89599700 -1.87642000 -0.09794600  
 H -3.70771600 -3.42819700 -0.12836900  
 H 1.08210600 4.15620900 -0.03325000  
 H -8.16445200 0.01188200 -0.07826500  
 Fe 2.11730300 -0.88898500 0.18475900

O 3.15921100 -2.71255800 -0.12823800  
H 4.08553200 -2.50989600 -0.41456900  
O 0.60351600 -1.66212600 1.51390700  
H -0.27231100 -1.52127900 1.07850600  
O 3.14852900 -0.61931100 2.03637800  
O 0.79985700 -1.77817700 -1.38939700  
H 0.93689500 -1.42199700 -2.27965900  
H 2.75759000 -3.25960200 -0.81951700  
H 0.65773700 -2.59889500 1.75156900  
H 4.08143400 -0.32081700 1.87541500  
H -0.10082400 -1.47813900 -1.11193600  
O 3.92922400 0.16891500 -0.69606200  
O 5.55461300 -1.63435000 -0.72607700  
O 5.58992800 0.00980700 1.12794300  
O 6.32288200 0.68970100 -1.13329300  
S 5.46910300 -0.20233700 -0.34226800  
O 3.03053000 2.36941400 -0.09882200  
H 2.74715900 0.01477100 2.64809100

**TS4**

E(6-31+G\*) = -3279.202458; E(Def2-QZVP) = -  
3280.187247; G<sub>corr</sub> = 0.277207

0 5

N 0.82057000 3.15384800 -0.11010300  
C 1.72595600 2.17429100 -0.35091100  
H 2.76748800 2.37370100 -0.59879800  
N 1.10410200 0.98640100 -0.54276400  
C -0.22005800 1.23506200 -0.35700100  
C -1.34954200 0.36798100 -0.37773100  
O -1.34385000 -0.86483300 -0.56447900  
N -2.53311100 1.04002300 -0.16225500  
H -3.40365000 0.45580000 -0.17479900  
C -2.63755200 2.39030100 0.07327000  
N -3.85690900 2.87733900 0.26288600  
H -4.70487300 2.28648300 0.24432300  
H -3.94340700 3.86783700 0.44072300  
N -1.58370000 3.21420600 0.11977200  
C -0.43164700 2.59644700 -0.09007700

N -7.24975300 -0.67118600 -0.02389600  
C -7.27231600 -2.00732700 -0.25155800  
C -6.07373300 0.06196800 -0.00103800  
H -8.24718400 -2.48142300 -0.24818100  
C -6.11519300 -2.67987100 -0.46768000  
N -4.90880700 -0.59043700 -0.21394400  
O -6.14070300 1.28572600 0.21380800  
H -6.10707000 -3.74699400 -0.65138300  
C -4.90596400 -1.91277400 -0.44139600  
N -3.72884200 -2.50357900 -0.64581900  
H -2.86395300 -1.95997800 -0.62714400  
H -3.67562500 -3.49532600 -0.82312200  
H 1.03557300 4.13580200 0.01099400  
H -8.10911600 -0.16089600 0.13737400  
Fe 2.23139100 -0.38145600 0.68882100  
O 3.07261100 -1.81553700 1.95620800  
H 3.98765700 -1.97936400 1.55238000  
O 0.48833700 -0.49193500 2.01331200  
H 0.17543400 -1.33294000 2.37935600  
O 2.60874300 1.20652200 1.41407900  
O 1.05921000 -1.95228900 -0.17363000  
H 1.49024900 -2.23288900 -0.99628400  
H 2.61020200 -2.66791900 1.93034600  
H 0.63018200 0.10227700 2.76660900  
H 5.08839100 3.25853300 -0.65032000  
H 0.14778600 -1.63138700 -0.41867500  
O 3.54797300 -0.81819700 -0.67108000  
O 5.29333000 -1.94891500 0.64223300  
O 5.77348100 0.21919800 -0.42820000  
O 5.46984800 -1.80105700 -1.81958100  
S 5.08448900 -1.09433700 -0.58259500  
O 4.66330500 2.60531900 -1.22171600  
H 5.05111800 1.74116100 -0.95127200

**I5**

E(6-31+G\*) = -3279.250260; E(Def2-QZVP) = -  
3280.236451; G<sub>corr</sub> = 0.277704

0 5

N 0.80907000 3.04648900 0.16604000  
 C 1.83291500 2.06338500 -0.21972700  
 H 2.39496400 2.42137800 -1.09359100  
 N 1.05271500 0.858869500 -0.55873700  
 C -0.22589600 1.16159100 -0.39146000  
 C -1.36662500 0.29899200 -0.40356700  
 O -1.33527500 -0.93785000 -0.55279100  
 N -2.55361900 0.96729700 -0.20842500  
 H -3.42922900 0.38752100 -0.22813800  
 C -2.63773600 2.30889600 0.07393900  
 N -3.85037400 2.81340600 0.21862300  
 H -4.70882900 2.24191700 0.12519900  
 H -3.92595000 3.79566600 0.44411800  
 N -1.57451800 3.11588300 0.22757300  
 C -0.40906200 2.52825300 0.02158200  
 N -7.25857100 -0.70430900 -0.11609700  
 C -7.28034800 -2.05551600 -0.22511600  
 C -6.08059500 0.02489400 -0.12298400  
 H -8.25710100 -2.52531600 -0.20524500  
 C -6.12107300 -2.74716100 -0.35139500  
 N -4.91428500 -0.64649600 -0.25049000  
 O -6.14530300 1.26282100 -0.01197700  
 H -6.11310300 -3.82635900 -0.43958400  
 C -4.90987100 -1.98326800 -0.36425800  
 N -3.73027200 -2.59071900 -0.49144700  
 H -2.86474400 -2.04892100 -0.51505300  
 H -3.67675200 -3.59348600 -0.58874000  
 H 1.00538900 4.01766600 0.36869500  
 H -8.11985400 -0.18074100 -0.02072000  
 Fe 2.26683700 -0.21993800 0.70196900  
 O 3.38420300 -0.88499800 2.33121300  
 H 4.24107000 -1.23376400 1.92107700  
 O 0.69718100 0.07126700 2.20470600  
 H 0.37867000 -0.68893300 2.71570000  
 O 2.66992400 1.65580700 0.79304900  
 O 1.02353900 -1.91578000 0.37942200  
 H 1.47719900 -2.49753500 -0.25154600  
 H 3.03516000 -1.57843100 2.91076100

H 0.90769100 0.76358600 2.85041600  
 H 4.75043500 2.72332100 -2.34911600  
 H 0.16060500 -1.66056600 -0.04256300  
 O 3.49322100 -1.05174700 -0.53791900  
 O 5.42097100 -1.57875100 0.90012800  
 O 5.65019200 0.06535300 -0.92679900  
 O 5.36465500 -2.33527800 -1.45159200  
 S 5.04687300 -1.23567700 -0.51969500  
 O 4.23686200 1.91239500 -2.45745600  
 H 4.70400500 1.24419900 -1.90899000

**TS5**

$E(6-31+G^*) = -3279.240697$ ;  $E(\text{Def2-QZVP}) = -3280.227368$ ;  $G_{\text{corr}} = 0.276641$

0 5

N 0.69277900 3.18288100 0.27285100  
 C 1.78423900 2.15923000 0.17392000  
 H 2.26635800 2.30284200 -0.81584700  
 N 1.00122900 0.89611200 0.05427700  
 C -0.23949100 1.18431000 0.02804000  
 C -1.40326700 0.27853700 -0.02471400  
 O -1.32505700 -0.94657700 0.00330000  
 N -2.58513800 0.94860300 -0.10014400  
 H -3.46046700 0.35607100 -0.15417600  
 C -2.70478800 2.33085400 -0.06716200  
 N -3.92283800 2.80627600 -0.15269800  
 H -4.76766800 2.20050600 -0.23971400  
 H -4.03389400 3.81197900 -0.12234200  
 N -1.67933900 3.19182400 0.05721700  
 C -0.48975600 2.63315300 0.11625500  
 N -7.26006300 -0.72132000 -0.40262300  
 C -7.28574000 -2.07615800 -0.37106000  
 C -6.08309200 0.00195700 -0.33500300  
 H -8.26269900 -2.54204800 -0.43045900  
 C -6.12892400 -2.77553300 -0.26948300  
 N -4.91710400 -0.67513800 -0.23455800  
 O -6.14796100 1.24526200 -0.36884400  
 H -6.12343500 -3.85784000 -0.24265300

C -4.91684500 -2.01743600 -0.19992600  
 N -3.74197000 -2.63779600 -0.09764600  
 H -2.87434100 -2.10749400 -0.05332200  
 H -3.69149700 -3.64501000 -0.06566700  
 H 0.86694000 4.17901300 0.33482500  
 H -8.11897200 -0.19006800 -0.47501300  
 Fe 2.46171400 -0.45379100 0.95174300  
 O 3.89984500 -1.53744100 2.08737900  
 H 4.58756400 -1.78146900 1.39393600  
 O 1.74510200 0.31605800 2.82302300  
 H 2.31571000 0.08623200 3.57216700  
 O 2.62284500 2.07266600 1.19441200  
 O 1.07913600 -2.08620000 0.83868600  
 H 1.39853800 -2.76201600 0.22080700  
 H 3.58908200 -2.36471700 2.48291900  
 H 2.00918100 1.23844200 2.52536800  
 H 4.32005400 3.01308300 -2.24052900  
 H 0.21644300 -1.77950600 0.47976500  
 O 3.26269000 -1.04934800 -0.78376200  
 O 5.43613800 -1.89881300 0.01933000  
 O 5.31803200 0.23835800 -1.20301700  
 O 4.90823900 -1.89216500 -2.39251900  
 S 4.77035300 -1.15446800 -1.11494500  
 O 3.79959000 2.20927600 -2.36786900  
 H 4.33718400 1.48986900 -1.95915200

**TS6**

$E(6-31+G^*) = -3279.186664$ ;  $E(\text{Def2-QZVP}) = -3280.175169$ ;  $G_{\text{corr}} = 0.274366$

0 5

N -0.85399500 3.21575900 -0.26227600  
 C -1.72181400 2.19878800 -0.46227600  
 H -3.04698300 2.49123300 -0.66470300  
 N -1.16302600 1.02531600 -0.41837700  
 C 0.19325200 1.28352300 -0.23127500  
 C 1.32259200 0.44030900 -0.16173600  
 O 1.32821500 -0.81988300 -0.23988600  
 N 2.49821200 1.12560700 0.01795400

H 3.36846000 0.54188600 0.07243600  
 C 2.59926300 2.49549500 0.11424900  
 N 3.81686900 3.00057500 0.28919200  
 H 4.66052200 2.41150300 0.36712600  
 H 3.90188400 4.00393800 0.36116800  
 N 1.54475400 3.30663800 0.04079200  
 C 0.39772900 2.66028700 -0.12982500  
 N 7.21780300 -0.55448800 0.41826800  
 C 7.25125000 -1.90195300 0.27565300  
 C 6.03983000 0.17393500 0.35706500  
 H 8.22652900 -2.37072400 0.34036000  
 C 6.10332300 -2.59178300 0.06532500  
 N 4.88318100 -0.49590700 0.14938100  
 O 6.09786500 1.40861000 0.49539200  
 H 6.10389000 -3.66848900 -0.05007800  
 C 4.89175600 -1.83012800 0.00701500  
 N 3.72316000 -2.43898900 -0.19397900  
 H 2.85585400 -1.90067000 -0.22301600  
 H 3.67662100 -3.44077900 -0.30350200  
 H -1.07723000 4.20358500 -0.26651700  
 H 8.06991800 -0.03088000 0.57549600  
 Fe -2.28508500 -0.78149300 -0.57302300  
 O -2.98175300 -2.78207000 -0.49102500  
 H -3.90159400 -2.65909500 -0.11352100  
 O -0.73984800 -1.50035600 -1.81353600  
 H 0.14899900 -1.39901700 -1.38764000  
 O -3.40267800 -0.27492300 -1.91479100  
 O -0.97351800 -1.59224100 1.01055300  
 H -1.17697700 -1.19622500 1.87203400  
 H -2.48114300 -3.26095300 0.18984200  
 H -0.82219500 -2.42580000 -2.09203300  
 H -4.29455800 -0.01306500 -1.60783300  
 H -0.02002100 -1.43374600 0.83398400  
 O -3.40733300 -0.34168000 0.96065400  
 O -5.24816700 -1.93058000 0.59249400  
 O -5.47525900 0.42401000 -0.11005300  
 O -5.45486000 -0.14648500 2.30076600  
 S -4.96583500 -0.50413300 0.96021100

O -4.10600400 2.77550200 -0.46599300  
H -4.55149400 1.91059800 -0.25683600

### I6

E(6-31+G\*) = -3279.204341; E(Def2-QZVP) = -  
3280.191000; G<sub>corr</sub> = 0.281255

0 5

N 0.90320300 3.15903300 0.01143900  
C 1.78319700 2.13481900 0.08535600  
H 3.49593200 1.48827500 1.71112900  
N 1.18517800 0.97576500 0.18978100  
C -0.18180100 1.25040800 0.12015200  
C -1.31370300 0.42031400 0.05296500  
O -1.32423600 -0.84635300 0.07170000  
N -2.49332200 1.11800600 -0.05576700  
H -3.36868500 0.54366900 -0.09407800  
C -2.58323200 2.48855800 -0.12666800  
N -3.80538400 3.01064600 -0.22325900  
H -4.65805200 2.43245200 -0.25283000  
H -3.88205200 4.01501000 -0.28608800  
N -1.51712800 3.28698700 -0.10677600  
C -0.36808800 2.62688600 0.00843200  
N -7.24245300 -0.52834600 -0.24398500  
C -7.27293200 -1.88153800 -0.17104900  
C -6.05893900 0.19428300 -0.22482900  
H -8.25269500 -2.34484500 -0.19452700  
C -6.11706500 -2.58352900 -0.07510800  
N -4.89493700 -0.48796800 -0.13012300  
O -6.11922100 1.43440900 -0.29558000  
H -6.11586400 -3.66479600 -0.01531800  
C -4.90042900 -1.82758600 -0.05660700  
N -3.72375700 -2.44699400 0.03580800  
H -2.85380800 -1.91060800 0.04943800  
H -3.67551800 -3.45309900 0.09173400  
H 1.14267500 4.13748100 -0.08556500  
H -8.10049300 0.00397800 -0.31682900  
Fe 2.26769900 -0.77482100 0.46967600  
O 3.10773900 -2.72974900 0.59091200

H 4.06142900 -2.51034200 0.39736200  
O 0.69388700 -1.48806000 1.69808900  
H -0.18664300 -1.42537800 1.24806300  
O 3.29875900 -0.22641700 1.91553700  
O 1.02816800 -1.71234200 -1.06565200  
H 1.26453100 -1.37878800 -1.94539300  
H 2.80165500 -3.29305400 -0.13782900  
H 0.79864500 -2.40112900 2.00744000  
H 4.21575600 -0.54959300 1.85751500  
H 0.07632900 -1.50267600 -0.92341400  
O 3.44706000 -0.40187800 -1.01783900  
O 5.36898500 -1.39132300 0.14218900  
O 5.39420800 1.00593300 -0.46751700  
O 5.55387400 -0.71169900 -2.23553500  
S 5.01489400 -0.36682100 -0.90727000  
O 3.66987600 2.34753200 1.24424100  
H 4.28371400 2.04191400 0.53389000

### TS7

E(6-31+G\*) = -3279.202292; E(Def2-QZVP) = -  
3280.188720; G<sub>corr</sub> = 0.282135

0 5

N 0.96039100 3.09523400 -0.08289300  
C 1.84633000 2.05619900 -0.11335200  
H 3.21755100 1.41912400 1.58065200  
N 1.21153000 0.89918400 0.06095700  
C -0.14715400 1.20164700 0.07669800  
C -1.28879800 0.39119000 0.01685300  
O -1.31522100 -0.87830300 -0.01098900  
N -2.46513700 1.10568400 -0.03248800  
H -3.34823800 0.54492200 -0.06756700  
C -2.53603600 2.47619100 -0.06686100  
N -3.75289200 3.02038300 -0.09960300  
H -4.61480500 2.45611300 -0.10538800  
H -3.81555000 4.02673500 -0.14119000  
N -1.45688600 3.25950400 -0.07433500  
C -0.31300400 2.58343000 -0.01312200  
N -7.23799600 -0.47777000 -0.17174500

C -7.28020200 -1.83255100 -0.19082200  
 C -6.04686400 0.23188200 -0.13384000  
 H -8.26479200 -2.28522400 -0.21945900  
 C -6.12958300 -2.54940000 -0.17399700  
 N -4.88826200 -0.46550100 -0.11693600  
 O -6.09555000 1.47441600 -0.11748400  
 H -6.13787100 -3.63217900 -0.18737600  
 C -4.90515100 -1.80675900 -0.13561100  
 N -3.73246900 -2.44018800 -0.11713900  
 H -2.85683600 -1.91260500 -0.08346000  
 H -3.69306700 -3.44816300 -0.13056000  
 H 1.19671000 4.06388000 -0.25325000  
 H -8.09231100 0.06525800 -0.18475500  
 Fe 2.23409800 -0.81851800 0.41763700  
 O 3.17677100 -2.71634000 0.67195000  
 H 4.12651600 -2.44944300 0.52791000  
 O 0.66023700 -1.56778700 1.63122900  
 H -0.21572900 -1.49339500 1.17305100  
 O 3.17740800 -0.13716300 1.90524300  
 O 1.05071300 -1.82026200 -1.11059100  
 H 1.30507700 -1.51716800 -1.99637800  
 H 2.95796600 -3.34207500 -0.03666200  
 H 0.76418800 -2.48932200 1.91438700  
 H 4.10343600 -0.43697500 1.92472000  
 H 0.10408500 -1.57417400 -0.98802000  
 O 3.50123100 -0.44782600 -1.00869000  
 O 5.39853100 -1.27093000 0.30883100  
 O 5.28908500 1.11353300 -0.34430600  
 O 5.71171800 -0.60971800 -2.06105200  
 S 5.04519200 -0.29447400 -0.78486600  
 O 3.28837800 2.29217200 1.05680300  
 H 4.04243900 2.05671400 0.44869300

**I7**

$E(6-31+G^*) = -3279.339957$ ;  $E(\text{Def2-QZVP}) = -3280.329754$ ;  $G_{\text{corr}} = 0.282372$

0 5

N 0.82293400 3.22706900 -0.04293400

C 1.73203200 2.20725300 -0.06933700  
 H 3.47493300 1.57034400 -0.37839800  
 N 1.16040700 1.01884500 -0.00064600  
 C -0.20688100 1.28890800 0.03577800  
 C -1.32783600 0.44880300 -0.01941900  
 O -1.32872600 -0.81813300 -0.09352300  
 N -2.52665300 1.12997100 -0.00231300  
 H -3.39158600 0.54345900 -0.03198800  
 C -2.64396200 2.49611400 0.02562400  
 N -3.87962700 3.00122700 0.05262600  
 H -4.72270700 2.41026700 0.04801300  
 H -3.97538800 4.00562900 0.05957600  
 N -1.59125600 3.31154400 0.02026100  
 C -0.42728200 2.66498900 0.01415400  
 N -7.26040700 -0.60037100 -0.08602900  
 C -7.25913000 -1.95332000 -0.17160900  
 C -6.09192400 0.14623500 -0.04137300  
 H -8.22899300 -2.43673500 -0.20048600  
 C -6.08590200 -2.63113300 -0.21667200  
 N -4.91139600 -0.51206400 -0.08477900  
 O -6.18029500 1.38420800 0.03637900  
 H -6.05947700 -3.71160000 -0.28463000  
 C -4.88551400 -1.85058800 -0.16890400  
 N -3.69267300 -2.44423600 -0.20756900  
 H -2.83391700 -1.88865000 -0.17007000  
 H -3.62091400 -3.44856200 -0.27035300  
 H 1.04411300 4.21240900 -0.10722100  
 H -8.13204500 -0.08643400 -0.05142900  
 Fe 2.18373900 -0.83224900 0.29211100  
 O 3.13042200 -2.74533600 0.16121200  
 H 4.04390300 -2.55740000 -0.19571100  
 O 0.63267400 -1.59194500 1.57699700  
 H -0.23392800 -1.49362000 1.11710200  
 O 3.21192600 -0.41173700 2.10853600  
 O 0.96747600 -1.65930400 -1.36059800  
 H 1.13218200 -1.27109500 -2.23269800  
 H 2.68632800 -3.30691100 -0.49149400  
 H 0.70720200 -2.51623300 1.85475800

H 4.14733600 -0.16802100 1.85072400  
H 0.04431500 -1.40789900 -1.12115000  
O 3.82491000 0.09522000 -0.72930600  
O 5.42855200 -1.76736900 -0.70401100  
O 5.57009000 0.02535100 0.99488900  
O 6.17760600 0.49812100 -1.35479400  
S 5.31559200 -0.29154800 -0.45421500  
O 3.00940900 2.45625000 -0.16752300  
H 2.86866300 0.30421100 2.66218000

### I8

E(6-31+G\*) = -3279.325940; E(Def2-QZVP) = -  
3280.313572; G<sub>corr</sub> = 0.282876

0 5

N 0.62033400 3.51623200 0.08192900  
C 1.69271700 2.67720100 -0.08437500  
H 1.65755700 0.96263900 -1.17501500  
N 1.17667100 1.39714300 -0.38476600  
C -0.23543800 1.53231000 -0.43437700  
C -1.26072600 0.58171400 -0.37937700  
O -1.14562100 -0.67730700 -0.37669400  
N -2.52102500 1.14016800 -0.26893200  
H -3.32479200 0.46904200 -0.25317400  
C -2.75619400 2.47266100 -0.07765000  
N -4.02259300 2.87206600 -0.00299000  
H -4.81560300 2.21784500 -0.08288400  
H -4.19751800 3.85132700 0.16839400  
N -1.76916900 3.36432700 0.05471900  
C -0.56201900 2.84452600 -0.11354700  
N -7.06136600 -1.00181200 -0.11771500  
C -6.94030600 -2.35119300 -0.07008600  
C -5.96399500 -0.15571100 -0.17266200  
H -7.86387600 -2.91722400 -0.02699400  
C -5.71222300 -2.92549100 -0.07841700  
N -4.73059100 -0.70992900 -0.18540200  
O -6.16048300 1.07201800 -0.20745200  
H -5.59167400 -4.00096000 -0.04254700  
C -4.58582500 -2.04288300 -0.14097500

N -3.34488100 -2.52950700 -0.15677400  
H -2.54233500 -1.89922600 -0.22232600  
H -3.18109000 -3.52474800 -0.13302000  
H 0.71132700 4.48132800 0.37230500  
H -7.97499000 -0.56533900 -0.10857000  
Fe 2.31209300 -0.57793500 0.79841600  
O 3.23572800 -2.35048100 1.52054000  
H 3.99438200 -2.47394800 0.87371900  
O 0.51559000 -0.64126000 1.93120400  
H -0.24469800 -0.86876900 1.35715900  
O 3.65858800 0.81337300 1.66922900  
O 1.19159200 -1.92073200 -0.54076900  
H 1.68765100 -1.92643300 -1.37415000  
H 2.65740800 -3.11797000 1.39401200  
H 0.45415200 -1.20649300 2.71570000  
H 4.51338800 0.55733700 1.21555500  
H 0.30048100 -1.53909000 -0.72774700  
O 3.44990700 -0.49538800 -0.90051900  
O 5.05648400 -2.28343500 -0.38580300  
O 5.63493900 0.06760900 0.07642400  
O 5.48679200 -0.73119500 -2.26252000  
S 4.95571200 -0.86602100 -0.89131500  
O 2.87546100 2.96503500 0.03011700  
H 3.47499100 1.69780700 1.29007200

### TS8

E(6-31+G\*) = -3279.208212; E(Def2-QZVP) = -  
3280.190504; G<sub>corr</sub> = 0.280391

0 5

N 0.86665500 3.24120800 -0.38577000  
C 1.78807900 2.25804200 -0.23018400  
H 2.84808900 2.41541600 -0.37408200  
N 1.24322400 1.10591900 0.09582600  
C -0.11726500 1.36169200 0.24868300  
C -1.22113600 0.44575900 0.07886600  
O -1.13775300 -0.80469000 0.09742000  
N -2.41914100 1.06875000 -0.09876300  
H -3.26776100 0.44896800 -0.14201900

C -2.57312800 2.43356900 -0.22088900  
 N -3.81313100 2.89390000 -0.28286800  
 H -4.64184900 2.27575000 -0.23618200  
 H -3.93912400 3.88732300 -0.41772100  
 N -1.54248900 3.28056400 -0.32116500  
 C -0.36827400 2.70255200 -0.16781600  
 N -7.05732200 -0.78554400 -0.29816100  
 C -7.02202700 -2.13972500 -0.34788100  
 C -5.91020300 -0.01212100 -0.22345500  
 H -7.97838700 -2.64645500 -0.40742800  
 C -5.83318600 -2.79091100 -0.32097000  
 N -4.71416000 -0.64271900 -0.19394000  
 O -6.02891900 1.22585000 -0.18645800  
 H -5.77992700 -3.87185600 -0.35774700  
 C -4.65445300 -1.98252400 -0.23644900  
 N -3.44932500 -2.55071500 -0.19773000  
 H -2.60893500 -1.97939200 -0.10972000  
 H -3.35245800 -3.55465300 -0.21730900  
 H 1.06197300 4.19077400 -0.67913800  
 H -7.94074600 -0.29115400 -0.31752500  
 Fe 2.46952100 -0.56925800 0.54805600  
 O 3.23658600 -2.53486200 0.69609300  
 H 4.15455400 -2.42256400 0.29912600  
 O 0.88855800 -1.20987200 1.82139600  
 H 0.03098400 -1.31967000 1.34589000  
 O 3.46548500 0.12704400 1.90391000  
 O 1.25566500 -1.62962300 -0.99858500  
 H 1.51682600 -1.31654700 -1.87840800  
 H 2.75068900 -3.10617800 0.07900400  
 H 1.04798000 -2.01703300 2.33477500  
 H 4.34128500 0.43173500 1.58030800  
 H 0.30028900 -1.43191100 -0.90032000  
 O 3.66217700 -0.18577900 -0.92725200  
 O 5.47395200 -1.77702600 -0.45925200  
 O 5.69220000 0.58561700 0.23606600  
 O 5.77294800 -0.01089000 -2.16721600  
 S 5.22836900 -0.33999500 -0.83732100  
 O -0.39736400 1.56052300 2.15916700

H 0.19618500 0.84020200 2.44242200

**I9**

$E(6-31+G^*) = -3279.245454$ ;  $E(\text{Def2-QZVP}) = -$   
 $3280.231470$ ;  $G_{\text{corr}} = 0.279428$

0 5

N 0.82765000 2.95496700 -0.91943500  
 C 1.68902300 1.86780000 -0.89729300  
 H 2.70175000 1.94484400 -1.27673200  
 N 1.19851300 0.79461100 -0.38297600  
 C -0.11844400 1.16641000 0.12880800  
 C -1.32537800 0.30825600 -0.25252000  
 O -1.30750000 -0.89907900 -0.43833700  
 N -2.49665700 1.01203500 -0.21746300  
 H -3.39697900 0.44945800 -0.21358400  
 C -2.55761700 2.38277100 -0.17702000  
 N -3.71748700 2.93940700 0.02329800  
 H -4.58918300 2.37818700 0.17410100  
 H -3.77101200 3.95049100 -0.01478200  
 N -1.48336600 3.18177800 -0.44244000  
 C -0.35633400 2.55775700 -0.43310500  
 N -7.19603500 -0.43338800 0.22776500  
 C -7.30850000 -1.76976100 0.02937000  
 C -5.98544300 0.22940100 0.15424800  
 H -8.30638100 -2.18613700 0.10810600  
 C -6.20801900 -2.51141900 -0.24870300  
 N -4.87587300 -0.49092900 -0.12213500  
 O -5.96918700 1.46048700 0.34669900  
 H -6.27230500 -3.58028300 -0.40873100  
 C -4.95836400 -1.81737200 -0.31276500  
 N -3.83078500 -2.48052700 -0.56751100  
 H -2.93462400 -1.99949800 -0.57457100  
 H -3.83866400 -3.48067500 -0.70112800  
 H 1.02132700 3.84627300 -1.36240700  
 H -8.01223800 0.12783200 0.43807200  
 Fe 2.56603600 -0.98067700 -0.19291400  
 O 3.82638500 -2.40647400 -1.25988500  
 H 4.72918700 -1.99400800 -1.09906600



O 0.60821900 -0.79381800 2.79422500  
H 0.72391500 -0.53554700 3.71921600  
O 2.82381300 -1.34543700 1.67224700  
O 0.98810700 -2.34747000 -0.65625900  
H 1.06168400 -2.94199300 -1.41568900  
H 3.71776900 -2.44487500 -2.22079700  
H 1.54666800 -1.01475300 2.43272300  
H 3.63552800 -0.87171300 1.93786400  
H 0.10823800 -1.91801400 -0.69951900  
O 4.07256100 0.43608900 -0.52102800  
O 5.99531000 -1.09613300 -0.58367000  
O 5.37732500 0.03456100 1.52698300  
O 6.35325400 1.33621400 -0.33673000  
S 5.48541300 0.18955700 0.03976400  
O -0.13904200 1.30440700 1.51063600  
H 0.15054100 0.43956400 1.97755500

### I10

E(6-31+G\*) = -3279.258100; E(Def2-QZVP) = -  
3280.243053; G<sub>corr</sub> = 0.281993

0 5

N 0.81795600 2.84966500 -0.92629500  
C 1.67844100 1.76674300 -0.81409200  
H 2.68983300 1.80671900 -1.20419000  
N 1.18095900 0.73770000 -0.22747900  
C -0.16098800 1.14683300 0.27122400  
C -1.33800400 0.24105200 -0.07022200  
O -1.32355000 -0.98642500 -0.03795900  
N -2.51544600 0.92481300 -0.23145800  
H -3.40615800 0.35921500 -0.21454000  
C -2.59130100 2.28869800 -0.34663700  
N -3.77531300 2.83935700 -0.30502300  
H -4.64885600 2.28361800 -0.17366500  
H -3.83632200 3.83937100 -0.45146600  
N -1.51261100 3.08072900 -0.59825400  
C -0.38092800 2.46927400 -0.45938400  
N -7.25219500 -0.55849600 -0.12041400  
C -7.32538900 -1.90956100 -0.20562800

C -6.04694400 0.12063400 -0.10338600  
H -8.32076100 -2.33874300 -0.21620300  
C -6.19192100 -2.65086600 -0.27096900  
N -4.90565900 -0.59987400 -0.16586800  
O -6.06457700 1.36423300 -0.03094700  
H -6.22629500 -3.73091500 -0.33747200  
C -4.95076000 -1.93885100 -0.24134400  
N -3.79194900 -2.59592500 -0.28895300  
H -2.90756600 -2.09350900 -0.22851200  
H -3.77099500 -3.60371400 -0.33531400  
H 1.02198500 3.70461000 -1.43148000  
H -8.09452300 0.00142600 -0.07208400  
Fe 2.42968300 -0.93656900 0.24278300  
O 3.43195100 -2.81119700 0.03106800  
H 4.33322200 -2.56129500 -0.34016200  
O 1.98238200 1.75902700 2.92136100  
H 2.33309200 2.62357800 2.66755900  
O 3.39748600 -0.23997900 1.91362600  
O 0.86785800 -2.01593400 1.18092400  
H 0.93471000 -2.97909800 1.24673400  
H 3.04903500 -3.46182600 -0.57501400  
H 2.94243600 0.54650700 2.33531700  
H 4.27999300 0.06546200 1.56167200  
H 0.00144900 -1.80400400 0.76331100  
O 3.82547400 -0.12323400 -1.07149300  
O 5.66164700 -1.73906400 -0.82513700  
O 5.62096500 0.31623100 0.54823900  
O 6.07891300 0.45949800 -1.87658600  
S 5.33791700 -0.26140600 -0.81649100  
O -0.22346000 1.30261100 1.60395500  
H 1.13312600 1.64024800 2.38944200

### TS9

E(6-31+G\*) = -3279.229019; E(Def2-QZVP) = -  
3280.216986; G<sub>corr</sub> = 0.278995

0 5

N 0.45713400 2.39534400 -1.63197600  
C 1.43432700 1.48618700 -1.37056700

H 2.27101300 1.32393700 -2.03883900  
 N 1.24731900 0.83165600 -0.26178500  
 C 0.04649600 1.34485900 0.33202600  
 C -1.42724700 0.39434500 -0.50783600  
 O -1.25641600 -0.79213200 -0.70974300  
 N -2.59903700 1.01254600 -0.30457000  
 H -3.48441400 0.42709900 -0.25773600  
 C -2.63628400 2.40017500 -0.23848900  
 N -3.80425300 2.95218900 0.04238000  
 H -4.65236100 2.37959400 0.17537200  
 H -3.87235400 3.96017500 0.04644000  
 N -1.55439600 3.08928400 -0.52512700  
 C -0.45399600 2.34584400 -0.61747500  
 N -7.19045100 -0.65127800 0.21961600  
 C -7.23525500 -1.99118600 0.02014000  
 C -6.01407100 0.07534600 0.13979000  
 H -8.20911100 -2.45930600 0.10676200  
 C -6.10186400 -2.67728000 -0.27011500  
 N -4.87430700 -0.59421300 -0.15148200  
 O -6.05002000 1.30183700 0.33666400  
 H -6.11493700 -3.74778700 -0.43167800  
 C -4.89058300 -1.91963000 -0.35045400  
 N -3.73424300 -2.52379700 -0.62896800  
 H -2.86613700 -1.99645900 -0.68044000  
 H -3.69612500 -3.51987600 -0.78475300  
 H 0.34525400 2.90861800 -2.49839300  
 H -8.03336900 -0.13402500 0.43706200  
 Fe 2.46144800 -0.85662100 0.19960700  
 O 3.44304600 -2.72061900 -0.13732500  
 H 4.37466500 -2.44499500 -0.40213300  
 O 1.76142400 1.19962400 3.34901700  
 H 2.09410600 2.10572400 3.40817900  
 O 3.35265800 -0.45392300 2.00127200  
 O 0.76302200 -1.99825900 0.78166000  
 H 0.81817900 -2.96438200 0.80739400  
 H 3.10655800 -3.28545900 -0.84810000  
 H 2.86122400 0.20365500 2.56764700  
 H 4.24262300 -0.07280900 1.75746600

H -0.02561500 -1.76574300 0.25067100  
 O 3.94958700 0.06716400 -0.91499700  
 O 5.74209900 -1.60073900 -0.68936400  
 O 5.62883800 0.32083600 0.86109200  
 O 6.26377100 0.67525000 -1.50139600  
 S 5.43743700 -0.12350600 -0.56815500  
 O -0.23909500 1.22119700 1.55495600  
 H 1.00935900 1.23429700 2.70235600

**III**

E(6-31+G\*) = -3279.289669; E(Def2-QZVP) = -  
 3280.275610; G<sub>corr</sub> = 0.278382

0 5

N -0.17303500 -1.61238900 -1.80185300  
 C -1.39374100 -1.38140500 -1.36498100  
 H -2.21331200 -1.13144600 -2.02837500  
 N -1.54735200 -1.45556400 -0.04316200  
 C -0.31768400 -1.80296600 0.47358600  
 C 1.56082200 -0.48348300 -0.45354100  
 O 1.14725900 0.66559000 -0.32328400  
 N 2.82277400 -0.92031400 -0.41390700  
 H 3.66452800 -0.29080300 -0.27065300  
 C 2.83140500 -2.30719500 -0.58757400  
 N 4.00976000 -2.92028300 -0.56607300  
 H 4.87007200 -2.38039800 -0.43072600  
 H 4.05111400 -3.92150200 -0.68587800  
 N 1.65455600 -2.85325100 -0.75089700  
 C 0.72135700 -1.78176300 -0.67182400  
 N 7.28330700 0.89359800 0.11233600  
 C 7.22952400 2.24107300 0.25518500  
 C 6.14651400 0.11552900 -0.04628900  
 H 8.18003900 2.74926800 0.37197700  
 C 6.03668600 2.88917200 0.24807900  
 N 4.95293400 0.75323100 -0.05347900  
 O 6.25656700 -1.11413300 -0.17384000  
 H 5.97807800 3.96443100 0.36091100  
 C 4.86803600 2.08039800 0.08477400  
 N 3.64980300 2.62900800 0.06569700

H 2.81690000 2.05809800 -0.05288700  
 H 3.52888200 3.62585600 0.16354100  
 H 0.12335700 -1.57396200 -2.76878700  
 H 8.17366400 0.41113500 0.11697400  
 Fe -2.90481700 -0.08695200 0.96966900  
 O -4.13698300 1.32527300 2.00633900  
 H -3.68084900 2.02233500 2.49923300  
 O -2.35806800 -1.09209900 2.78560100  
 H -2.34066300 -0.61543500 3.62805300  
 O -4.58934700 -1.40674500 0.77479400  
 H -5.08111000 -1.01266400 -0.00612200  
 O -1.18073600 1.29409600 1.15782900  
 H -0.80399300 1.36348400 2.04744000  
 H -4.62738800 1.78026700 1.25879400  
 H -4.32763100 -2.29989100 0.50701700  
 H -0.41438900 1.11218700 0.57100400  
 O -0.05332600 -2.00313000 1.64771000  
 H -1.46684100 -1.49089000 2.65224200  
 S -4.73175000 1.21136900 -1.26159500  
 O -5.22635400 2.19609400 -0.22863300  
 O -5.59659900 -0.02689000 -1.23768400  
 O -4.68553400 1.81581700 -2.61115600  
 O -3.30987100 0.78292300 -0.85077000

## I12

$E(6-31+G^*) = -3354.336372$ ;  $E(\text{Def2-QZVP}) = -3355.356149$ ;  $G_{\text{corr}} = 0.279545$

0 5

N 0.03862000 1.51996300 -1.84299100  
 C 1.24467200 1.21160300 -1.41092600  
 H 2.05256900 0.93449300 -2.07828600  
 N 1.39802400 1.24350700 -0.08849000  
 C 0.19085200 1.64921000 0.43514900  
 C -1.72959900 0.42643000 -0.50841300  
 O -1.35360300 -0.73756300 -0.40174300  
 N -2.97480500 0.90694700 -0.44787500  
 H -3.83614800 0.30630100 -0.29788500  
 C -2.93564500 2.29667700 -0.59354100

N -4.09112900 2.95050700 -0.54744700  
 H -4.96773400 2.43990700 -0.40294100  
 H -4.09706600 3.95553100 -0.63910700  
 N -1.74197300 2.80416700 -0.75949700  
 C -0.84665200 1.70022100 -0.70804200  
 N -7.48610900 -0.74584700 0.17254300  
 C -7.47903600 -2.09518700 0.30704800  
 C -6.32573000 -0.00993000 -0.01372400  
 H -8.44435800 -2.56818400 0.44764400  
 C -6.31197400 -2.78735900 0.26382300  
 N -5.15756300 -0.69170600 -0.05774100  
 O -6.39318800 1.22378800 -0.13140600  
 H -6.29116300 -3.86472100 0.36959900  
 C -5.11860900 -2.02180100 0.07300100  
 N -3.92256300 -2.61518600 0.01913500  
 H -3.07214600 -2.07464600 -0.11573200  
 H -3.83561300 -3.61593100 0.11309800  
 H -0.25940700 1.51587600 -2.81007400  
 H -8.35710400 -0.23026400 0.20518000  
 Fe 2.74804600 -0.12209300 0.91724900  
 O 3.94713900 -1.56751800 1.96531200  
 H 3.46789300 -2.29345100 2.39018700  
 O 2.18614800 0.83347800 2.74025800  
 H 2.10205100 0.29876700 3.54336300  
 O 4.52719400 1.14734900 0.90156600  
 H 5.04224000 0.78636200 0.10170600  
 O 1.02098100 -1.51790600 0.96037200  
 H 0.67866500 -1.77408700 1.82901700  
 H 4.48538000 -1.98224400 1.22902000  
 H 0.23047700 -1.26276000 0.43725800  
 O -0.06214700 1.84335300 1.61375100  
 H 1.31153800 1.26609300 2.58666100  
 S 4.72416800 -1.29292700 -1.26023400  
 O 5.16724900 -2.32441100 -0.25434500  
 O 5.58402200 -0.05399500 -1.12833000  
 O 4.74323100 -1.81998300 -2.63925100  
 O 3.28419800 -0.87795700 -0.89412300  
 O 4.26018200 2.50393900 0.53199300

H 4.89557600 2.97795900 1.09442600

### TS10

E(6-31+G\*) = -3354.311566; E(Def2-QZVP) = -3355.328853;  $G_{\text{corr}} = 0.278558$

0 5

N 0.06876700 1.50421600 -1.88010600

C 1.27504900 1.20695000 -1.45233700

H 2.07735300 0.91103700 -2.11773100

N 1.43632400 1.28321300 -0.12979500

C 0.23413600 1.71282300 0.39198000

C -1.67726400 0.43782200 -0.49975100

O -1.28415400 -0.71572400 -0.35623400

N -2.92764700 0.90619800 -0.45666900

H -3.78393500 0.30100400 -0.28988800

C -2.90460400 2.29079100 -0.64786600

N -4.06622100 2.93279100 -0.62488500

H -4.93868700 2.41705900 -0.47096500

H -4.08268900 3.93361700 -0.75442600

N -1.71614500 2.80773200 -0.82804100

C -0.80948300 1.71800800 -0.74357400

N -7.42713600 -0.76544700 0.18620300

C -7.40902600 -2.10925200 0.36678800

C -6.27206000 -0.02544500 -0.01494500

H -8.37118900 -2.58633900 0.51507900

C -6.23532200 -2.79133500 0.35728300

N -5.09713200 -0.69707100 -0.02577100

O -6.35015500 1.20287700 -0.17503200

H -6.20537200 -3.86421100 0.49977200

C -5.04741000 -2.02166000 0.15041900

N -3.84589800 -2.60579100 0.12697300

H -2.99924600 -2.06332200 -0.02130800

H -3.75118000 -3.60213200 0.25456900

H -0.23557700 1.48051800 -2.84536000

H -8.30304200 -0.25723200 0.19354500

Fe 2.84621000 0.04052400 0.89113000

O 3.74562900 -1.51381800 2.02525200

H 3.08379400 -2.17779200 2.27537800

O 2.27230200 1.03408600 2.66466200

H 2.27605800 0.58211400 3.52177600

O 4.46687100 0.99791500 0.75340300

H 4.97827200 0.67280500 -0.04503300

O 1.03321200 -1.28128600 1.21187700

H 0.59320000 -1.23977600 2.07388600

H 4.31204700 -1.96410600 1.32711300

H 0.30806400 -1.17478900 0.55907900

O -0.00565900 1.95084800 1.56404800

H 1.38323600 1.44991000 2.54251900

S 4.51957100 -1.51728400 -1.22095500

O 4.98529300 -2.42831100 -0.11604000

O 5.43065800 -0.32702900 -1.33465800

O 4.35432800 -2.22607400 -2.50222900

O 3.12467300 -0.96958300 -0.78288100

O 4.53150900 2.69926200 0.29970500

H 5.00975300 2.94614700 1.10954800

### I13

E(6-31+G\*) = -3354.329823; E(Def2-QZVP) = -3355.346775;  $G_{\text{corr}} = 0.277498$

0 5

N 0.14485500 1.55241100 -1.82523900

C 1.33896300 1.23037800 -1.39173500

H 2.15536200 0.96514700 -2.05285900

N 1.47076500 1.24576100 -0.06066700

C 0.26008800 1.66645000 0.45791200

C -1.62227400 0.42201100 -0.52290400

O -1.22123600 -0.73214600 -0.41354700

N -2.87555800 0.88162700 -0.48789100

H -3.73031100 0.26754300 -0.33859200

C -2.85688100 2.27341300 -0.61982000

N -4.02118900 2.90833100 -0.59265400

H -4.89283900 2.38382300 -0.46323700

H -4.03931800 3.91443800 -0.67221800

N -1.66777600 2.80405600 -0.75676200

C -0.75777200 1.71827800 -0.69803400

N -7.36158400 -0.80883200 0.17477800

C -7.33695800 -2.15170500 0.36110800  
 C -6.21179100 -0.06638800 -0.04531600  
 H -8.29544500 -2.63077400 0.52577800  
 C -6.16148400 -2.83038600 0.33779100  
 N -5.03524600 -0.73489800 -0.07302000  
 O -6.29570300 1.16144600 -0.20625600  
 H -6.12647900 -3.90240600 0.48545100  
 C -4.97888500 -2.05837800 0.11052800  
 N -3.77612500 -2.63912500 0.07423200  
 H -2.93277600 -2.09462300 -0.08371600  
 H -3.67613000 -3.63388200 0.20985800  
 H -0.13681600 1.58784000 -2.79748100  
 H -8.23847300 -0.30262000 0.19476100  
 Fe 2.89323600 -0.00052400 0.90174000  
 O 3.76736000 -1.53908700 2.01232700  
 H 3.12305400 -2.21866100 2.26903600  
 O 2.27576600 0.91581700 2.69144000  
 H 2.32014800 0.45825100 3.54477800  
 O 4.38342500 1.07818600 0.75364400  
 H 4.93734900 0.79035900 -0.00833600  
 O 1.07265200 -1.29920600 1.18305100  
 H 0.60950900 -1.25787500 2.03323800  
 H 4.35712700 -1.98044800 1.32058600  
 H 0.36423400 -1.21463700 0.50809500  
 O 0.00219300 1.85962200 1.63227100  
 H 1.38200000 1.33078800 2.60448100  
 S 4.55405400 -1.53062200 -1.21729400  
 O 5.05514200 -2.40168600 -0.09606400  
 O 5.42981000 -0.33852500 -1.40501400  
 O 4.31860500 -2.28721700 -2.45765100  
 O 3.15308500 -0.98883800 -0.73060200  
 O 3.40049500 3.53482100 0.18992800  
 H 3.81300500 2.64848100 0.41699600

**TS11**

$E(6-31+G^*) = -3354.316197$ ;  $E(\text{Def2-QZVP}) = -$   
 $3355.332747$ ;  $G_{\text{corr}} = 0.281506$

0 5

N 0.18538200 1.79987400 -1.67896700  
 C 1.40316800 1.44469000 -1.26352200  
 H 2.10216600 0.93945400 -1.91778100  
 N 1.42747200 1.23774600 0.09853300  
 C 0.22303300 1.68316300 0.60558700  
 C -1.58255000 0.49335600 -0.51402700  
 O -1.14705600 -0.65401000 -0.47426700  
 N -2.85150100 0.91044200 -0.46557500  
 H -3.68542100 0.26562400 -0.35589400  
 C -2.87008800 2.30912000 -0.46383000  
 N -4.05600500 2.90443600 -0.39208800  
 H -4.91046100 2.34517800 -0.30914200  
 H -4.10363600 3.91203500 -0.36032000  
 N -1.69777700 2.88307800 -0.53648300  
 C -0.75170700 1.82194700 -0.57279600  
 N -7.27320300 -0.97855500 0.14558600  
 C -7.19415900 -2.32697000 0.26538300  
 C -6.15530700 -0.18159200 -0.05006300  
 H -8.13123400 -2.85083100 0.41675700  
 C -5.99374400 -2.95740900 0.19667700  
 N -4.95517700 -0.80224700 -0.12467700  
 O -6.28732600 1.04864900 -0.14792700  
 H -5.91580100 -4.03313800 0.29136600  
 C -4.84473100 -2.12922500 -0.00486700  
 N -3.61972800 -2.65795600 -0.08059000  
 H -2.80040000 -2.07108600 -0.21664800  
 H -3.47757600 -3.65280400 0.00943200  
 H -0.10179200 1.77317500 -2.64723400  
 H -8.16865700 -0.50892000 0.20101800  
 Fe 2.92905000 0.05883400 0.94650600  
 O 3.99561100 -1.32023400 2.06728500  
 H 3.45042200 -1.99614400 2.50096700  
 O 2.34922300 0.96713700 2.75802100  
 H 2.45644500 0.53213100 3.61764800  
 O 4.22624100 1.29996200 0.47852100  
 H 4.81179900 0.92606300 -0.22015800  
 O 1.15096000 -1.29981700 1.28793600  
 H 0.67220800 -1.24218100 2.12848900

H 4.53264600 -1.81062600 1.36054000  
H 0.46100900 -1.22309500 0.59635100  
O -0.04258000 1.81216100 1.78709800  
H 1.43422100 1.33669300 2.71288000  
S 4.52175300 -1.53066300 -1.18591600  
O 5.13562100 -2.30974200 -0.05116600  
O 5.32835200 -0.31641500 -1.49953800  
O 4.24643400 -2.37256700 -2.36103800  
O 3.13276800 -1.02514000 -0.63750100  
O 2.42571700 2.89767000 -0.83031400  
H 3.23923500 2.47794900 -0.41110300

#### I14

$E(6-31+G^*) = -3354.364269$ ;  $E(\text{Def2-QZVP}) = -3355.380792$ ;  $G_{\text{corr}} = 0.281888$

0 5

N -0.06647100 -1.42690800 -2.12435200  
C -1.42725500 -1.29685700 -1.64076300  
H -2.01418000 -0.65384100 -2.30875700  
N -1.30223500 -0.65521600 -0.34719600  
C -0.07236800 -0.68944400 0.10538100  
C 1.95244500 -0.16352600 -1.23731000  
O 1.85871500 0.92332900 -1.75431700  
N 3.04056100 -0.68409500 -0.59604600  
H 3.95075200 -0.14487600 -0.39572900  
C 2.78267700 -1.96738800 -0.24042100  
N 3.64359100 -2.69506600 0.41931500  
H 4.55329600 -2.28024000 0.69593800  
H 3.40761400 -3.64846600 0.66522600  
N 1.56092000 -2.41408900 -0.64341000  
C 0.85813500 -1.27106900 -1.07086800  
N 7.41742300 0.47936500 0.98530500  
C 7.72793300 1.75431300 0.64340900  
C 6.21486300 -0.11009400 0.63980800  
H 8.69788800 2.11491200 0.96615700  
C 6.85171100 2.51206300 -0.06411100  
N 5.33351000 0.63606200 -0.06518200  
O 5.98941000 -1.28366000 0.98248600

H 7.08646100 3.53149600 -0.34285900  
C 5.60986200 1.89822700 -0.41704300  
N 4.68429500 2.56585600 -1.10951800  
H 3.80235800 2.13292800 -1.36324500  
H 4.83992200 3.51861900 -1.40337700  
H 0.08381900 -2.24120600 -2.71102000  
H 8.07072500 -0.08531200 1.51462400  
Fe -2.97593700 -0.22707200 0.77281100  
O -4.24358700 0.28553800 2.38998300  
H -3.80984700 0.95192000 2.94769600  
O -2.02097800 -1.42594800 2.28762000  
H -2.37756600 -1.33982600 3.18543100  
O -3.99490000 -1.58653200 0.04073000  
H -4.70990500 -1.20127400 -0.51604900  
O -1.73909900 1.36036100 1.71770200  
H -0.79706700 1.09163800 1.69751800  
H -4.99734300 0.77039100 1.92854000  
H -1.80671400 2.16753300 1.18347400  
O 0.39324900 -0.34697400 1.19622300  
H -1.06160500 -1.25176800 2.34974400  
S -5.24748200 1.41388200 -0.55692400  
O -5.91399300 1.51589500 0.78978400  
O -5.69218600 0.18888200 -1.28320900  
O -5.39224600 2.64732500 -1.34913400  
O -3.71113000 1.23295700 -0.25469900  
O -2.01920900 -2.55824600 -1.53534600  
H -2.86607000 -2.41300000 -1.03909300

#### TS12

$E(6-31+G^*) = -3354.336683$ ;  $E(\text{Def2-QZVP}) = -3355.354293$ ;  $G_{\text{corr}} = 0.279431$

0 5

N -0.31478300 -2.29222100 -1.44354700  
C -1.66061800 -1.98602400 -1.29081800  
H -2.02155400 -0.98370000 -1.87428500  
N -1.85705100 -1.58311600 0.05055800  
C -0.69683600 -1.61704300 0.72187100  
C 1.34384500 -0.71737000 -0.44001100

O 1.01184000 0.39024100 -0.82051600  
 N 2.56485300 -1.13797600 -0.05937700  
 H 3.42348200 -0.51865300 -0.05022700  
 C 2.51088400 -2.48657700 0.25897900  
 N 3.63177000 -3.08204100 0.64788000  
 H 4.50424800 -2.54762700 0.70934200  
 H 3.61688000 -4.06263800 0.88675500  
 N 1.32585900 -3.04076600 0.14456200  
 C 0.44376900 -1.99550700 -0.26038400  
 N 7.03667500 0.67374200 0.39295600  
 C 7.04854100 1.98283800 0.03875500  
 C 5.88459500 -0.09738600 0.35342600  
 H 8.00414100 2.49026500 0.10764200  
 C 5.91086500 2.59750300 -0.37472700  
 N 4.74661000 0.50761900 -0.05761800  
 O 5.93220300 -1.29169800 0.68879900  
 H 5.90556500 3.64211600 -0.65949400  
 C 4.72606900 1.79647100 -0.41201500  
 N 3.55743200 2.31257400 -0.80366500  
 H 2.71336700 1.74489100 -0.83190400  
 H 3.48554700 3.27992000 -1.08137200  
 H 0.03501800 -2.91944300 -2.15892300  
 H 7.88602500 0.21698800 0.70174600  
 Fe -3.34401700 -0.17777300 0.25736500  
 O -5.09382100 0.90308000 0.54463100  
 H -5.65446200 0.75399700 1.32119500  
 O -4.68561700 -1.82835100 -0.10150000  
 H -4.95626200 -2.30539700 0.69910600  
 O -3.16936500 0.02866000 -1.64255800  
 H -2.77263600 0.91814800 -1.82780300  
 O -3.15161700 -0.69862900 2.32596700  
 H -2.19232700 -0.94358600 2.42427000  
 H -4.81752800 1.87284300 0.53560800  
 H -3.28921100 0.05305300 2.92450500  
 O -0.52908900 -1.33442300 1.90875400  
 H -4.17615400 -2.47421700 -0.63626000  
 S -2.48604800 2.80648600 0.00692900  
 O -3.90753300 3.21576600 0.28257200

O -2.25257000 2.60395500 -1.45430500  
 O -1.50645000 3.70875600 0.63230500  
 O -2.32547200 1.39382400 0.68621200  
 O -2.58526400 -2.96361600 -1.67992600  
 H -2.77709600 -2.88530300 -2.62843600

### I15

$E(6-31+G^*) = -3354.453925$ ;  $E(\text{Def2-QZVP}) = -3355.478565$ ;  $G_{\text{corr}} = 0.279202$

0 5

N -0.25663900 -1.37443100 1.92926600  
 C 1.03176200 -1.19345000 1.67568000  
 H 3.93098000 -1.20542600 2.00284700  
 N 1.35008300 -1.01352400 0.38881600  
 C 0.16408700 -1.09132600 -0.29949500  
 C -2.00186300 -0.15102000 0.62693000  
 O -1.78675200 1.02729600 0.86025300  
 N -3.15469800 -0.72659100 0.23874200  
 H -4.06135300 -0.20237500 0.10999300  
 C -2.96848200 -2.10140700 0.13269500  
 N -4.01469100 -2.84162400 -0.22492400  
 H -4.92594300 -2.40310400 -0.38530300  
 H -3.91422200 -3.84329700 -0.29380600  
 N -1.75962600 -2.52197500 0.40185600  
 C -1.00102700 -1.34258800 0.68856100  
 N -7.75024800 0.58718700 -0.63712500  
 C -7.89025900 1.92668200 -0.47711400  
 C -6.54075400 -0.06363700 -0.44155800  
 H -8.88032400 2.33041100 -0.65647700  
 C -6.83097700 2.69348200 -0.11207900  
 N -5.48034400 0.69329200 -0.07789200  
 O -6.47081300 -1.29242600 -0.60304300  
 H -6.92826100 3.76372300 0.01974900  
 C -5.58695000 2.01519600 0.08738000  
 N -4.48693900 2.68406600 0.44664300  
 H -3.60114500 2.20341200 0.58956000  
 H -4.50953300 3.68378600 0.58071900  
 H -0.66731900 -1.58357900 2.83033500

H -8.54115200 0.01637800 -0.90925300  
 Fe 3.30342500 -0.58602400 -0.52255500  
 O 5.18724400 -0.58982700 -1.64428700  
 H 4.99701900 -0.62632000 -2.59351300  
 O 3.42531000 -2.70229000 -0.99368500  
 H 2.91399300 -3.28864100 -0.41509300  
 O 4.49683500 -0.97145100 1.25161000  
 H 4.84405400 -0.05639800 1.45719700  
 O 2.38718900 -0.21884900 -2.46833700  
 H 1.43481600 -0.44188100 -2.34064400  
 H 5.51778900 0.33962200 -1.47387900  
 H 2.41841400 0.73302200 -2.64857600  
 O 0.00103700 -0.97601600 -1.50363000  
 H 4.33857900 -3.02663800 -0.95537400  
 S 4.66310500 2.17009900 0.14878800  
 O 5.66832400 1.92025100 -0.94785800  
 O 5.16770800 1.58662000 1.44469600  
 O 4.34452700 3.60781100 0.28158600  
 O 3.37163900 1.40701800 -0.22864800  
 O 1.97207200 -1.18684600 2.58342000  
 H 1.63881300 -1.32436700 3.48707300

**TS13**

E(6-31+G\*) = -3354.316682; E(Def2-QZVP) = -  
 3355.336095; G<sub>corr</sub> = 0.274775

0 5

N -0.21414500 -1.77251700 -1.77483300  
 C -1.41850100 -1.52745400 -1.31997300  
 H -2.27786300 -1.34510500 -1.95605000  
 N -1.51778300 -1.53854900 0.01476000  
 C -0.27610500 -1.87978900 0.51002300  
 C 1.53163900 -0.55043600 -0.51649500  
 O 1.08629600 0.58614100 -0.39860500  
 N 2.80471600 -0.95589600 -0.50863700  
 H 3.63261900 -0.30607400 -0.36292200  
 C 2.84382900 -2.34740600 -0.63065000  
 N 4.03552500 -2.93116900 -0.62448100  
 H 4.88514600 -2.36937100 -0.50760800

H 4.09572700 -3.93648900 -0.69162600  
 N 1.67658400 -2.92992800 -0.73978700  
 C 0.72046600 -1.88385800 -0.66648800  
 N 7.21083900 0.92609200 0.17695100  
 C 7.12281300 2.26035800 0.40190700  
 C 6.09728000 0.13690200 -0.06652600  
 H 8.05737600 2.77924900 0.58280400  
 C 5.91675100 2.88348800 0.39553500  
 N 4.89106800 0.75055400 -0.07963300  
 O 6.23830300 -1.08097000 -0.26022700  
 H 5.83104200 3.94790400 0.57401500  
 C 4.77194100 2.06381500 0.14303000  
 N 3.54281700 2.58727200 0.12117700  
 H 2.72642800 2.00692600 -0.05222500  
 H 3.39470300 3.57134100 0.28793100  
 H 0.04694300 -1.81519100 -2.75237300  
 H 8.11053900 0.46151300 0.18503700  
 Fe -2.92643300 -0.29887600 0.98200100  
 O -3.75251800 1.17457200 2.19198000  
 H -3.05748500 1.74778700 2.55571100  
 O -2.36340000 -1.32843600 2.74567600  
 H -2.42953700 -0.90170500 3.61366500  
 O -4.46443300 -1.23378100 0.72284100  
 H -4.79332700 -1.61916600 -0.28887300  
 O -1.05459300 0.90615600 1.47718700  
 H -0.49941900 0.63927700 2.22494800  
 H -4.22820700 1.74296000 1.50279800  
 H -0.43713400 0.98181000 0.71964600  
 O 0.01260000 -2.05103400 1.68186000  
 H -1.45060300 -1.69688000 2.65566200  
 S -3.99161800 1.85968600 -1.08911900  
 O -4.72266500 2.38835500 0.11503600  
 O -4.90032000 1.04784800 -1.95208200  
 O -3.29787700 2.92339900 -1.83519200  
 O -2.89003700 0.88054900 -0.54503800  
 O -4.61090200 -1.60196400 -1.47905000  
 H -4.76546100 -0.64440300 -1.71255100



**I16**

E(6-31+G\*) = -3354.346897; E(Def2-QZVP) = -3355.362395;  $G_{\text{corr}} = 0.284299$

0 5

N -0.22933600 -1.88308700 -1.70703800  
C -1.43815500 -1.63079900 -1.26782400  
H -2.30682900 -1.48424100 -1.91161500  
N -1.54045400 -1.60593800 0.06872000  
C -0.30285000 -1.94063900 0.57885300  
C 1.48432500 -0.60693400 -0.46209000  
O 1.01513500 0.52337500 -0.35906400  
N 2.76424900 -0.98389800 -0.45144000  
H 3.57939400 -0.31141900 -0.32837300  
C 2.83221500 -2.37726600 -0.54742000  
N 4.03594400 -2.93478000 -0.53249600  
H 4.87366400 -2.35197400 -0.43301800  
H 4.11821200 -3.93952400 -0.58333000  
N 1.67688300 -2.98554300 -0.64159800  
C 0.70002800 -1.95862700 -0.59165100  
N 7.13043500 1.01549000 0.12019600  
C 7.01549000 2.35538700 0.29377800  
C 6.03184600 0.19348500 -0.07801800  
H 7.94026200 2.90153600 0.44162100  
C 5.79593900 2.95145600 0.27891100  
N 4.81206400 0.77973100 -0.09762800  
O 6.19724000 -1.02747400 -0.22783100  
H 5.68869600 4.02002500 0.41617400  
C 4.66652600 2.09811300 0.07362700  
N 3.42636200 2.59422800 0.04578300  
H 2.62039400 1.99056100 -0.09316100  
H 3.25949300 3.58089200 0.17536400  
H 0.03800300 -1.95262700 -2.68136100  
H 8.04040600 0.57145200 0.13316000  
Fe -2.85188700 -0.25764000 1.00776000  
O -3.73448900 1.16598500 2.25078300  
H -3.06258100 1.78677800 2.57790400  
O -2.42012000 -1.35768200 2.75448000  
H -2.51695200 -0.92591300 3.61759800

O -4.23769900 -1.00228800 0.70543700  
H -4.49161100 -1.81531800 -1.18903400  
O -1.08617900 0.81344900 1.48633200  
H -0.55528200 0.53547900 2.24934400  
H -4.25856900 1.68563400 1.56297700  
H -0.45060600 0.88183700 0.73648600  
O -0.02073400 -2.08899400 1.75572200  
H -1.50886800 -1.73613800 2.70168000  
S -3.95947000 1.86933000 -1.03682300  
O -4.79465500 2.27096100 0.14575800  
O -4.75630700 1.08936300 -2.02058300  
O -3.25637100 3.01280200 -1.64594000  
O -2.82278300 0.92184000 -0.47823900  
O -4.36189400 -1.62954500 -2.13323200  
H -4.52104800 -0.66050500 -2.17447900

**TS14**

E(6-31+G\*) = -3354.319350; E(Def2-QZVP) = -3355.336861;  $G_{\text{corr}} = 0.281899$

0 5

N -0.06527100 1.21598700 -1.24176400  
C -1.32276000 1.29948900 -0.79099300  
H -1.98833500 2.10317500 -1.10788100  
N -1.40322900 0.79322800 0.51550500  
C -0.16857900 0.28003300 0.84101200  
C 2.14385000 0.98371100 -0.07343000  
O 2.41070800 2.10733300 0.31609700  
N 2.99914700 -0.03684000 -0.30235800  
H 4.04666400 0.03061500 -0.17361800  
C 2.30315200 -1.13633600 -0.77353000  
N 2.97713400 -2.24173500 -1.05429300  
H 3.99670300 -2.26437400 -0.93930800  
H 2.48709300 -3.04904000 -1.41097400  
N 1.00876000 -0.94293000 -0.89710700  
C 0.75639300 0.38905600 -0.39834500  
N 7.76136700 -0.93088200 -0.06867700  
C 8.42451000 0.16982400 0.36467700  
C 6.38489600 -0.95267200 -0.23438300

H 9.50044500 0.07604100 0.45847600  
 C 7.75109400 1.31181400 0.65699000  
 N 5.70580100 0.18105700 0.05382300  
 O 5.83130400 -1.99013700 -0.63338200  
 H 8.26836900 2.19745000 1.00377400  
 C 6.33136700 1.28197100 0.48310000  
 N 5.58184600 2.35688000 0.74496600  
 H 4.57171100 2.33609800 0.62549900  
 H 6.00084500 3.21385300 1.07380500  
 H 0.22759900 1.55439700 -2.14903700  
 H 8.26486900 -1.78208900 -0.28643100  
 Fe -2.74728000 -0.66828300 0.12419800  
 O -3.95408000 -2.23681400 -0.49247500  
 H -3.82826600 -3.08862900 -0.04650100  
 O -1.23453100 -2.23342100 -0.19697800  
 H -0.34983000 -1.90499800 -0.56288500  
 O -2.40719000 0.00086000 -1.39983500  
 H -3.83283700 3.40128400 -2.27594200  
 O -2.45159500 -1.32484700 2.09023600  
 H -1.57132700 -0.99757900 2.39594500  
 H -4.91241800 -1.94423500 -0.35928500  
 H -3.11764200 -0.92287200 2.67424600  
 O 0.11117000 -0.27801100 1.88917300  
 H -1.02091100 -2.79245000 0.56557400  
 S -5.78363500 0.36264200 0.23507600  
 O -6.21291500 -1.02614600 -0.14715500  
 O -5.72977100 1.25878400 -0.94929100  
 O -6.57173700 0.90862700 1.35198700  
 O -4.30430700 0.21409700 0.77174000  
 O -3.72889200 3.15071800 -1.34847600  
 H -4.42304700 2.47341100 -1.19021500

**H17**

E(6-31+G\*) = -3354.346062; E(Def2-QZVP) = -  
 3355.365605; G<sub>corr</sub> = 0.277177

0 5

N -0.15040500 1.05596000 -1.80237800  
 C -1.45038800 1.18230600 -1.14802300

H -1.85698800 2.19133900 -1.27437700  
 N -1.23210500 0.86923900 0.24662800  
 C -0.04486700 0.35579000 0.47386400  
 C 2.11868900 1.05680900 -0.63281700  
 O 2.35338600 2.22251800 -0.41144200  
 N 2.99162600 0.00990200 -0.56750100  
 H 4.01376700 0.09321700 -0.25084700  
 C 2.37418900 -1.12948000 -0.98028800  
 N 2.99702200 -2.28051600 -0.99958000  
 H 3.98405800 -2.32959200 -0.69183600  
 H 2.50714700 -3.11121200 -1.30614600  
 N 1.08839000 -0.93870700 -1.35461900  
 C 0.76938500 0.37276600 -0.99294000  
 N 7.54602400 -0.99784500 0.57793700  
 C 8.20780400 0.12922400 0.94009200  
 C 6.21429800 -0.98857000 0.20195500  
 H 9.24911700 0.00686000 1.21515500  
 C 7.57449500 1.32966800 0.94662900  
 N 5.57285500 0.20285300 0.20735800  
 O 5.66234500 -2.05406200 -0.12186700  
 H 8.08984900 2.23832600 1.23116900  
 C 6.19893400 1.33300900 0.55754400  
 N 5.49652800 2.46802100 0.53212800  
 H 4.52088900 2.48028900 0.25179000  
 H 5.92356900 3.34651600 0.78501500  
 H -0.20765200 0.72382100 -2.76049500  
 H 8.01989800 -1.89305300 0.57088200  
 Fe -2.72526500 -0.70441100 -0.01452100  
 O -4.02800000 -2.11047700 -0.72610500  
 H -3.84988700 -3.05374000 -0.59419400  
 O -1.28458000 -2.21552500 -0.56313400  
 H -0.44890600 -1.93556600 -1.01424700  
 O -2.37480900 0.24042700 -1.59446000  
 H -4.06328600 3.51727100 -1.72374400  
 O -2.05551500 -1.38768200 1.90456300  
 H -1.15650900 -1.05416900 2.11480600  
 H -4.95446900 -1.88928100 -0.37954600  
 H -2.64847900 -1.01539600 2.57857900

O 0.46700200 -0.15492200 1.45557700  
H -1.02172300 -2.84131700 0.12992800  
S -5.68373500 0.27348100 0.71995200  
O -6.16943500 -1.06856800 0.23897000  
O -5.83463900 1.30906000 -0.33734200  
O -6.29244300 0.65479000 2.00611000  
O -4.14134800 0.10232500 0.98182700  
O -4.00580300 3.37077100 -0.77067100  
H -4.61780900 2.62396800 -0.59568300

**I18**

E(6-31+G\*) = -3354.401620; E(Def2-QZVP) = -  
3355.424818; G<sub>corr</sub> = 0.278782

0 5

N 0.22747500 0.68672300 1.94060400  
C 1.04176000 1.79456000 1.31321500  
H 1.03017900 2.64324900 2.00592000  
N 0.38705600 2.16908700 0.05745400  
C -0.12398400 3.22695200 -0.26074500  
C -2.10792100 0.72475900 0.89001200  
O -2.39807800 1.88994100 0.73792300  
N -2.90222000 -0.35719800 0.65220300  
H -3.90430600 -0.30739400 0.27361500  
C -2.27370100 -1.47424300 1.11041300  
N -2.82468700 -2.64947100 1.02427200  
H -3.76839300 -2.73909800 0.60419500  
H -2.33863600 -3.46022600 1.38722400  
N -1.03556300 -1.23426500 1.63158300  
C -0.84903900 0.07285700 1.50000600  
N -7.26422000 -1.56892300 -0.93880500  
C -7.96897600 -0.46622100 -1.29492300  
C -5.97965700 -1.49634600 -0.42993400  
H -8.96649900 -0.63861900 -1.68248800  
C -7.42833800 0.77163100 -1.16115600  
N -5.43105700 -0.26747500 -0.29291100  
O -5.38362900 -2.54298300 -0.12154500  
H -7.97898300 1.66092100 -1.44069600  
C -6.10062500 0.83958800 -0.63616000

N -5.48626600 2.01345900 -0.47175400  
H -4.54316300 2.06825600 -0.10110800  
H -5.94588700 2.87835800 -0.71433200  
H 0.83534300 0.10381800 2.51244400  
H -7.66805800 -2.49240200 -1.03907600  
Fe 2.74062000 -0.35961000 0.14568100  
O 3.86322800 -1.20515000 1.77643500  
H 3.55688500 -2.08287000 2.04624300  
O 1.37290400 -2.06220900 0.11948800  
H 0.62691500 -2.03453300 0.75506500  
O 2.26192000 1.29757100 1.11995100  
H 3.77197200 2.28375100 0.62513800  
O 1.58292500 0.19127700 -1.68250300  
H 1.05583500 0.97701900 -1.43854300  
H 4.76301300 -1.33703200 1.35203700  
H 2.21233500 0.48699800 -2.35754500  
O -0.62710900 4.19476000 -0.67852400  
H 0.94773100 -2.05692700 -0.75296300  
S 5.62810900 -0.81539000 -1.04516500  
O 6.03503600 -1.33394600 0.31542900  
O 5.91792500 0.64999800 -1.15181600  
O 6.27668500 -1.58825000 -2.13072200  
O 4.09649000 -1.00901900 -1.16933500  
O 4.62749600 2.64630300 0.32380400  
H 5.05077600 1.91170700 -0.17177100

**TS15**

E(6-31+G\*) = -3354.309203; E(Def2-QZVP) = -  
3355.330629; G<sub>corr</sub> = 0.273954

0 5

N -0.21164500 -1.82313900 -1.60819100  
C -1.41305000 -1.56494800 -1.16972300  
H -2.39826200 -1.46194600 -2.02828800  
N -1.55013300 -1.51211300 0.14078400  
C -0.31346900 -1.85838400 0.68705800  
C 1.52172700 -0.54730700 -0.36839600  
O 1.07513400 0.58993900 -0.27594100  
N 2.79831400 -0.94470500 -0.38860300

H 3.62982000 -0.28480900 -0.29839000  
 C 2.84093700 -2.33618100 -0.45773100  
 N 4.02707500 -2.92180700 -0.46210900  
 H 4.88201300 -2.35701700 -0.39314400  
 H 4.08276900 -3.92939900 -0.50121600  
 N 1.66774500 -2.92839200 -0.50412600  
 C 0.71614200 -1.89044400 -0.46460000  
 N 7.21915700 0.95013700 0.05432800  
 C 7.14216600 2.29479900 0.21196900  
 C 6.09635700 0.15432300 -0.10871200  
 H 8.08375500 2.81833100 0.33298600  
 C 5.93813800 2.92179300 0.21466400  
 N 4.89177400 0.77125700 -0.11158900  
 O 6.22773600 -1.07274800 -0.24382300  
 H 5.86082000 3.99435900 0.34053200  
 C 4.78338100 2.09515900 0.04516500  
 N 3.55606200 2.62259800 0.03796700  
 H 2.73197000 2.03858000 -0.07373600  
 H 3.41773200 3.61517300 0.15508700  
 H 0.06342700 -1.96077000 -2.57341300  
 H 8.11761100 0.48290900 0.05516900  
 Fe -2.94590400 -0.19390400 1.07157200  
 O -3.75614300 1.37992300 2.19912000  
 H -3.05111300 1.99984900 2.44936600  
 O -2.48038800 -1.21903700 2.84589300  
 H -2.59483800 -0.78578400 3.70590300  
 O -4.52211700 -1.03241300 0.74365800  
 H -4.96141800 -0.72304500 -0.07587000  
 O -1.06808400 0.98338000 1.54503800  
 H -0.54407000 0.77517900 2.33290700  
 H -4.28882600 1.85615000 1.49471200  
 H -0.42054800 1.01656000 0.80890200  
 O -0.06812300 -1.99934300 1.86633700  
 H -1.57339400 -1.60372000 2.81827400  
 S -4.15686500 1.60529400 -1.12949500  
 O -4.86705000 2.31494500 -0.01556100  
 O -4.98400800 0.45552100 -1.63854800  
 O -3.71864000 2.50922900 -2.20361900

O -2.87517500 0.95400100 -0.50163700  
 O -3.30056800 -1.42627900 -2.77312700  
 H -3.89712600 -0.74046300 -2.36842200

**I19**

$E(6-31+G^*) = -3354.328692$ ;  $E(\text{Def2-QZVP}) = -3355.349646$ ;  $G_{\text{corr}} = 0.280122$

0 5

N 0.21049800 1.75056800 -1.42075900  
 C 1.36553900 1.27416400 -1.01826100  
 H 2.89986800 2.37214900 -2.70447800  
 N 1.48620800 1.14978500 0.30022000  
 C 0.30070000 1.56829600 0.86556100  
 C -1.58743700 0.49273000 -0.28083300  
 O -1.20198700 -0.67233800 -0.31168300  
 N -2.83951600 0.95651700 -0.22131100  
 H -3.70252100 0.33983900 -0.20343400  
 C -2.80534600 2.35255200 -0.17666700  
 N -3.96543400 2.99268200 -0.10247700  
 H -4.84487200 2.46666400 -0.07864100  
 H -3.97449200 4.00130600 -0.06528100  
 N -1.60744200 2.88124700 -0.20748100  
 C -0.70935500 1.78901100 -0.27700700  
 N -7.36134900 -0.77272100 -0.11459000  
 C -7.34853500 -2.12759600 -0.17205100  
 C -6.19875700 -0.01685400 -0.11742900  
 H -8.31577900 -2.61712500 -0.16481200  
 C -6.17416100 -2.80555500 -0.23476900  
 N -5.02318800 -0.68471800 -0.17899500  
 O -6.27036800 1.22114000 -0.06424500  
 H -6.14904700 -3.88689600 -0.28198200  
 C -4.97888300 -2.01976700 -0.23680800  
 N -3.77627000 -2.59923400 -0.29668200  
 H -2.92359700 -2.04578500 -0.30222600  
 H -3.68675000 -3.60309500 -0.34364400  
 H -0.09645900 1.80435400 -2.38373500  
 H -8.23868200 -0.26855600 -0.06982100  
 Fe 2.89560900 -0.17953700 1.11320700

O 3.86665200 -1.91623000 1.81861500  
H 3.28481200 -2.69199500 1.76731700  
O 2.20639000 0.37728000 3.02069000  
H 2.13304000 -0.25581000 3.75068600  
O 4.38132600 0.86929600 1.21345000  
H 4.88861800 0.90438700 0.37753500  
O 1.10617400 -1.57907100 1.14924500  
H 0.65763600 -1.71659200 1.99693100  
H 4.53790800 -2.04104100 1.08744000  
H 0.39065800 -1.32582900 0.52637300  
O 0.04244900 1.62923400 2.05718100  
H 1.34310400 0.85899100 2.94249500  
S 4.49259700 -1.04647600 -1.37459800  
O 5.33703900 -1.84978500 -0.43073200  
O 5.03014500 0.35709100 -1.50544900  
O 4.30119800 -1.69767500 -2.68039600  
O 3.09204700 -0.90029100 -0.69689700  
O 3.08480200 2.26260700 -1.75813200  
H 3.77508400 1.54579300 -1.70962000

**TS16**

E(6-31+G\*) = -3354.328394; E(Def2-QZVP) = -  
3355.349109; G<sub>corr</sub> = 0.281915

0 5

N 0.25845000 1.86682900 -1.35364000  
C 1.40224100 1.30993600 -0.97455100  
H 2.80211500 2.53628600 -2.41704600  
N 1.47859800 1.09145800 0.34685700  
C 0.29223100 1.48034300 0.90757000  
C -1.56940600 0.52409500 -0.35169800  
O -1.19072600 -0.63793300 -0.47861400  
N -2.81936500 0.98508200 -0.24811800  
H -3.68225000 0.37028400 -0.25336600  
C -2.77875800 2.37312500 -0.08620200  
N -3.93872400 3.00719400 0.04750800  
H -4.81753200 2.48064900 0.04958100  
H -3.94521500 4.00731100 0.18246700  
N -1.58074700 2.89782500 -0.08298400

C -0.68360900 1.80823100 -0.23703400  
N -7.33482900 -0.76662200 -0.08063200  
C -7.31903200 -2.11767700 -0.19662900  
C -6.17602500 -0.00477600 -0.09782800  
H -8.28327600 -2.61254400 -0.17116200  
C -6.14555900 -2.78582600 -0.33586800  
N -5.00182100 -0.66273000 -0.23837500  
O -6.24971900 1.22917300 0.01372500  
H -6.11869400 -3.86406700 -0.42982300  
C -4.95432300 -1.99388800 -0.35265200  
N -3.75217900 -2.56270500 -0.48418300  
H -2.90283500 -2.00361200 -0.49563200  
H -3.65913900 -3.56336500 -0.57370200  
H -0.05295600 1.89844400 -2.31637900  
H -8.21134100 -0.26995700 0.02362000  
Fe 2.84690800 -0.29595800 1.11511000  
O 3.85066600 -2.06868700 1.69477100  
H 3.30869700 -2.85862500 1.53764400  
O 2.07866900 0.08075500 3.03254000  
H 1.94024300 -0.62259800 3.68470900  
O 4.31090300 0.76105900 1.36761100  
H 4.83994200 0.90614800 0.55895300  
O 1.07885200 -1.69997600 0.93437800  
H 0.60279000 -1.93627700 1.74421000  
H 4.55912200 -2.09115800 0.99263900  
H 0.38334100 -1.36774600 0.32539900  
O -0.00647800 1.44591900 2.09511900  
H 1.22858800 0.58962600 2.94320000  
S 4.54008900 -0.87597100 -1.39021500  
O 5.42141900 -1.68239400 -0.48712400  
O 4.97626100 0.57410900 -1.40152800  
O 4.42741500 -1.43188200 -2.74768700  
O 3.12177700 -0.87246500 -0.74298100  
O 2.94082200 2.29412200 -1.48518500  
H 3.69626400 1.62153400 -1.49057800

**I20**

E(6-31+G\*) = -3354.419540; E(Def2-QZVP) = -

3355.446058;  $G_{\text{corr}} = 0.276646$

0 5

N -0.03586200 -0.78182500 2.04924100  
C 1.22762400 -0.70322900 1.64882500  
H 1.95457200 -0.16894200 3.32947600  
N 1.44050300 -1.01960300 0.36918900  
C 0.22060600 -1.35511500 -0.14767000  
C -1.85217000 -0.05801700 0.50310200  
O -1.59680200 1.11168600 0.26610900  
N -3.04252700 -0.68178400 0.43791000  
H -3.94909700 -0.19615900 0.20215200  
C -2.88938500 -2.00487500 0.84144600  
N -3.97474600 -2.77453700 0.86114500  
H -4.88916600 -2.38201300 0.62051800  
H -3.89904000 -3.73227500 1.16963600  
N -1.66958700 -2.35238400 1.16057200  
C -0.87024900 -1.18787100 0.93666100  
N -7.68307400 0.46375100 -0.43422400  
C -7.78920200 1.78114300 -0.73836100  
C -6.46790100 -0.13689500 -0.13861300  
H -8.78750000 2.14520300 -0.95314600  
C -6.68807000 2.57502400 -0.76436100  
N -5.36583400 0.64707700 -0.16348700  
O -6.43049100 -1.34738500 0.13361200  
H -6.75686600 3.62832700 -1.00586300  
C -5.43872600 1.94867300 -0.45764700  
N -4.29987300 2.64823000 -0.45650000  
H -3.40989800 2.20631100 -0.23573900  
H -4.29902500 3.63478400 -0.66746800  
H -0.37900600 -0.64789900 2.99173300  
H -8.50526300 -0.12685300 -0.41380900  
Fe 3.23580400 -0.74404700 -0.82782900  
O 5.05797400 -0.21919500 -2.17484600  
H 5.37516200 0.60806900 -1.75741400  
O 2.53374000 -2.30282600 -2.19072000  
H 2.75268900 -2.16280700 -3.12346600  
O 4.63688800 -1.75539000 0.00433800  
H 5.06693000 -1.29941700 0.74182700

O 1.99927200 0.52269400 -2.19468300  
H 1.08214700 0.22694200 -2.30697400  
H 5.44283000 -0.91618500 -1.59972700  
H 1.94926500 1.38330500 -1.74744000  
O -0.00759800 -1.70577100 -1.29791100  
H 1.55485500 -2.27430300 -2.12801000  
S 4.55796900 1.92476400 0.56365400  
O 5.68836200 1.88256400 -0.37956700  
O 5.02418700 0.87030600 1.72909500  
O 4.32242600 3.21612400 1.21007000  
O 3.30638200 1.31629600 0.01690000  
O 2.22999200 -0.35977200 2.41588600  
H 4.22519500 0.59275800 2.21533600

#### TS of 1,2-H shift in Fig. 5

$E(6-31+G^*) = -3279.233161$ ;  $E(\text{Def2-QZVP}) = -3280.220912$ ;  $G_{\text{corr}} = 0.277825$

0 5

N -0.26985300 3.70123600 0.05877400  
C -1.43276600 2.88232300 0.10879700  
H -1.39729800 2.30999300 1.24693900  
N -0.93524100 1.51762900 0.05630600  
C 0.40212400 1.60085700 0.00318000  
C 1.39436800 0.56801600 0.07803700  
O 1.17692100 -0.65819900 0.15035900  
N 2.67255800 1.05136000 0.00844200  
H 3.44213000 0.33278500 0.00971900  
C 2.99918500 2.39103400 -0.04058300  
N 4.28401900 2.68805300 -0.09517700  
H 5.02895500 1.96715200 -0.10267000  
H 4.53731800 3.66599400 -0.12791900  
N 2.09362200 3.37681500 -0.02883300  
C 0.84109600 2.95342100 -0.01567000  
N 7.06122600 -1.34675900 -0.08731200  
C 6.87054700 -2.68824200 -0.04687600  
C 6.01095500 -0.44402100 -0.06876200  
H 7.76279100 -3.30349200 -0.06745700  
C 5.61482500 -3.19489200 0.01626600

N 4.74982600 -0.92847700 -0.00563200  
O 6.27256800 0.77193400 -0.11124100  
H 5.43760700 -4.26254300 0.05016200  
C 4.53664800 -2.25303900 0.03668300  
N 3.27469400 -2.67696800 0.09939400  
H 2.50393200 -2.00987400 0.12056800  
H 3.06278600 -3.66276200 0.13377800  
H -0.31146800 4.71320000 0.05696400  
H 7.99582200 -0.95968000 -0.13496200  
Fe -2.34322600 -0.20960500 0.03054400  
O -1.12413100 -1.20176600 -1.46083300  
H -0.19364700 -1.28828800 -1.18279400  
O -3.47267000 0.57478000 1.68089800  
H -3.14232800 0.65916900 2.58585600  
O -3.39152200 0.96880700 -1.34369000  
H -3.38163100 1.89841000 -1.01231400  
O -1.12613300 -1.30330700 1.42225200  
H -1.19667200 -1.13353500 2.37262800  
H -4.29281900 -0.00744300 1.70975200  
H -1.44944200 -2.09982600 -1.62680000  
H -4.32524900 0.61551700 -1.31894900  
H -0.18297800 -1.17068500 1.17782700  
S -5.21355600 -1.52805400 -0.12796000  
O -3.69686200 -1.73166800 -0.30013500  
O -5.63182100 -0.43259700 -1.07906700  
O -5.91316100 -2.80033900 -0.41791400  
O -5.45693000 -1.08170300 1.29701800  
O -2.57312100 3.27675400 -0.22580500