

Supporting Information for

Theoretical Study of the Water Oxidation Mechanism with Non-heme Fe(Pytacn) Iron Complexes. Evidence that the Fe^{IV}(O)(Pytacn) Species Cannot React with the Water Molecule to Form the O-O Bond.

Ferran Acuña-Parés, Miquel Costas, Josep M. Luis* and Julio Lloret-Fillol*

Institut de Química Computacional i Catàlisi (IQCC) and Departament de Química,
Universitat de Girona. Campus Montilivi, E-17071 Girona, Catalonia (Spain)

*To whom correspond should be addressed to emails: josepm.luis@udg.edu, julio.lloret@udg.edu

Contents:

SI.1 – Structural and free energy data for iron and nitrate species

SI.2 – Cartesian coordinates of optimized structures

SI.3 – References

SI.1 – Structural and free energy data for iron and nitrate species.

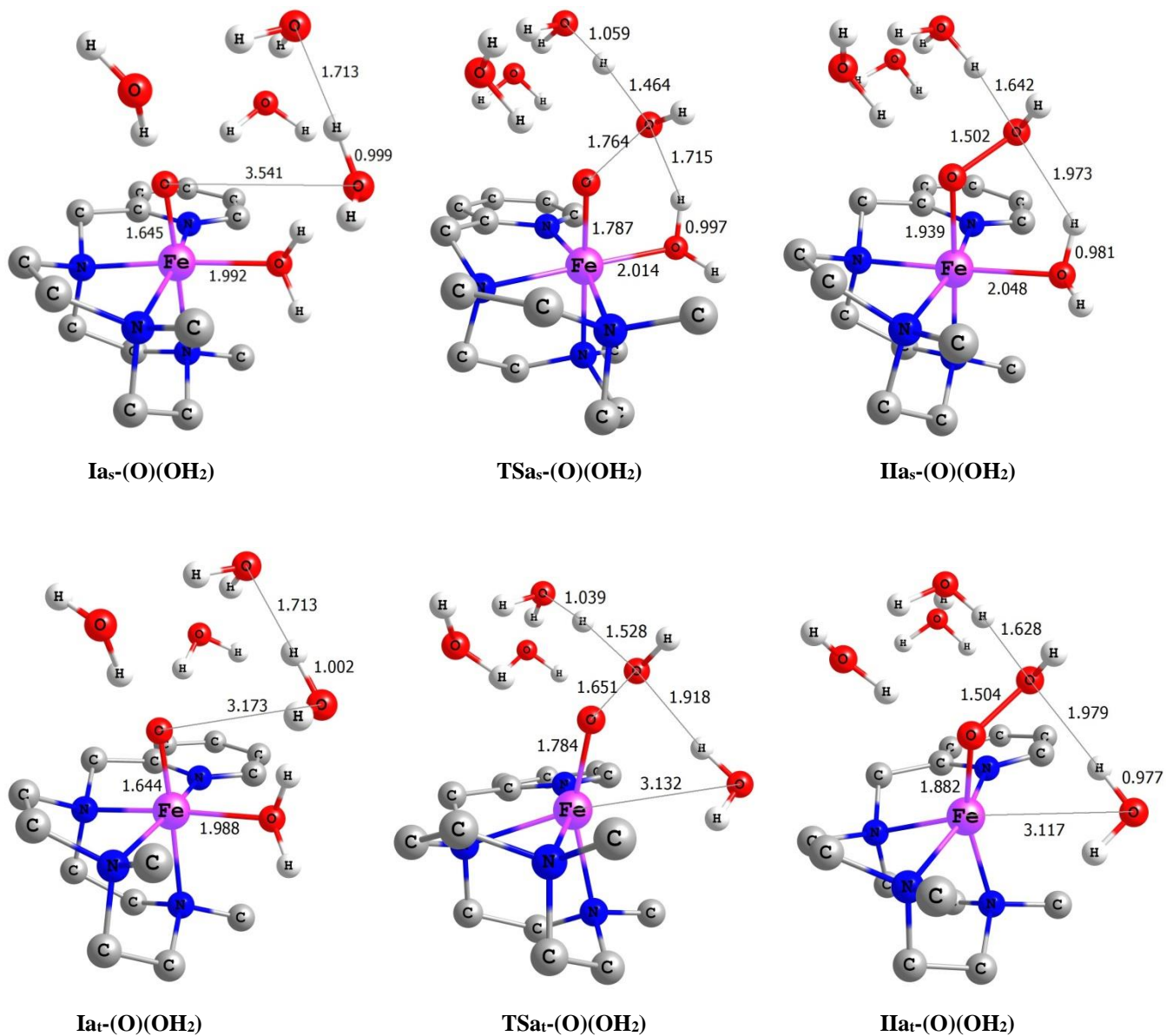


Figure SI.1. Optimized structures of $S = 0$ and $S = 1$ intermediates involved in the O-O bond formation mechanism by the $[\text{Fe}^{\text{IV}}(\text{O})(\text{OH}_2)(\text{Pytacn})]^{2+}$ complex in the tautomeric form **a**. Selected bond distances (\AA) are indicated in the figures. H atoms of the Pytacn ligand have been omitted for clarity.

Table SI.1: Effect of the inclusion of explicit water molecules on the proton dissociation free energy differences (ΔG) and pK_a values for $[\text{Fe}^{\text{IV}}(\text{O})(\text{OH}_2)(\text{Pytacn})]^{2+}$ in its two tautomeric forms (**a** and **b**).

<i>Tautomer a</i>		
	ΔG (kcal·mol ⁻¹)	pK_a^a
$[\text{Fe}^{\text{IV}}(\text{O})(\text{OH}_2)(\text{Pytacn})]^{2+}$	9.7	7.1
$[\text{Fe}^{\text{IV}}(\text{O})(\text{OH}_2)(\text{Pytacn})]^{2+} \cdot \text{H}_2\text{O}$	13.5	9.9
$[\text{Fe}^{\text{IV}}(\text{O})(\text{OH}_2)(\text{Pytacn})]^{2+} \cdot 4\text{H}_2\text{O}$	13.4	9.8
<i>Tautomer b</i>		
	ΔG (kcal·mol ⁻¹)	pK_a^a
$[\text{Fe}^{\text{IV}}(\text{OH}_2)(\text{O})(\text{Pytacn})]^{2+}$	10.8	7.9
$[\text{Fe}^{\text{IV}}(\text{OH}_2)(\text{O})(\text{Pytacn})]^{2+} \cdot \text{H}_2\text{O}$	11.6	8.5

^aThe pK_a values are evaluated at room temperature and atmospheric pressure.

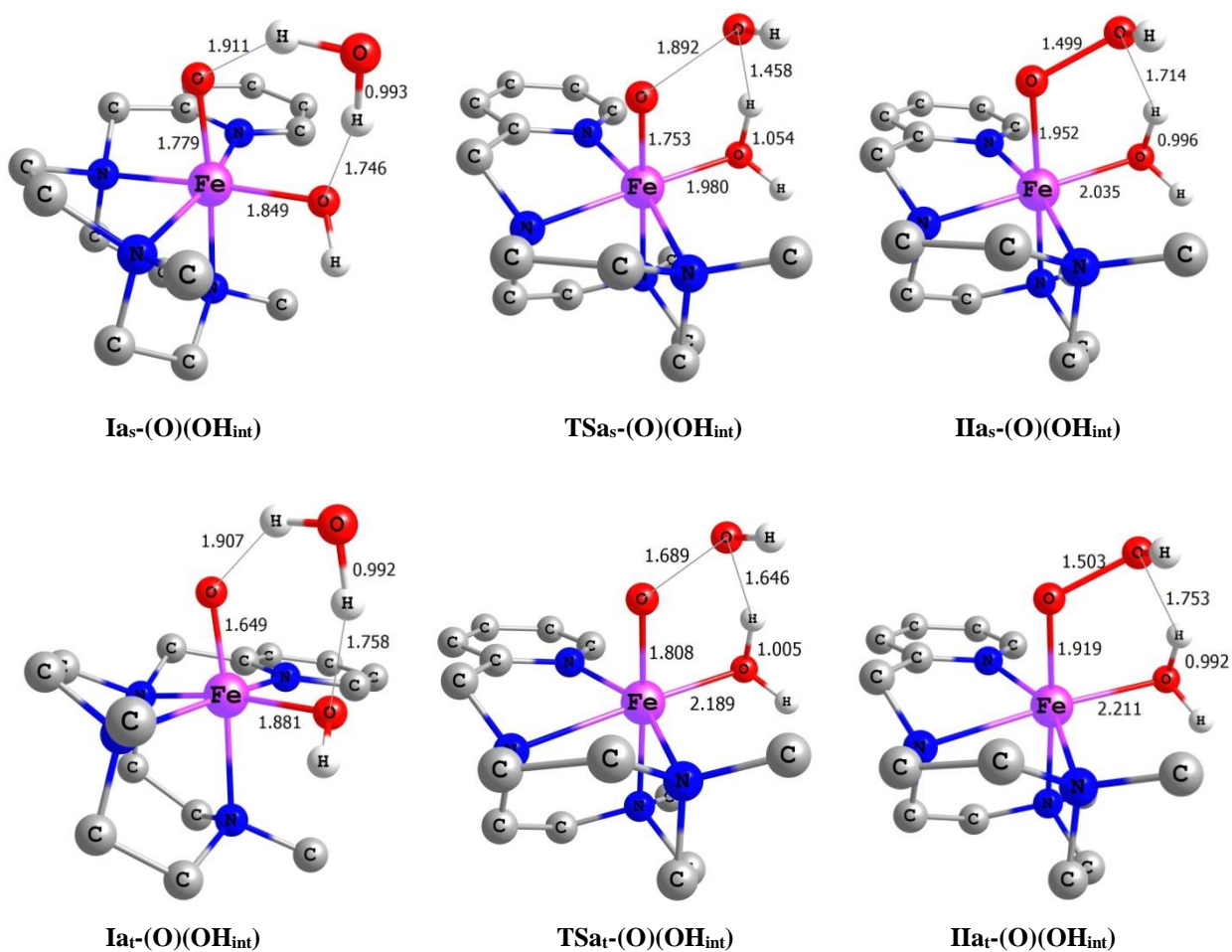


Figure SI.2. Optimized structures of $S = 0$ and $S = 1$ intermediates involved in the O-O bond formation internal mechanism by the $[\text{Fe}^{\text{IV}}(\text{O})(\text{OH})(\text{Pytacn})]^+$ complex in the tautomeric form **a**. Selected bond distances (\AA) are indicated in the figures. H atoms of the Pytacn ligand have been omitted for clarity.

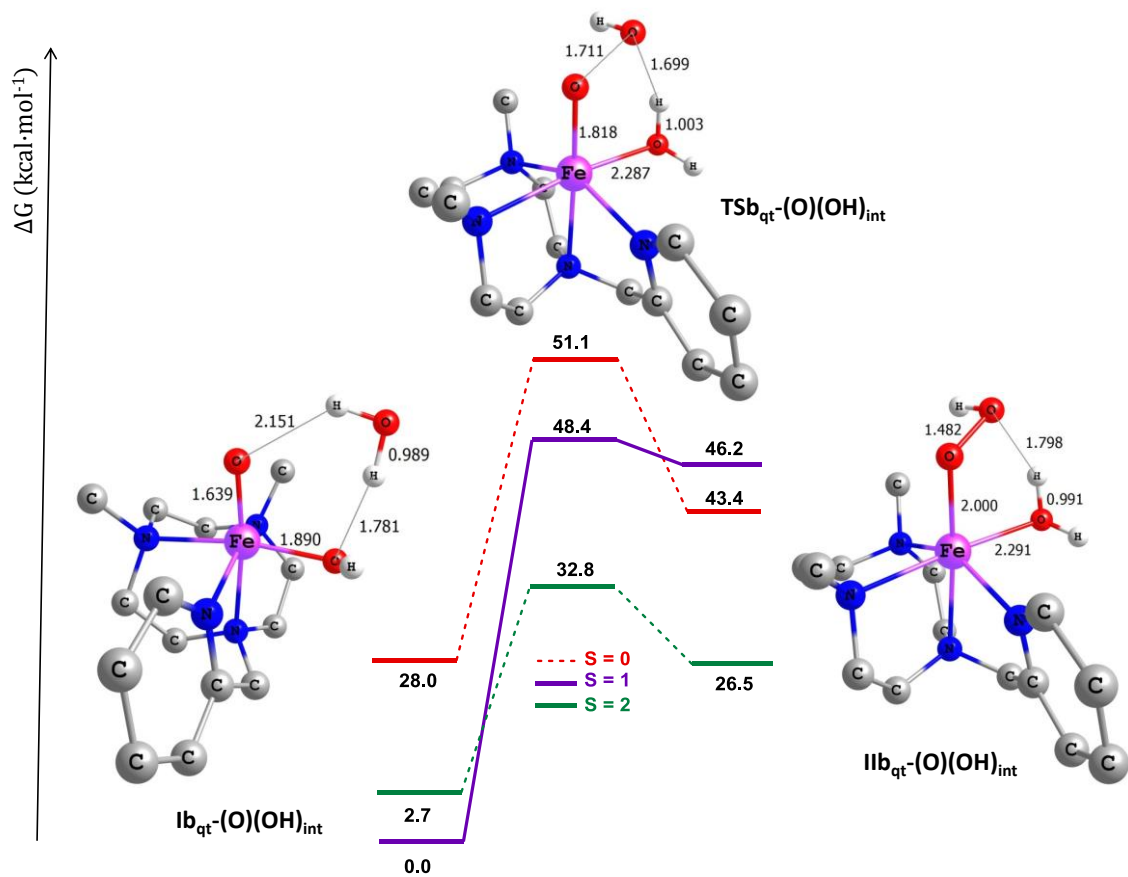


Figure SI.3. Internal base assisted O-O bond formation mechanism from the $[\text{Fe}^{\text{IV}}(\text{O})(\text{OH})(\text{Pytacn})]^+$ intermediate by tautomer **b**. Gibbs energy values are given in $\text{kcal}\cdot\text{mol}^{-1}$. Selected bond distances in Å are indicated in the figures corresponding to the stationary points of the $S=2$ reaction profile.

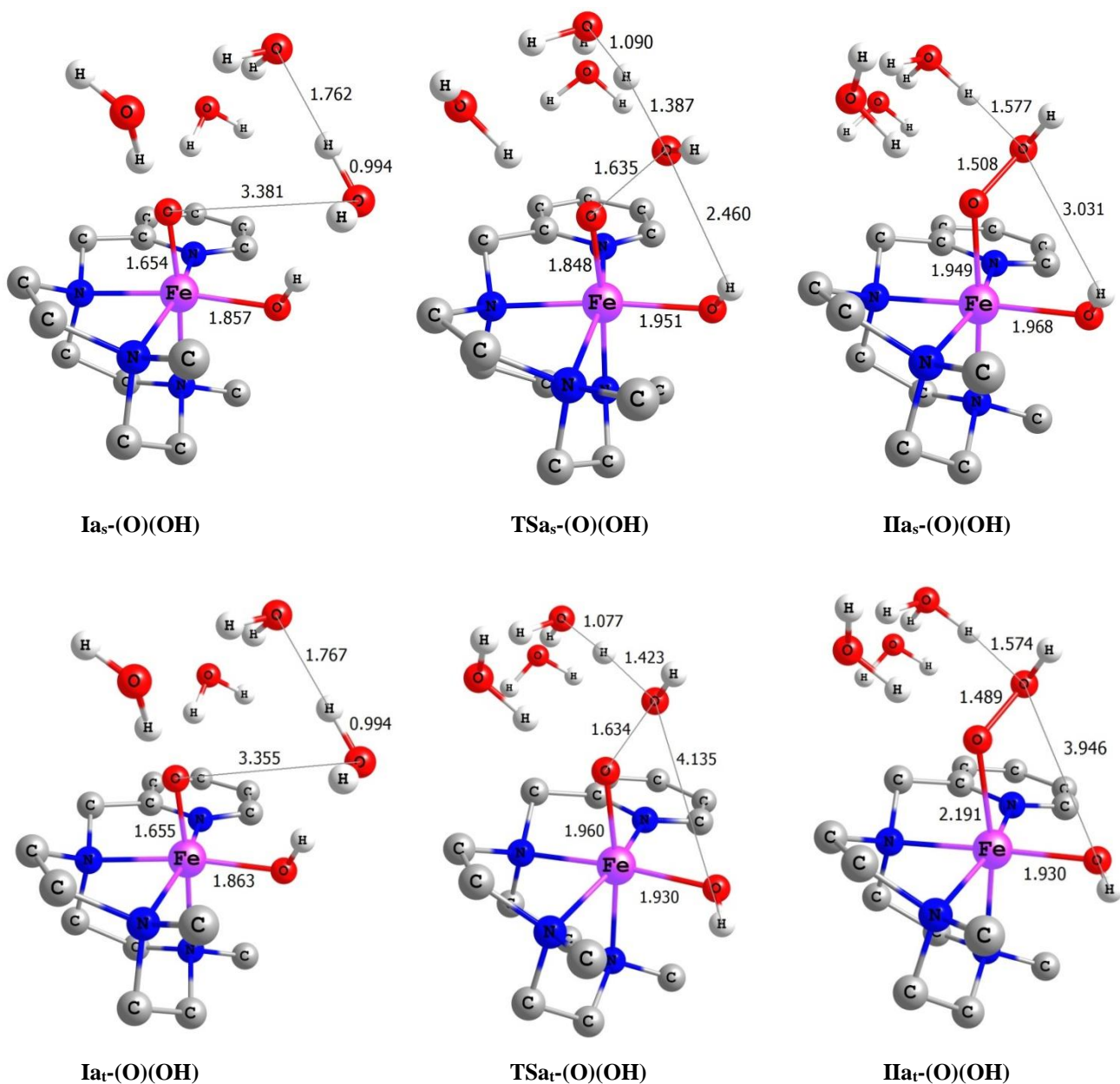


Figure SI.4. Optimized structures of $S = 0$ and $S = 1$ intermediates involved in the O-O bond formation external mechanism by the $[\text{Fe}^{\text{IV}}(\text{O})(\text{OH})(\text{Pytacn})]^+$ complex. Selected bond distances (\AA) are indicated in the figures. H atoms of the Pytacn ligand have been omitted for clarity.

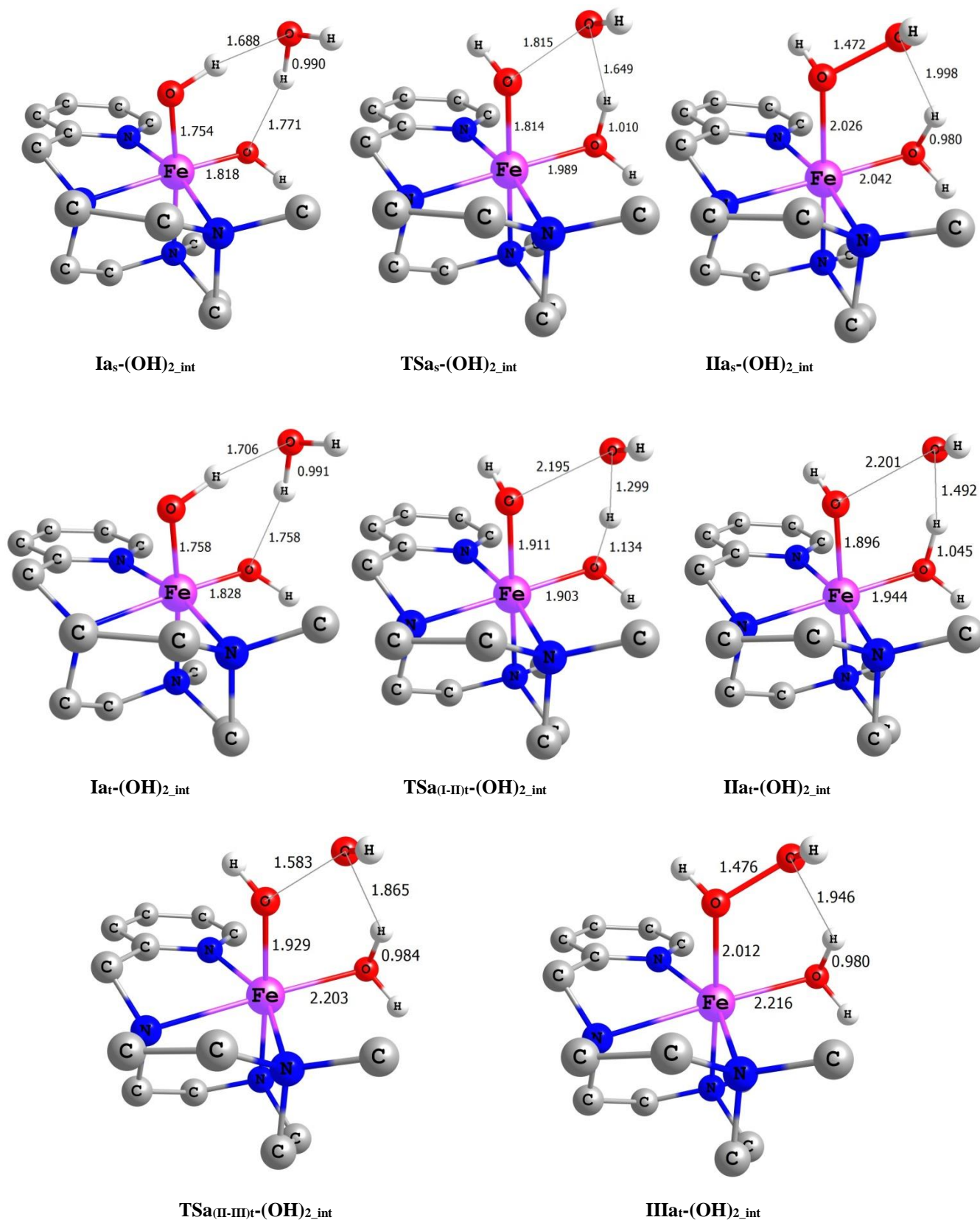


Figure S1.5. Optimized structures of $S = 0$ and $S = 1$ intermediates involved in the O-O bond formation external mechanism by the $[\text{Fe}^{\text{IV}}(\text{OH})(\text{OH})(\text{Pytacn})]^+$ complex in the tautomeric form **a**. Selected bond distances (\AA) are indicated in the figures. H atoms of the Pytacn ligand have been omitted for clarity.

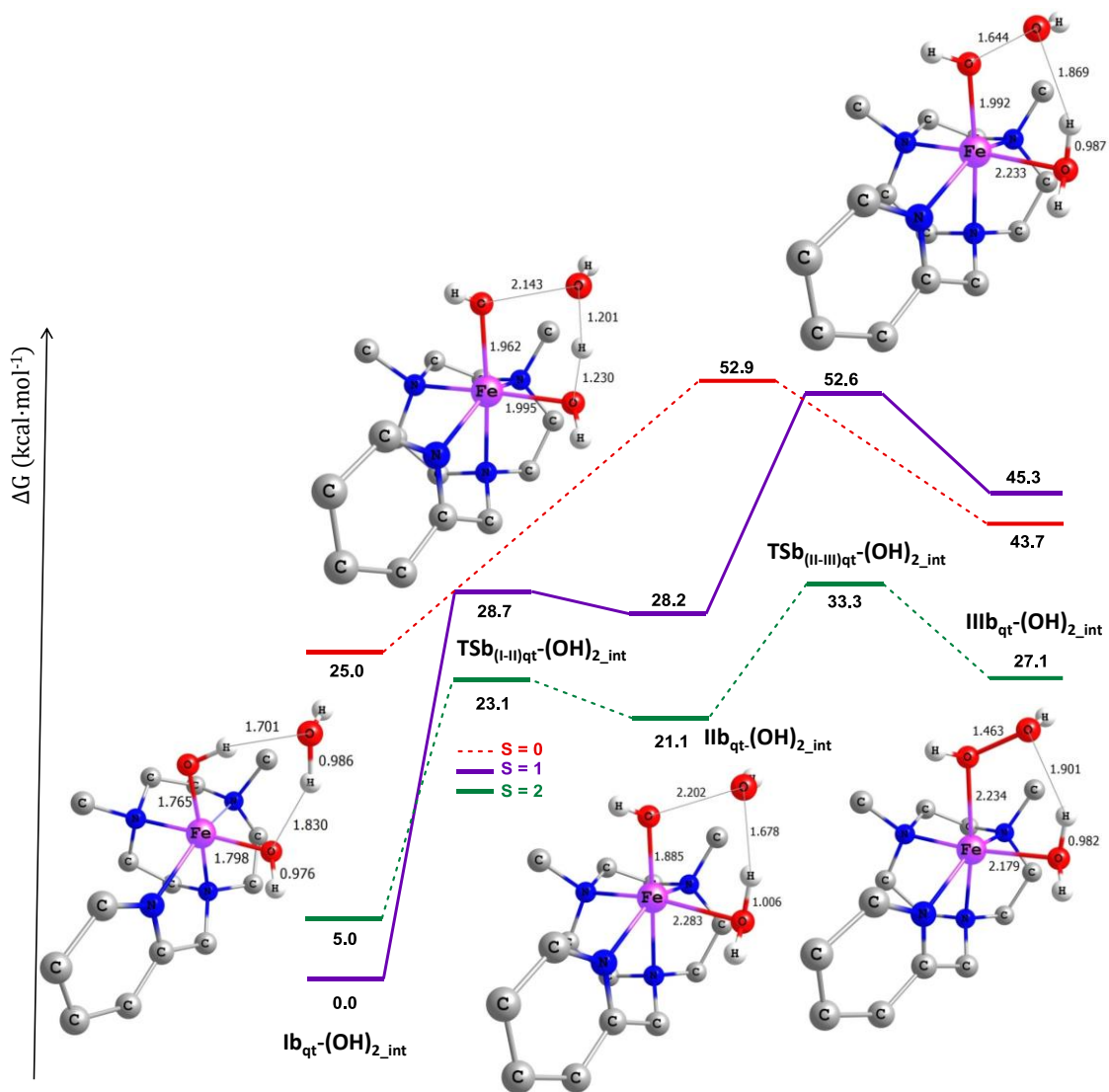


Figure SI.6. O-O bond formation profiles found for $[\text{Fe}^{\text{IV}}(\text{OH})(\text{OH})(\text{Pytacn})]^{2+}\cdot\text{H}_2\text{O}$ in the $S = 0$, $S = 1$ and $S = 2$ spin states, by the tautomeric form **b**. Gibbs energy values are given in $\text{kcal}\cdot\text{mol}^{-1}$. Figures inserted correspond to the $S = 2$ spin state, where selected bond distances (\AA) are presented.

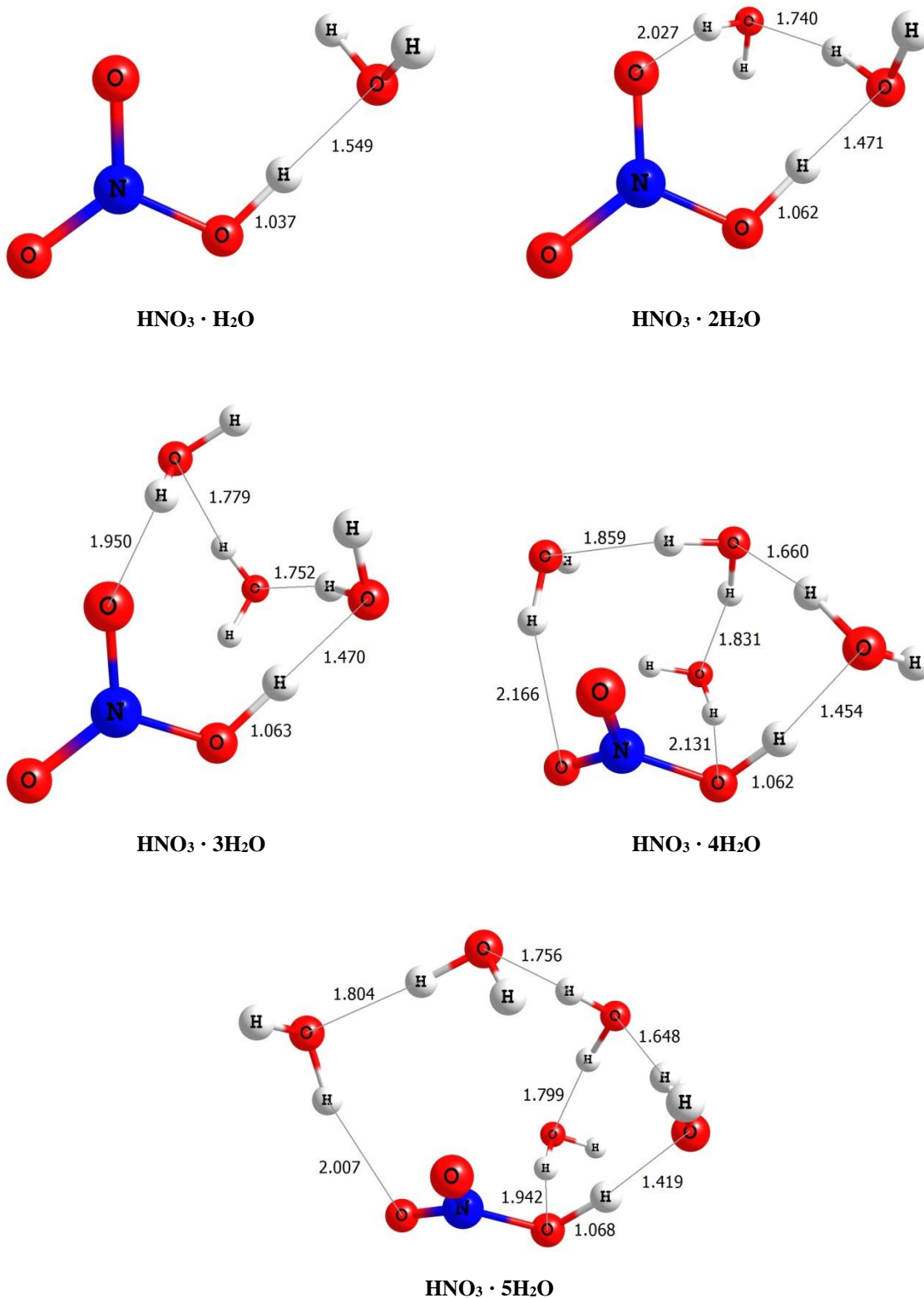


Figure SI.8. Structures of the HNO₃ hydrated cluster geometries in aqueous phase, optimized at the B3LYP-D₂/6-31G*/SMD level. The O-H bond of the HNO₃ was restricted in **HNO₃ · 4H₂O** and **HNO₃ · 5H₂O**, due to tendency to freely evolve to the deprotonated form. Indeed, this fact clearly reflects the acidic character of HNO₃ species when the bulk solvent is becoming properly described. Selected bond distances (Å) are indicated in the figures.

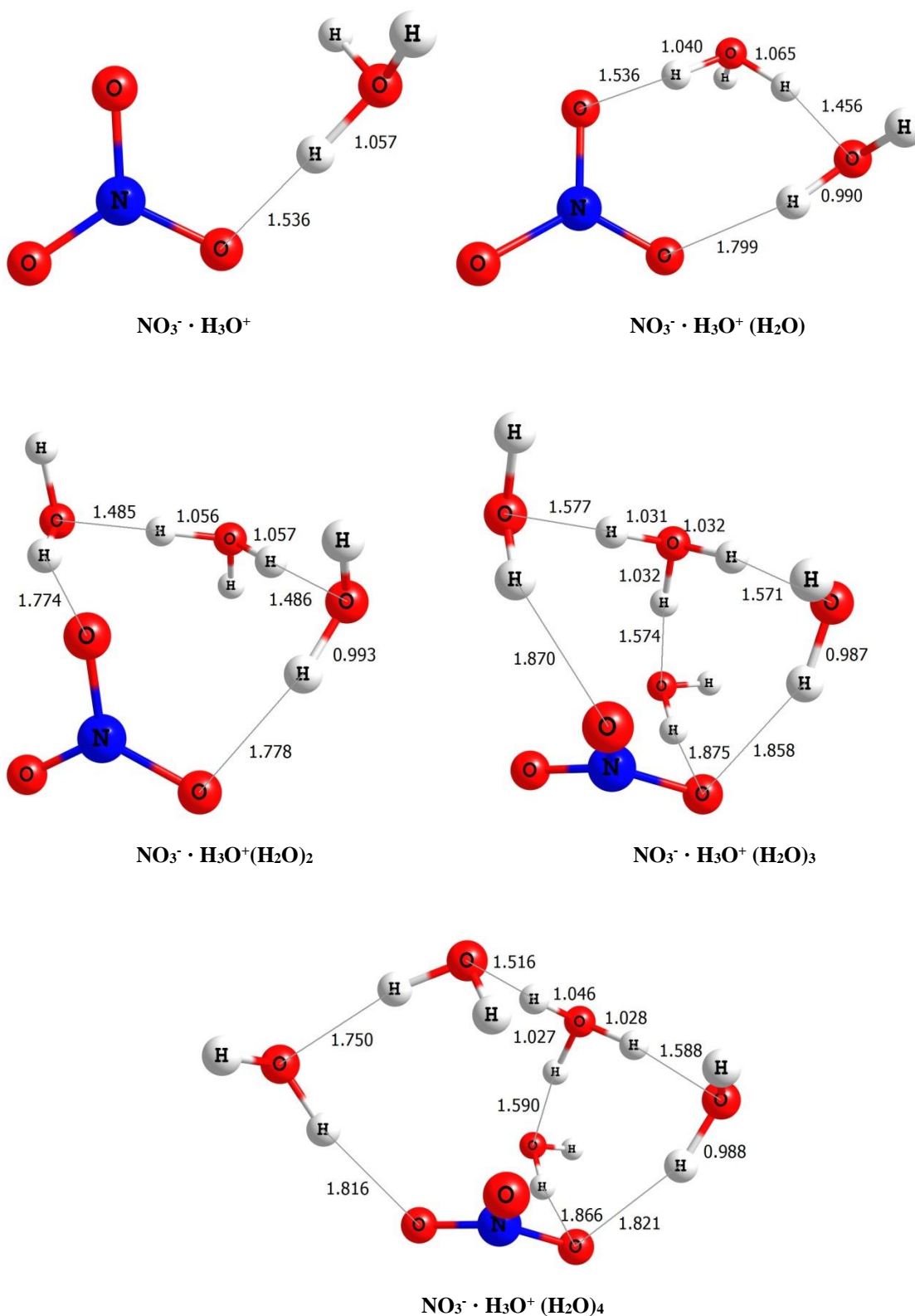


Figure SI.9. Structures of the NO_3^- hydrated cluster geometries in aqueous phase optimized at the B3LYP- $\text{D}_2/6\text{-}31\text{G}^*/\text{SMD}$ level. The O(nitrate)-H bond was restricted for the $\text{NO}_3^- \cdot \text{H}_3\text{O}^+$, $\text{NO}_3^- \cdot \text{H}_3\text{O}^+ (\text{H}_2\text{O})$ and $\text{NO}_3^- \cdot \text{H}_3\text{O}^+ (\text{H}_2\text{O})_2$ clusters, due to the fact that freely evolves to the protonated form. This results evidence the inaccurate description of the bulk solvent which leads to a basic character for the NO_3^- anion. Selected bond distances (\AA) are indicated in the figures.

Table SI.2: Free energy differences (ΔG) and pK_a values for the proton dissociation step in aqueous phase for several HNO_3 -water clusters.

	ΔG (kcal·mol ⁻¹)		pK_a^a
	HNO_3	125.7 (270) ^b	
$\text{HNO}_3 \cdot \text{H}_2\text{O}$		5.9	4.3
$\text{HNO}_3 \cdot 2\text{H}_2\text{O}$		1.2	0.9
$\text{HNO}_3 \cdot 3\text{H}_2\text{O}$		0.8	0.6
$\text{HNO}_3 \cdot 4\text{H}_2\text{O}$		-4.6	-3.4
$\text{HNO}_3 \cdot 5\text{H}_2\text{O}$		-4.2	-3.1
Exp. ^c		-1.9	-1.4

^aThe pK_a values are evaluated at room temperature and atmospheric pressure. ^bIn parenthesis are shown the electronic energy difference obtained from ref. 1 and the corresponding pK_a value. ^cExperimental pK_a obtained from reference 2.

SI.2 – Cartesian coordinates of optimized structures.

In parenthesis are indicated the free energy values (G) in atomic units. The spin multiplicity is also shown in parenthesis by iron complexes without solvent explicit water molecules.

$[\text{Fe}^{II}(\text{O})(\text{OH})_2(\text{Pytncn})]^{2+}$ (G = -2182.196103) (singlet)				1	-5.419649000	0.274091000	0.098845000	1	-3.687739000	-1.043995000	1.076658000
				1	-3.839601000	2.177687000	0.530919000	1	-1.860212000	-1.762978000	2.727255000
				1	2.726102000	-0.382792000	-0.382710000	1	-2.114900000	-0.140860000	-0.439780000
				1	4.182719000	-0.218799000	-1.352151000	1	1.505053000	-1.654800000	1.449276000
				1	0.157045000	-3.201457000	0.608514000	1	-0.832719000	-3.084997000	0.141925000
				1	-0.084761000	-2.898438000	2.348127000	1	0.872018000	-3.208019000	-0.253323000
				1	-1.315841000	-2.571512000	1.174198000	1	-2.394271000	0.073764000	-2.303650000
				1	-0.955107000	-2.571374000	-0.916593000	1	-3.379537000	-1.263662000	-1.695470000
				8	0.596282000	-1.950308000	-1.547830000	1	-0.918081000	-1.589304000	-2.911488000
				1	0.559718000	-1.794231000	-2.591152000	1	-1.545326000	-2.750810000	-1.742838000
				1	1.128425000	-2.529978000	-1.264083000	1	1.598306000	-2.237103000	-0.862398000
				1	0.066984000			1	1.933937000	1.999173000	1.230278000
				1	0.054882000			1	4.432292000	1.808770000	1.194227000
				1	-0.481325000			1	5.477826000	-0.027310000	5.477826000
				1	-0.721643000			1	3.981085000	-1.460722000	-1.597750000
				1	-0.530366000			1	-3.205588000	1.415111000	0.862398000
				7	2.388421000	0.232503000	-0.324877000	1	-2.876330000	1.807549000	-0.849962000
				6	2.724555000	0.023709000	1.120393000	1	-4.237450000	0.722465000	0.722465000
				6	1.909655000	-1.114139000	1.686011000	1	-0.215180000	0.859672000	3.159905000
				6	0.449042000	-0.996221000	1.363178000	1	0.272281000	-0.754462000	3.730263000
				6	-0.276775000	0.016128000	2.190274000	1	1.354931000	0.179183000	2.661847000
				6	0.021215000	1.459080000	1.796443000	1	0.976166000	-0.877293000	-2.627571000
				6	1.449899000	-1.636539000	3.311920000	8	-0.496283000	1.989078000	1.001469000
				6	2.455632000	1.662019000	-0.618964000	8	-0.392329000	1.181346000	-1.564293000
				6	1.320827000	2.487625000	-0.069643000	1	-0.695546000	2.764430000	0.273879000
				6	-1.122642000	0.124900000	-0.272487000	8	-1.246171000	1.981312000	-1.981312000
				6	-2.155935000	1.020890000	-0.286385000	8	-1.028311000	3.758796000	-0.858925000
				6	-1.691104000	-0.214458000	-0.492943000	1	-1.982397000	3.914681000	-0.739879000
				6	-2.534861000	-1.259292000	-0.544906000	1	-0.993962000	3.054123000	-1.538660000
				6	-3.906510000	-1.101209000	-0.337884000				
				6	-4.392383000	-0.765710000	-0.065502000				
				6	-3.508138000	-1.255225000	-0.018399000				
				6	0.388634000	-0.382366000	-0.677736000				
				6	3.290505000	-0.578522000	-1.179638000	7	-2.295754000	-0.151115000	-0.199973000
				6	-1.784255000	-2.036428000	2.642140000	6	-2.607424000	-1.167745000	-0.868341000
				6	2.562098000	0.964820000	1.656625000	6	-1.715064000	-0.938628000	2.067971000
				6	3.793737000	-0.200064000	1.211611000	7	-0.281078000	-0.729196000	1.683469000
				6	2.038787000	-1.190118000	2.771959000	6	0.444072000	-1.990840000	1.345632000
				6	-2.194955000	0.202709000	-0.202709000	6	-0.060972000	-0.202709000	-0.202709000
				6	-0.019583000	-0.139068000	3.245067000	7	-0.073091000	-1.037829000	-1.037829000
				6	-1.340813000	-0.190987000	2.068104000	6	-2.459455000	-0.747286000	-2.222210000
				6	0.932134000	1.802898000	2.279931000	6	-1.245756000	-1.618924000	-1.957892000
				6	-2.790985000	-0.202709000	2.171128000	6	-0.202709000	2.145242000	-0.202709000
				6	2.368359000	1.687660000	-1.805361000	6	-2.195837000	-0.470033000	-0.319203000
				6	0.678737000	0.432315000	0.432315000	7	1.639896000	0.448517000	-0.093454000
				6	0.997148000	3.246119000	-0.784924000	6	2.420697000	1.237628000	0.663250000
				6	1.686494000	3.010562000	0.816385000	6	3.806414000	1.130426000	0.631505000
				6	-1.483860000	3.013116000	0.258010000	6	4.389112000	0.171383000	-0.198270000
				6	-2.089199000	-2.227091000	-0.746362000	6	3.572110000	-0.641789000	-0.985602000
				6	-4.554596000	-1.965078000	-0.379863000	26	-0.337587000	0.383114000	-0.125530000
				6	-0.968056000	0.069056000	1.143970000	6	-3.212090000	1.010782000	-0.064161000
				6	-3.849802000	2.262101000	0.195551000	6	0.403495000	-0.136275000	2.864769000
				6	3.252273000	-1.619310000	-0.849803000	1	-2.492357000	-2.166070000	0.448725000
				6	2.952670000	-0.598115000	-2.215423000	1	-3.656876000	-1.066643000	1.156902000
				6	4.316092000	-0.1199302000	-1.091443000	1	-1.789370000	-1.731790000	2.774945000
				6	0.311551000	-3.094514000	1.055690000	1	-2.033863000	-0.023140000	2.573315000
				6	-0.070680000	-2.548411000	2.709468000	1	0.236855000	-2.751909000	2.105932000
				6	-1.238776000	-2.277370000	1.389941000	1	1.510311000	-1.759253000	1.372345000
				6	-0.929057000	-2.392328000	-1.315923000	1	-0.878685000	-3.052682000	0.009515000
				6	0.558699000	-2.420863000	-1.392435000	1	0.821718000	-3.209494000	-0.385622000
				6	0.396204000	-2.246921000	-2.181326000	1	-2.546523000	0.087128000	-2.257475000
				1	0.879252000	-2.330529000	-2.308725000	1	-3.389618000	-1.325918000	-1.586383000
				1	1.294842000	-0.851131000	-0.917398000	1	-0.943155000	-1.943559000	-2.971174000
				1	-1.488177000			1	-1.488177000	-2.682673000	-1.594361000
				1	1.598489000			1	1.598489000	-2.176501000	-2.113252000
				1	1.907252000			1	1.907252000	1.949993000	1.297753000
				1	4.408365000			1	4.408365000	-1.782316000	-1.254387000
				1	5.467759000			1	5.467759000	0.055263000	-2.319957000
				1	3.985581000			1	3.985581000	-1.397927000	-1.643792000
				1	-3.184777000			1	1.372654000	-0.965581000	0.300578000
				1	-2.884941000			1	-2.884941000	-1.796907000	-2.640683000
				1	-4.233049000			1	-4.233049000	0.694858000	-0.901767000
				1	-0.066526000			1	0.810453000	0.810453000	3.131484000
				1	-0.319394000			1	-0.319394000	-0.831363000	3.709924000
				1	1.457995500			1	1.457995500	0.026425000	-2.640683000
				1	1.005299000			1	-0.592252000	-2.661835000	-2.661835000
				1	-0.503789000			1	-0.503789000	2.023354000	-1.012341000
				1	-0.441976000			1	-0.441976000	1.200893000	-1.546364000
				1	-0.736930000			1	-0.736930000	2.806198000	0.414958000
				1	-1.221377000			1	-1.221377000	1.988208000	-1.988208000
				1	-1.050673000			1	-1.050673000	3.767815000	-0.875893000
				1	-2.014680000			1	-2.014680000	3.890994000	-0.829787000
				1	-0.942088000			1	-0.942088000	2.951867000	-1.419865000
				1	2.952670000	0.127415000	-0.258301000				
				7	-2.632483000	-1.139506000	0.800785000				
				6	-1.768999000	-0.919140000	2.032030000				
				6	-0.325550000	-0.687287000	1.700515000				
				6	-0.449760000	-2.439236000	0.616621000				
				6	0.090826000	-2.519543000	0.078859000				
				6	-0.070052000	-1.423656000	-0.961946000				
				6	-0.419266000	-0.742910000	-1.611288000				
				6	-1.248107000	-0.576760000	-1.427190000				
				6	-2.117470000	-1.260695000	-1.733357000				
				6	2.000369000	-0.488182000	-0.960720000				
				6	1.649429000	0.462137000	-0.116536000				
				26	-2.451794000	-0.439236000	0.616621000				
				6	3.825008000	1.143493000	0.590719000				
				6							

1	-0.053410000	-3.147363000	0.444814000	1	0.878844000	-2.654865000	-0.463195000	8	0.263733000	0.964652000	-2.017107000
1	-0.274730000	-2.977803000	2.209900000	8	-0.442104000	1.598136000	-1.685137000	1	1.089651000	-2.239202000	-1.462689000
1	-1.460930000	-2.298107000	1.131130000	8	-0.319194000	-1.127849000	-2.020989000	1	0.627200000	0.513990000	-2.801901000
1	-0.916197000	2.603519000	-0.816050000	1	0.596023000	-1.225034000	-2.330894000				
8	0.405649000	-1.819422000	-1.536488000								
8	0.376382000	-2.053892000	-2.053892000								
1	1.215838000	-1.887042000	-2.064465000								

$[Fe^2(OH)(OH)(Pytaen)]^2 (G = -2181.765100)$ (quintuplet)

$[Fe^2(OH)(OH)(Pytaen)]^2 (G = -2182.207787)$ (quintuplet)

$[Fe^2(OH)(OH)(Pytaen)]^2 (G = -2181.762231)$ (quintuplet)											
7	2.454881000	0.279273000	-0.289484000	7	-2.501895000	-0.239489000	-0.200922000	7	2.463881000	0.331700000	-0.247158000
6	2.771129000	-0.100449000	1.113590000	6	-2.788694000	0.427830000	1.092416000	6	2.782444000	-0.163521000	1.119224000
6	1.970263000	-1.333579000	1.502550000	6	-1.929817000	1.643900000	1.238672000	6	1.993687000	-1.433137000	1.400020000
6	-0.241002000	-0.346059000	2.123940000	6	-0.075458000	-0.770459000	2.057776000	7	0.526620000	-1.365970000	1.073547000
6	0.016575000	1.143152000	-0.923126000	6	-1.131659000	-2.327997000	0.573863000	6	-0.259514000	-0.547101000	2.094307000
7	0.142842000	1.517819000	0.472296000	6	1.123425000	-2.037241000	0.334755000	6	-0.001244000	0.945238000	2.081026000
6	0.514646000	-1.216489000	-0.498356000	6	-2.1397447000	-1.039730000	0.009736000	7	0.114283000	1.433457000	0.588385000
6	1.298331000	2.439803000	0.227067000	7	1.781885000	0.103984000	-0.545180000	6	0.526620000	2.258181000	2.408181000
6	-1.123923000	2.097208000	-0.023052000	6	2.670397000	1.054918000	-0.870487000	6	1.251037000	2.408181000	0.428904000
6	-2.190973000	1.030482000	-0.103388000	6	4.024000000	0.934470000	-0.570382000	6	-1.170630000	2.055386000	0.158027000
6	-1.175472000	-0.180239000	-0.498436000	6	4.489739000	-0.231498000	0.005959000	6	-2.227739000	0.999707000	-0.002363000
6	-2.628385000	-1.186648000	-0.655218000	6	3.532175000	-1.202031000	0.431281000	6	-4.481708000	1.890441000	-0.340368000
6	-3.989427000	-1.024716000	-0.413542000	26	-0.394940000	0.211850000	-0.818002000	26	0.374842000	-0.299137000	-0.751599000
6	-4.447310000	0.224288000	0.010097000	6	-3.417948000	0.245689000	-1.251133000	6	-0.036274000	-2.697590000	1.031301000
6	-1.234783000	-1.824859000	-0.573950000	6	-1.599617000	0.1599617000	0.712367000	1	2.573220000	0.218216000	0.427381000
26	0.400626000	-0.344019000	-0.781376000	1	-2.623409000	-0.072300000	1.908049000	1	3.851528000	-0.393325000	1.193126000
6	3.387368000	-0.381419000	-1.226376000	1	-3.845141000	0.270369000	1.140922000	1	2.087055000	-1.731700000	2.449222000
6	-0.071841000	-2.577895000	1.276396000	1	-2.031850000	2.103512000	2.239375000	1	2.380022000	-2.238177000	0.170313000
1	2.567650000	-1.720180000	-0.573950000	1	-2.827270000	-0.504533000	1.007381000	1	-0.073810000	1.125169000	0.2251508000
1	3.840723000	-0.323981000	1.210518000	1	-0.024167000	1.167687000	3.002609000	1	-1.311055000	-0.766573000	1.318310000
1	2.087237000	-1.550064000	2.571703000	1	1.302796000	0.873473000	1.866312000	1	0.907462000	1.201147000	2.555319000
1	2.243597000	-2.187950000	0.931986000	1	-1.010251000	-0.955288000	2.579921000	1	-0.823082000	1.473208000	2.510733000
1	-2.469828000	-1.741255000	-0.498356000	6	-2.107744000	-1.328170000	0.009736000	1	2.949105000	-2.362121000	0.218216000
1	-1.298504000	-0.562397000	1.969067000	1	-2.630058000	-2.089336000	-1.125167000	1	3.381655000	2.218650000	0.044515000
1	0.918256000	1.443737000	2.450957000	1	-2.071696000	0.432755000	1.0896767000	1	0.896767000	3.281280000	-0.122610000
1	-0.810876000	1.702154000	2.373409000	1	-0.993561000	-3.184774000	-0.025101000	1	1.557620000	2.748718000	1.417434000
1	1.282625000	-1.573950000	-1.573950000	1	-1.547125000	-0.077434000	-1.041396000	1	-0.474202000	-0.127381000	0.628745000
1	3.424081000	2.164269000	-0.158620000	1	1.419345000	-2.735538000	1.127202000	1	-2.220493000	-2.096969000	-1.109756000
1	0.967227000	-0.391507000	2.270410000	1	2.270410000	1.927163000	-1.376865000	1	-4.685962000	-0.382690000	-0.730938000
1	1.629793000	2.859161000	1.197939000	1	4.713335000	1.724538000	-0.847178000	1	-5.540789000	0.328696000	0.180110000
1	-4.257104000	-2.927747000	0.613237000	1	5.506076000	-0.634671000	0.355642000	1	-3.900260000	-2.177895000	0.642612000
1	-2.210389000	-2.134850000	-0.975787000	1	3.829479000	-2.105605000	0.953017000	1	3.461126000	-1.310569000	-1.125923000
1	-4.467039000	-1.860661000	-0.547985000	1	-3.379878000	1.337498000	-1.282116000	1	0.011810000	-2.249183000	-0.214830000
1	-5.500976000	0.383104000	0.218681000	1	-3.092835000	-0.154229000	-2.214915000	1	4.396421000	0.209470000	-1.104143000
1	-2.948585000	-2.252936000	0.502394000	1	-0.502394000	-0.079550000	-0.079550000	1	-0.507913000	-3.148130000	-0.629210000
1	-3.572126000	-1.458698000	-0.104636000	1	-0.318892000	-0.592610000	-0.051836000	1	0.071254000	-3.148130000	-0.202021000
1	3.059817000	-0.183379000	-2.249561000	1	0.049511000	3.349083000	1.700229000	1	-1.091875000	-2.563095000	0.764085000
1	4.406615000	0.032325000	-1.081909000	1	1.220428000	2.634142000	0.557371000	1	-1.002378000	2.533173000	-0.811349000
1	4.444410000	-0.502394000	-0.502394000	1	0.970151000	-2.620251000	-1.041396000	8	-1.763169000	0.162596000	0.589485000
1	0.037769000	-2.946594000	2.304941000	1	-0.544009000	1.504791000	-1.814350000	8	0.281082000	0.811601000	-2.142433000
1	-1.131934000	-2.537790000	1.019979000	8	-0.428114000	-1.097223000	-2.109812000	1	1.534810000	-2.301480000	-1.386608000
1	-0.948640000	2.473986000	-1.032446000	1	-0.596589000	-0.684287000	-2.972221000	1	0.788594000	0.400840000	-2.889415000
8	0.573525000	-2.034552000	-1.504028000								
8	0.391747000	0.419327000	-2.193217000								
1	0.657066000	-1.950490000	-2.467997000								

$[Fe^2(OH)(OH)(Pytaen)]^2 (G = -2181.720353)$ (singlet)

$[Fe^2(OH)(OH)(Pytaen)]^2 (G = -2182.178564)$ (singlet)

$[Fe^2(OH)(OH)(Pytaen)]^2 (G = -2181.559386)$ (quadruplet)

7	-2.362272000	-0.104100000	-0.424058000	7	2.361508000	0.058464000	-0.402218000	7	2.327842000	0.161867000	-0.386619000
6	-2.764657000	0.5211739000	0.880433000	6	2.758470000	-0.612597000	0.894640000	6	2.739074000	-0.334848000	-2.574762000
6	-0.396524000	1.648310000	1.208851000	6	1.767290000	-1.697906000	1.536469000	6	1.888192000	-1.325682000	1.365875000
6	0.181840000	0.559376000	2.176295000	6	2.746846000	-1.234021000	1.134717000	6	0.429036000	-1.280287000	1.125316000
6	-0.266083000	-0.888014000	2.144407000	6	-0.105316000	-0.357368000	2.255161000	6	-0.224540000	-0.439332000	2.172365000
6	-2.266610000	1.839977000	0.733287000	6	0.405793000	1.028851000	2.669936000	6	0.152436000	1.025996000	2.042063000
6	-2.457732000	-1.582689000	-0.349176000	7	-0.276390000	-1.431791000	0.629534000	7	0.233017000	1.460412000	0.589485000
6	-1.446824000	-2.268360000	0.474996000	6	2.624448000	1.509113000	-0.306412000	6	2.488151000	1.647692000	-0.484095000
6	1.038782000	-2.039830000	0.413689000	6	1.409064000	2.237181000	0.229206000	6	1.409043000	2.263568000	0.338505000
6	-2.082167000	1.098593000	0.502394000	6	-1.067560000	-0.077434000	-1.041396000	6	-0.507913000	-3.148130000	-0.629210000
6	3.383636000	0.088261000	-0.587802000	6	-2.097918000	-0.899398000	0.070576000	6	-2.104167000	-0.2097428000	0.386146000
6	2.511262000	1.029537000	-0.981696000	6	-1.643455000	-0.099538000	-0.573431000	6	-1.625692000	-0.115273000	-0.505852000
6	3.873596000	0.926234000	-0.723018000	26	0.333719000	-0.172141000	-0.682137000	26	-0.180297000	-0.666627000	0.170430000
4	4.388320000	-0.166046000	-0.019440000	6	3.193917000	-0.570109000	-1.501733000	6	3.147950000	-0.498467000	-1.440879000
4	4.429493000	-1.161431000	0.010400000	6	-0.315104000	-0.101040000	-0.117532000	6	-2.451010000	-2.606104000	0.136546000
26	-0.354553000	0.189577000	-0.709761000	2	2.840265000	0.134343000	1.677522000	1	2.662327000	0.483716000	1.683912000
6	-3.194114000	0.444450000	-1.518839000	3	3.752353000	-1.054716000	0.775276000	1	3.791795000	-0.629198000	0.609034000
6	0.358414000	2.611783000	0.971636000	1	1.943089000	-2.059662000	2.272422000	1	2.047807000	-1.783542000	2.418523000
1	-2.533812000	-0.481921000	-0.481921000	1	4.948355000	-0.448355000	-0.052124000	1	1.653925000	2.163836000	0.165414000
1	-3.791590000	0.886397000	0.811714000	1	0.232426000	-0.077928000	3.207584000	1	0.056359000	-0.807913000	1.365317000
1	-2.015413000	2.041503000	2.229479000	1	-1.196520000						

6	2.293546000	-0.094614000	-0.990309000	7	-1.165116000	-1.807488000	-1.002423000	1	0.473756000	2.311022000	-2.213822000
7	1.800476000	0.579147000	0.059331000	6	-1.553450000	-1.928329000	0.007941000	1	2.383904000	3.878312000	-1.855534000
6	2.602089000	1.111017000	0.978068000	7	-1.528696000	-2.084599000	1.452050000	1	3.790612000	3.611531000	2.162521000
6	3.985146000	0.989432000	0.886740000	7	-0.600295000	-0.909503000	1.576040000	1	3.229366000	1.793288000	1.801623000
6	4.522727000	0.284388000	-0.192076000	6	1.770528000	-1.770528000	1.553211000	1	-3.450588000	-1.083816000	-1.774146000
6	-0.4658738000	-0.1457358000	-0.591175000	7	0.591175000	-0.591175000	2.413808000	1	-2.208835000	-2.357463000	-1.804768000
26	-0.3906202000	0.572748000	0.146072000	6	-1.327320000	0.292327000	2.085598000	1	-3.709256000	-2.599160000	-0.856381000
6	-3.454222000	0.639248000	0.151715000	6	-2.037791000	0.997709000	0.963214000	1	-2.408953000	2.529260000	-1.560222000
6	0.283030000	-0.694753000	2.858268000	7	-1.433865000	0.918418000	-0.243148000	1	-2.729868000	3.491157000	-0.084918000
1	-2.222216000	-0.159685000	-0.1906762000	6	-1.906762000	-1.906762000	-1.284655000	1	-1.057703000	3.248212000	-0.649213000
1	-3.566147000	-1.756200000	0.753600000	6	-3.025917000	2.437390000	-1.161546000	1	1.657548000	-1.047248000	0.905180000
1	-1.670152000	-2.517616000	2.249715000	6	-3.673810000	2.507274000	0.073448000	8	-2.1297254000	0.413812000	-2.364589000
1	-2.144355000	-0.815236000	2.445340000	6	-3.174690000	1.775931000	1.151081000	0	0.268028000	-1.508496000	-1.131267000
1	0.477329000	-2.035544000	-1.457923000	26	0.130975000	-0.216770000	-0.243931000	1	-1.427705000	-0.458149000	-2.767181000
1	1.627795000	-1.768138000	1.084174000	6	2.711901000	-1.616396000	-0.685353000	8	1.429088000	-1.142401000	-0.2021787000
1	-0.506191000	-3.011184000	-0.675301000	6	-1.926901000	-1.486600000	-2.235263000	1	1.325850000	-1.803700000	-2.703507000
1	1.203615000	-0.817932000	-0.988184000	1	0.448711000	-3.607457000	0.599133000	1	2.719451000	-1.640610000	-1.267336000
1	-2.481134000	0.440122000	-2.164479000	1	1.616267000	-3.785107000	-0.694663000	8	3.395910000	-2.215077000	-0.738687000
1	-3.275761000	-1.083927000	-2.014182000	1	-0.811804000	-3.855273000	-1.481951000	1	3.789177000	-1.641089000	0.107042000
1	-0.835362000	-0.741864000	-3.181643000	1	0.231807000	-2.659449000	-2.288467000	1	2.743914000	-2.897855000	-0.307677000
1	-1.282730000	-2.253108000	-2.403554000	1	-2.604146000	-3.101756000	-0.117862000	8	4.456129000	-0.792540000	1.159906000
1	2.123498000	1.637175000	1.797234000	1	-0.967930000	-2.391311000	1.667167000	1	1.833044000	-0.848938000	1.905445000
1	4.619311000	1.431337000	1.647427000	1	-2.313574000	-2.008714000	2.211295000	8	1.399578000	-3.589420000	-0.058866000
1	5.597114000	0.160560000	-0.287941000	1	2.615268000	-1.104689000	1.687254000	1	0.877215000	-2.794922000	-0.341228000
1	-3.463556000	0.711459000	1.242135000	1	2.081257000	-2.471197000	-1.362167000	1	1.277913000	-4.230931000	-0.582757000
1	-3.254177000	1.618842000	-0.272609000	1	0.296865000	-1.984971000	3.176870000				
1	-4.429697000	0.262729000	-0.193290000	1	-2.012885000	0.026588000	2.895515000				
1	-1.046320000	-1.894212000	-1.470463000	1	2.081257000	-2.471197000	-1.362167000				
1	0.290220000	-1.572891000	3.517740000	1	-3.382090000	2.395121000	-2.020474000				
1	1.304041000	-0.333787000	2.726567000	1	-4.558415000	3.125152000	0.196367000	7	1.435238000	-1.829825000	0.083941000
1	0.994581000	0.241321000	-2.630884000	1	-3.643931000	1.808375000	2.128370000	6	0.799297000	-3.148350000	-0.219324000
1	-2.618134000	0.440122000	-2.164479000	1	2.487147000	-1.928329000	0.007941000	6	-0.272580000	-2.949474000	-0.708194000
8	-0.494077000	1.729805000	-1.344180000	1	3.110817000	-0.628554000	-0.456519000	7	-1.185262000	-1.809892000	-0.898992000
1	-1.577319000	3.004035000	-0.733164000	1	3.435008000	-2.389988000	-0.399458000	6	-2.174307000	-2.105545000	0.088456000
1	0.254454000	2.349914000	-1.291075000	1	-1.232287000	-1.165832000	-3.011115000	6	-1.546436000	-2.053508000	1.471622000
1	-0.174539000	-1.454463000	-1.470463000	1	-2.471197000	-2.471197000	-1.362167000	7	-0.608938000	-0.898992000	-0.898992000
1	-1.939245000	3.237172000	0.652482000	1	-2.642015000	-0.689137000	-2.030733000	1	1.760323000	-1.786938000	1.551855000
				1	-0.579470000	0.989970000	2.473583000	6	0.591563000	-1.246401000	2.418947000
				6	0.599966000	0.052983000	-2.006089000	6	-1.307766000	0.326040000	2.086602000
				1	1.103242000	-1.103242000	1.028448000	6	1.028448000	1.028448000	0.842956000
				1	1.502312000	0.442987000	-2.011200000	7	-1.424522000	0.925445000	-0.924289000
				8	2.993937000	1.537511000	-2.214693000	1	-1.894172000	1.623993000	-1.295974000
7	-2.409347000	-0.321635000	-0.286561000	8	3.667204000	0.913784000	-1.808940000	6	-2.998827000	2.458365000	-1.173458000
6	-2.618098000	-1.297625000	0.812512000	1	2.970135000	-2.230290000	-1.501151000	6	-3.650616000	-2.556431000	-3.650616000
6	-1.835890000	-0.884813000	2.060111000	6	3.212807000	-1.167199000	-0.428128000	6	-1.990202000	0.078233000	2.2904776000
6	-0.113634000	1.790048000	0.473338000	1	1.806824000	-1.670544000	-0.752554000	6	-1.358648000	1.486093000	-2.364710000
6	-0.464727000	-1.715069000	1.573799000	1	-1.039580000	-0.511955000	-1.060529000	1	-1.039580000	1.486093000	-2.364710000
6	0.249687000	-2.438416000	0.242550000	1	3.363529000	-2.390995000	0.447550000	26	0.127500000	-0.303664000	-0.207805000
7	0.002926000	-1.516682000	-0.903454000	1	0.345242000	3.385082000	0.614782000	6	2.687449000	-1.663059000	-0.697231000
7	-0.194630000	-1.621270000	-1.470463000	1	-1.430377000	-1.430377000	-1.430377000	1	-1.945390000	-1.945390000	-1.945390000
6	-1.152577000	-1.924183000	-1.751148000	1	0.542783000	2.401172000	0.620021000	1	1.568343000	-3.822043000	-0.664090000
6	1.232455000	-1.301495000	-1.690370000	8	3.254531000	1.206486000	1.450976000	1	-0.863998000	-3.867303000	-1.447081000
6	2.243555000	-0.524392000	-0.880991000	1	3.409306000	1.959770000	2.336384000	1	0.195170000	-1.189170000	-0.842956000
6	1.744120000	-1.401373000	-0.812512000	1	2.875354000	0.569790000	1.129620000	1	-2.636888000	-3.084733000	-0.084523000
6	2.567665000	0.256211000	0.580580000					1	-2.950340000	-1.340154000	0.018092000
6	3.948959000	0.106344000	0.657414000					1	-1.000609000	-2.965885000	1.696653000
6	4.456805000	-0.062859000	-0.072911000					1	-2.350211000	-1.350211000	-2.350211000
6	5.598624000	-0.841092000	-0.852279000					1	2.611250000	-1.118044000	1.671049000
26	-0.4623145000	-0.4623145000	-0.069007000	7	2.352397000	1.125103000	-0.147508000	1	2.065663000	-2.789196000	1.867243000
6	-3.444314000	-0.227812000	-0.262149000	6	3.448228000	0.183198000	0.227980000	1	0.932877000	-0.395777000	-0.826577000
6	0.113961000	0.222639000	2.943163000	6	3.212807000	-1.167199000	-0.428128000	1	-1.990202000	0.078233000	2.2904776000
1	-2.239345000	-2.290216000	0.473338000	1	1.806824000	-1.670544000	-0.752554000	1	-1.358648000	1.486093000	-2.364710000
1	-3.488497000	-1.354463000	-1.470463000	1	-1.039580000	-0.511955000	-1.060529000	1	-1.039580000	1.486093000	-2.364710000
1	-1.894520000	-1.680249000	2.816937000	6	1.350751000	-1.147576000	2.125488000	1	-3.353136000	3.013899000	-2.026151000
1	-2.306699000	0.150560000	2.473068000	7	0.591600000	0.039791000	1.595257000	1	2.453101000	-1.746391000	3.188565000
1	0.919000000	-1.385960000	1.626227000	6	2.026428000	2.027070000	0.989553000	1	1.921440000	2.090480000	1.880697000
1	-0.582329000	-3.135509000	0.331638000	6	-0.850780000	-0.098350000	1.930896000	1	3.099599000	-0.677292000	-0.482968000
1	1.141437000	-3.047984000	0.045378000	1	-1.497774000	-1.071651000	0.980711000	1	-1.247799000	-3.403168000	-2.411890000
1	-2.239345000	-0.135845000	-2.339345000	7	-1.020544000	-1.020544000	-0.290656000	1	-2.499252000	-2.380309000	-2.548542000
1	-1.482920000	-1.482920000	-1.482920000	1	-1.623620000	-1.623620000	-1.262650000	1	-2.651912000	-0.680544000	-2.027651000
1	-0.851203000	-1.949518000	-2.802248000	6	-2.685904000	-2.635637000	-0.935820000	1	-1.547888000	-0.547888000	-0.547888000
1	-1.461022000	-2.939871000	-1.489602000	6	-3.140187000	-2.723970000	0.381271000	8	0.599888000	0.029660000	-2.018252000
1	1.670949000	-2.251057000	-2.028010000	6	-2.532814000	-1.922822000	1.353999000	1	-0.863998000	-3.867303000	-1.447081000
1	2.099440000	2.099440000	2.099440000	26	0.607843000	-0.939483000	-0.4078374000	1	1.123210000	0.807544000	0.468224000
1	4.567513000	1.629204000	-1.208416000	6	2.742440000	1.932548000	-1.310976000	1	1.484014000	-0.458629000	-0.210760000
1	5.516811000	-0.294541000	-0.029528000	6	1.590126000	-2.712326000	-1.274194000	8	0.1	0.1	0.1
1	3.963268000	-1.689173000	-1.422474000	1	3.495992000	0.103138000	1.312307000	1	2.969672000	2.236178000	1.546

7	-2.19341000	-1.42882000	-0.05624400	1	0.45194500	1.83225700	2.63477700	6	0.25697800	-2.27466900	0.83227600
6	-3.21866000	-0.78589400	0.83059300	1	1.78582200	2.39148000	3.10506600	6	-0.12292600	-0.40996000	-0.63049200
6	-3.43527000	0.68211800	0.48044000	1	-1.24775200	-0.25565300	2.89552100	7	-0.16691600	-1.04980800	-1.29797000
7	-2.17862800	1.44487800	0.34290200	1	-1.41122700	-1.64263500	-2.29192000	6	-2.48351600	-0.09764300	-1.65792800
6	-1.53130700	1.80815300	1.60422900	1	-3.26128400	-3.23465600	-1.73355000	6	-1.33711200	-0.95397300	-2.24975300
6	-0.87337700	-0.04481600	1.29121000	1	4.06893200	1.02675000	0.45846800	6	-4.23757000	-1.13969500	-0.78373200
6	-0.19028600	-0.34473500	1.41121800	1	-2.93412700	-1.89804700	2.36427400	6	2.15495200	-0.32052000	-0.96418100
7	-1.42300300	-2.43617500	0.72366300	1	3.51788100	1.16875100	-1.72538100	7	1.64724700	0.40066300	0.06186800
6	-0.48636600	-1.77183400	1.76428600	1	2.47643500	2.50235300	-1.30445600	6	2.48705900	0.92930000	0.97039700
6	-1.24530000	0.00161600	1.29121000	1	4.06893200	1.02675000	0.45846800	6	3.86346400	0.74604500	-0.14975900
6	1.46344300	1.19909000	0.50364200	1	2.06319800	-2.86987900	-2.28128000	6	4.38716500	-0.19988800	-0.14425100
6	0.66975900	1.26280800	-0.60234300	1	2.18295100	-3.78020300	-1.08509800	6	3.51789900	-0.56423300	-1.09577700
7	-0.81796600	2.31894300	-1.43110200	1	0.59177200	-3.00412100	-1.49467500	26	-0.32810400	0.40820300	0.08819200
6	1.73028000	2.35179000	-1.19223700	1	-1.33075300	0.93671500	1.63142800	6	-3.18978400	1.22148500	0.25050100
6	2.52254000	3.28926500	-0.04390500	8	0.97282800	-0.07077700	-2.68731000	6	0.29895400	-0.82954000	2.74664100
6	2.37674100	2.19808400	0.81821600	8	-0.11146500	1.93472700	-0.91670200	1	-2.65124700	-1.99917700	-1.16773600
26	-0.74501200	-0.06424400	-0.60968500	1	0.85565200	0.80466600	-3.09186600	1	-3.77810400	-1.07454800	0.85320400
6	-2.87628900	-2.09315500	-1.18072000	8	-1.34263000	2.08094900	-1.93357000	1	-1.98921200	-2.27136000	-2.25292500
6	-2.43130200	2.66943700	-0.42855000	1	-1.05712600	2.89495000	-2.39649000	1	-2.11554300	-0.51056000	2.49749100
1	-2.90616800	-0.89347700	1.86582500	1	-2.45896900	2.48031000	-1.08605400	1	-0.00988600	-3.18370700	1.38392800
1	-4.17253100	-1.31912500	0.73641600	8	-3.16551100	2.75803800	-0.34491600	1	1.33397700	-2.11997000	0.92252000
1	-4.10119200	1.13984400	1.22960600	1	-3.66522300	1.96010200	-0.09437800	1	-1.09136600	-2.73764100	-0.21764100
1	-3.94027100	0.73217900	-0.48965400	1	-2.53389400	3.01269300	0.41866700	1	0.60579700	-3.04297900	-1.14487200
1	-2.20918600	2.30813800	2.29496300	8	-4.47128200	0.56214100	0.14509300	1	-2.46588900	0.89407000	-2.10961500
1	-0.72896300	2.52628000	1.34429100	1	-4.17752800	-0.03511600	-0.56961600	1	-3.45841700	-0.53372400	-1.86608600
1	-0.33015000	0.09465700	2.91002200	1	-2.87653000	0.07853000	-0.19253000	1	-3.98618200	0.48169100	-0.21505000
1	-0.14765200	0.10319200	3.05724600	1	-1.11665100	3.30133200	1.12473300	1	-1.67734700	-1.96043200	-2.50046800
1	-0.83522000	-3.00722900	0.00390800	1	-0.64431900	0.73269800	0.39388600	1	1.48733300	-1.66475700	-2.52538300
1	-2.11071700	-3.13327300	1.22568100	1	-0.92775000	4.23229000	0.91432200	1	2.02420400	1.49800600	1.76800200
1	-0.44571700	-2.94516200	1.35124800	1	-0.92775000	4.23229000	0.91432200	1	4.50435300	1.18929200	-0.21472000
1	-0.92711200	-1.81776000	2.76319300	I_{2m}(OH)(G) = -2487.545604				1	5.45611600	-0.19372600	-0.21935500
1	1.71149900	0.06214100	2.32672600					1	3.88004100	-1.16523900	-1.91776800
1	0.16775800	3.25264600	-2.29826400					1	-3.19711400	1.26419800	1.34306600
1	4.80514200	-1.82421300	-1.85930600					1	-2.79456400	-2.15696600	-0.21174600
1	3.23206100	4.07938500	0.18108500	7	2.53427600	1.00333400	0.13252100	1	-4.21718000	1.07001200	-0.10372100
1	2.95786500	2.11601900	1.73192000	6	3.20310600	-1.37609700	-0.22086400	1	-0.12315400	0.05619300	3.22202700
1	-3.50587800	-1.37036600	-1.70015400	6	1.78188300	-1.17743600	-0.31545100	1	0.16661900	-1.69580800	3.40740200
1	-1.28167100	-2.46711000	-1.87145600	1	-1.87145600	-1.87145600	-1.87145600	1	-0.48169100	-0.21505000	-0.77185700
1	-3.51311600	-2.91812100	-0.81646500	6	1.23885300	-0.23750800	0.91822900	1	0.98377700	0.02290000	-2.70117700
1	-2.86002300	2.40543100	-1.39900800	7	0.49936000	-0.07889500	1.66782800	8	-0.43032300	1.79735700	-1.05252000
1	-3.12619000	3.34393200	0.09926300	6	2.07937300	1.84897600	1.24978900	8	-0.35814900	1.70262100	-1.18160100
1	-1.48728000	3.11640400	-0.59396000	6	1.20948200	1.07712900	2.27182900	1	-1.23601800	-1.76083200	-0.20509400
1	1.38464400	-0.88033700	0.81010300	6	-0.88033700	-0.88033700	-0.88033700	8	-0.43144900	-2.39505200	-0.04828200
1	-1.27392100	0.86797800	-2.43192100	6	-1.63913000	-0.98659400	0.91411300	1	-1.35384000	3.52163300	-0.81268200
8	0.60869900	-1.68705100	-1.18912400	7	-1.23039700	-0.88732300	-0.37015700	1	-0.51397500	2.61654300	0.92342600
8	-2.01552600	-2.69792200	-2.69792200	6	-1.81983400	-1.66729500	-1.29329900	1	0.50886900	1.94329900	-1.56230200
1	-1.59691000	-1.17145000	-1.79729200	6	-2.62862300	-1.93477600	-1.24677000				
1	1.80366900	-1.82289100	-2.70355100	6	-3.22758700	-2.70176900	0.35025500	I_{2m}(OH)_{2m}(G) = -2258.607874			
1	3.05137600	-1.50012300	-1.14172400	6	-2.61641700	-1.89530400	1.31378400				
1	3.79549500	-1.95495500	-0.52322700	26	0.63948000	1.04954600	-0.75152300				
1	1.38464400	-1.27605100	0.13240500	6	-3.98596200	-3.41414400	-0.89245600	7	2.32706800	0.08770700	0.11491300
1	3.12429200	-2.67295000	-0.08312200	6	1.63375500	-2.76304300	-1.39624000	6	2.65637600	-1.36534600	-0.03679000
1	4.54301700	-0.21447200	1.23189500	1	3.31600600	-0.24704000	1.64184800	6	1.78666500	-1.94770600	-1.36141400
1	4.32714200	0.63517800	0.80684600	1	4.49062600	2.01659700	0.43638300	7	0.34982500	-1.56770200	-0.96724900
1	0.81670000	-0.31670000	0.79459000	1	3.81222400	-2.11783700	0.20663200	6	-0.36572700	-2.39505200	-0.04820200
8	1.86480700	-3.49185300	-0.20975000	1	3.94516100	-1.19328600	-1.19328600	6	-0.00988600	-3.99416400	-0.82628200
1	1.28100700	-2.83546600	-0.32186600	1	1.88349500	-3.20218000	1.25780800	7	0.13806200	-0.48348000	1.58088300
1	1.92124900	-4.28172000	-0.35589300	1	0.26868400	-2.80327200	0.65349100	6	2.45362200	1.52036200	1.53536300
				1	2.00469000	1.78117500	2.59063000	6	1.33662400	-1.10209300	2.41554600
				1	1.86863000	-1.86863000	-1.86863000	6	-1.13539300	0.98634000	2.10276100
				1	1.49089700	2.65536700	0.80496600	6	-2.15618500	0.13205000	0.99421100
				1	2.93323000	2.30657800	1.77452400	1	-1.63956600	0.37393000	-0.23737800
				1	0.48242000	1.78117500	2.66463200	6	-2.48345600	0.50585800	-0.40333700
				1	1.42644700	-1.94767000	0.63425600	6	-3.86277900	-3.86277900	-3.86277900
				1	-1.23024000	-0.29841000	2.91056600	6	-4.39085000	0.09676000	0.11942000
				1	-1.45203600	-0.55544000	-2.30848100	6	-3.52056600	-0.02710900	1.20212900
				1	-3.72733000	-3.18125600	-1.76575100	26	0.32758900	0.32355000	-0.26015500
				1	-2.98592000	-0.95989200	0.63425600	6	3.24651200	-2.86592000	-0.72415700
				1	-2.98867900	-1.95825000	2.36252800	6	-0.31964100	-1.79742100	-2.22772400
				1	3.51047800	1.18043000	-1.71919000	1	2.51032000	-1.87030000	0.91493200
				1	2.46405900	2.55528400	-1.28245300	1	3.71411100	-1.48781200	-0.29599900
				1	4.06195000	4.06195000	4.06195000	1	1.88649400	-1.38649400	-1.38649400
				1	2.03108600	-2.35112300	-2.32631000	1	2.10539900	-1.52135000	-2.09192300
				1	2.16984100	-3.69720200	-1.16017600	1	-0.14443700	-3.45861800	-0.14443700
				1	0.57121400	-2.98823500	-1.53369600	1	-1.43311400	-2.24059800	-1.12034700
				1	-1.30732000	-1.30732000	-1.30732000	1	-2.35320000	-2.35320000	-2.35320000
				8	0.88187300	-0.03071100	-2.69672100	1	-1.92483000	-2.48236000	2.15476100
				8	-0.08767200	2.08463300	-0.93340500	1	2.38846800	1.02821100	1.54092000
				1	0.62949100	0.83033500	-1.06495300	1	3.43990000	0.23211600	1.92850500
				1	-1.32544000	-1.32544000	-1.32544000	1	1.03396600	-1.03396600	-1.03396600
				1	-1.02198700	2.95577200	-2.39398800	1	1.70194600	-0.97907000	2.95293000
				1	-2.47466900	2.47466900	-1.04891300	1	-1.50363000	-0.45673100	2.97302800
				6	-3.16255700	2.79135500	-0.31373700	1	-2.02273900	0.70267200	-2.23841400
				1	-0.80080800	-0.80080800	-0.80080800	6	3.49710300	-4.50049700	-1.17917200
				1	-2.52167200	2.98613300	0.45608900	1	5.46078500	-0.02215300	0.05298200
				1	-4.45783200	0.54328200	0.14642200				

1	-2.046221000	3.468896000	-0.928580000	1	-0.529954000	0.880490000	3.138598000	1	-0.379169000	-2.515150000	2.863084000
1	-0.106527000	3.129667000	0.729559000	1	-0.007282000	-0.898331000	3.831450000	1	-2.256646000	-0.104837000	-2.874279000
IM₀₂(OH)₂₀ (G = -2258.670524)											
7	-2.293153000	-0.496621000	-0.169788000	1	-0.537611000	2.560300000	-1.589056000	1	2.282015000	-1.817003000	-1.732361000
6	-2.294547000	-1.232576000	-1.117023000	1	-0.723205000	1.796370000	-2.153457000	1	2.935499000	-0.973045000	-0.297594000
6	-1.614612000	-0.739480000	2.189465000	8	-1.151744000	3.737161000	-0.562373000	1	3.029341000	-2.760240000	-0.412244000
6	-0.227566000	-0.591062000	1.709283000	6	-2.285526000	0.948046000	-1.797923000	1	-4.265287000	3.605524000	0.475925000
6	-1.455447000	-0.189376000	1.351296000	8	-0.227498000	1.626858000	-1.179719000	1	-3.651500000	1.951948000	-1.821562000
6	0.086329000	-2.419149000	0.006930000	8	-0.537611000	2.560300000	-1.589056000	1	2.282015000	-1.817003000	-1.732361000
7	0.062192000	-1.131889000	-1.013978000	8	-0.942685000	2.148016000	0.948046000	1	-4.265287000	3.605524000	0.475925000
6	-2.411819000	-1.398170000	-1.364308000	8	-0.227498000	1.626858000	-1.179719000	1	-3.651500000	1.951948000	-1.821562000
-1.024489000	-1.529711000	-2.048342000	-0.048342000	8	-0.537611000	2.560300000	-1.589056000	1	2.282015000	-1.817003000	-1.732361000
6	1.371013000	-1.190614000	-1.718817000	7	-2.389837000	-0.407567000	-0.319079000	1	1.768356000	0.793827000	-1.721437000
6	2.356247000	-0.428155000	-0.880480000	6	-2.636236000	-1.249716000	0.805040000	8	3.279128000	-1.212949000	-1.906488000
7	1.814571000	0.536076000	-0.113209000	6	-1.897478000	-0.684731000	2.093241000	1	3.758987000	0.371505000	-1.825814000
6	2.609478000	0.599409000	0.599409000	7	-0.473106000	-0.349177000	0.819844000	1	1.587645000	1.750934000	-1.123017000
6	3.993368000	1.226537000	0.579153000	6	0.430282000	-1.526502000	1.780801000	8	3.978475000	2.714680000	0.238584000
4	4.560311000	0.211564000	-0.195893000	6	0.268588000	-2.410195000	0.537635000	1	3.051561000	3.037479000	0.243371000
6	3.731069000	-0.628977000	-0.939049000	7	0.041559000	-1.638367000	-0.721675000	1	3.948327000	1.963752000	0.806059000
6	-3.404131000	-0.581572000	-0.304497000	6	-2.283308000	-1.189792000	-1.570442000	1	0.868209000	-2.208560000	-2.522947000
6	0.529005000	0.064911000	2.812190000	6	-1.090885000	-2.165822000	-1.539736000	8	1.259752000	3.163388000	-0.120050000
1	-2.474262000	-2.362269000	0.961420000	6	1.287287000	-1.520705000	-1.511471000	1	1.339960000	3.019967000	-1.078520000
1	-2.191741000	-1.689710000	0.961420000	6	2.280656000	-0.645201000	-0.792233000	1	1.162356000	2.242574000	2.242574000
1	-1.643058000	-1.426077000	3.041698000	6	1.758274000	0.649891000	-0.201119000	1	3.655190000	0.443708000	-1.814316000
1	-1.945003000	0.253049000	2.531941000	6	2.563716000	1.298540000	0.459846000	1	3.558050000	0.795896000	2.715207000
1	0.204675000	-2.621844000	2.156136000	6	4.483494000	-0.303557000	-0.054956000	1	3.558050000	0.795896000	2.715207000
26	-0.250010000	-1.638971000	1.422167000	6	3.443810000	-0.048342000	-0.731402000	1	2.729376000	0.422661000	1.474490000
1	-0.828282000	-2.908697000	0.005756000	26	-0.418541000	0.583881000	-0.177258000	1	2.729376000	0.422661000	1.474490000
1	0.820988000	-0.3170589000	-0.297249000	6	-3.421803000	0.639903000	-0.449571000	1	2.729376000	0.422661000	1.474490000
1	-3.029225000	-0.969838000	-2.112487000	6	0.007295000	0.597666000	2.836973000	7	2.3882629000	1.081166000	-0.095151000
1	-2.802262000	-1.073344000	-2.073344000	6	-2.357920000	-2.357920000	0.673338000	6	3.476106000	0.095078000	0.167575000
1	-0.899860000	-0.766666000	-2.780140000	1	-3.710219000	-1.277917000	1.103487000	6	3.170746000	-1.193743000	-0.573831000
1	-0.900443000	-2.520118000	-1.367760000	1	-1.967776000	-1.387399000	2.935303000	6	1.756443000	-1.656435000	-0.123399000
1	1.745915000	-2.180556000	-1.993801000	1	-2.384907000	-0.245256000	2.387203000	6	1.507196000	-2.292419000	0.932826000
1	2.118020000	-1.608976000	3.704849000	1	0.275119000	-2.444350000	2.676639000	7	1.409476000	-1.274150000	2.058006000
1	4.607131000	-1.900182000	1.166542000	1	1.449236000	-1.135810000	1.817884000	6	0.638820000	-0.050555000	1.618884000
1	5.636943000	-0.074942000	-0.220564000	1	-0.550514000	-3.106841000	0.684913000	6	2.135353000	-1.825477000	-1.625868000
4	4.131833000	-1.425771000	-1.556327000	1	1.175983000	-0.319672000	0.440838000	6	1.265081000	1.199737000	2.172868000
1	-2.346141000	0.946651000	-1.541404000	1	-0.761499000	-2.330353000	-2.569340000	6	-0.795042000	-1.094383000	2.007170000
1	-1.364038000	1.184892000	-1.182323000	1	-1.401091000	-3.139096000	-1.150827000	6	-1.492429000	-1.091380000	1.021507000
1	-4.402817000	0.042888000	-0.416488000	1	-1.272980000	-0.446214000	-0.721414000	6	1.265081000	1.199737000	2.172868000
0	0.088672000	1.041516000	3.014889000	1	-2.083438000	2.154263000	0.922845000	6	-1.691279000	-1.660674000	-1.223098000
1	0.454390000	0.176783000	2.535157000	1	4.522997000	1.798525000	1.103073000	6	-2.753044000	-2.520922000	-0.938262000
1	1.176819000	-0.761872000	-2.637890000	1	5.549262000	-0.232506000	0.005613000	26	-3.170778000	-2.680798000	0.368374000
1	1.199124000	-0.619571000	-2.637890000	1	0.549262000	-0.232506000	0.005613000	6	1.649466000	-2.636531000	-1.442042000
8	-0.897577000	-0.896376000	0.688985000	1	3.480474000	1.202666000	0.486037000	6	3.569398000	0.926353000	1.239863000
8	-0.897577000	-0.896376000	0.688985000	1	-3.141584000	1.320408000	-1.260373000	6	1.469466000	-2.636531000	-1.442042000
1	-2.814568000	-0.315966000	-0.803261000	1	-4.402817000	1.193601000	-0.667436000	1	4.436953000	0.497841000	-1.735670000
1	0.259669000	1.541714000	-2.120096000	1	-0.626911000	-0.626911000	3.904859000	1	3.861765000	-1.993253000	-0.278475000
1	-1.863292000	3.609655000	-0.859592000	1	1.034727000	0.866533000	2.655173000	1	3.289319000	-1.019094000	-1.645923000
1	-1.513811000	2.888975000	-1.434565000	1	1.031965000	-1.043254000	-2.464617000	1	2.924799000	-2.924799000	-1.151398000
1	-1.282440000	2.632965000	0.406805000	1	-0.824710000	-0.824710000	-2.446214000	1	0.559193000	-2.827084000	0.842111000
TS₀₁(OH)₂₀ (G = -2258.641631)											
7	-2.348818000	-0.396472000	-0.249660000	1	-0.498065000	1.254515000	-1.984362000	1	0.914693000	-1.728240000	2.922640000
6	-2.348818000	-0.396472000	-0.249660000	1	0.638861000	1.471266000	-2.503943000	1	3.089118000	2.249890000	1.537905000
6	-2.348818000	-0.396472000	-0.249660000	1	-1.111791000	-0.845980000	-1.214214000	1	0.466022000	1.878050000	1.427848000
6	-0.348174000	-0.445423000	1.797341000	1	-2.057845000	3.330709000	-0.791837000	1	1.845348000	0.951549000	3.065494000
6	0.348174000	-1.674245000	1.617979000	1	-0.077031000	2.882737000	0.899740000	1	-0.8970000	-0.565813000	-1.239863000
6	0.317644000	-2.426267000	0.307030000	1	1.034727000	0.866533000	2.655173000	1	3.289319000	-1.019094000	-1.645923000
7	0.056289000	-1.522543000	-0.865399000	1	1.031965000	-1.043254000	-2.464617000	1	-3.982736000	-3.357507000	0.615270000
6	2.284972000	-0.523907000	-0.892906000	7	-2.2213396000	-0.611370000	-0.240479000	1	-0.914693000	-1.728240000	2.922640000
6	1.746607000	-1.335023000	-1.659522000	6	-2.464165000	-1.285748000	1.075850000	1	1.899461000	2.551702000	-1.520356000
6	1.335234000	-1.318120000	0.520806000	6	-0.320775000	-0.155430000	1.814173000	1	3.600894000	2.603402000	-0.953773000
6	3.914490000	1.151200000	0.564952000	6	0.651923000	-2.709430000	1.883450000	1	-1.582520000	-2.169732000	-1.459732000
6	4.480634000	-0.093061000	-0.149349000	6	0.488212000	-3.228152000	0.795822000	1	0.449876000	-3.080800000	-3.311430000
6	3.655515000	-0.765688000	-0.888425000	6	-2.199484000	-1.560649000	-1.368436000	1	-1.260754000	-1.912060000	1.951168000
26	-0.392158000	0.651220000	-0.250075000	6	-0.942637000	-2.449113000	-1.249382000	1	-0.213522000	1.663449000	-0.359467000
6	-3.393846000	0.653122000	-0.250075000	6	1.381782000	-1.631094000	-1.389979000	1	-0.109543000	0.818867000	-2.534621000
6	0.186643000	0.327841000	2.911626000	6	-2.249638000	-2.328429000	0.601310000	6	-1.115953000	2.016975000	-1.833063000
1	-2.249638000	-2.328429000	0.601310000	6	-1.374133000	1.153714000	-0.438958000	8	-0.622304000	-6.223040000	2.831464000
26	-1.791293000	-1.598289000	2.909476000	7	1.738661000	0.560344000	-0.438958000	1	-2.373878000	2.443439000	-2.029382000
1	-2.231571000	-0.07036000	2.488549000	6	3.684267000	1.390824000	0.295765000	8	-3.205655000	2.729049000	-0.627861000
1	0.402205000	-2.37842000	2.459214000	6	4.480634000	-0.093061000	-0.149349000	1	-3.696969000	1.852228000	-0.426730000
1	-1.566241000	-1.300398000	1.639728000	6	3.884110000	-0.818271000	-0.647240000	1	-2.996574000	-2.742219000	-2.232479000
1	-0.511024000	-1.322362000	0.412709000	26	-0.411826000	0.514867000	-0.282713000	1	1.363006000	0.357760000	-2.843679000
1	1.208397000	-0.325966000	0.107130000	6	-3.407682000	0.348761000	-0.472916000				

1	-0.927413000	2.791472000	-0.049162000	1	-3.764651000	-2.087667000	0.127052000	1	-2.279799000	3.046157000	-0.893677000				
1	-1.340533000	4.306086000	-0.048533000	1	-3.337106000	-0.380510000	1.444646000	8	-3.070297000	3.081210000	-0.221200000				
$I_{\alpha}(O)(OH_2)(G = -2488.075312)$															
7	1.1657539000	-1.664160000	0.098741000	1	-1.378775000	2.298334000	-1.096029000	1	-3.689871000	0.193080000	-0.998168000				
6	1.191103000	-3.061690000	-0.228406000	1	-2.929026000	2.155827000	-1.861777000	1	-3.713032000	0.270517000	-0.5705182000				
6	0.097497000	-3.012224000	-1.275727000	1	-0.582792000	1.534150000	-2.995780000	1	-1.531492000	2.652786000	1.803669000				
6	-0.930310000	-1.969035000	-0.955881000	1	-2.006092000	1.446080000	-3.197744000	1	-0.984068000	2.626073000	-0.828263000				
6	-1.867747000	-2.165963000	0.140879000	1	1.161367000	-0.673650000	-3.013650000	1	-1.039786000	3.497326000	2.4627364000				
6	-1.242758000	-2.195127000	1.514282000	1	1.313245000	-1.129600000	2.349797000								
6	-0.437779000	-0.914874000	1.589625000	1	3.294272000	-2.633727000	2.097306000	$I_{\alpha}(O)(OH_2)(G = -2488.011044)$							
6	2.007469000	-1.546340000	1.558043000	1	4.118035000	-0.187840000	-0.223809000	7	2.566221000	0.906353000	0.262293000				
6	0.799660000	-1.144545000	2.423564000	1	2.968709000	-2.063001000	-2.174000000	6	3.463845000	-0.249581000	0.498688000				
6	-1.284505000	0.209977000	2.106359000	1	-3.224945000	-0.100106000	1.717827000	6	3.463845000	-0.249581000	0.498688000				
6	-2.099937000	0.790952000	0.989676000	1	-2.217009000	2.718797000	1.063859000	6	3.463845000	-0.249581000	0.498688000				
7	-1.520784000	0.701850000	-0.230463000	1	-1.613019000	-1.948378000	2.458496000	6	3.463845000	-0.249581000	0.498688000				
6	-2.081590000	-1.338916000	-1.284097000	1	-1.613019000	-1.948378000	2.458496000	6	3.463845000	-0.249581000	0.498688000				
6	-3.267245000	2.051203000	-1.156044000	1	-2.061360000	-3.406313000	1.521575000	6	1.200714000	-2.501625000	0.590560000				
6	-3.891355000	2.013360000	0.092347000	1	-0.373795000	-8.294930000	1.536921000	6	1.084728000	-1.704775000	1.894699000				
6	-3.201431000	1.461196000	1.180851000	1	-0.865184000	0.209225000	3.467094000	7	0.552195000	-0.321386000	1.710061000				
26	-1.156199000	-0.322275000	-0.212976000	8	-0.865184000	0.209225000	3.467094000	6	2.173737000	-1.604000000	1.502870000				
6	2.863566000	-1.347646000	-0.715610000	8	0.002899000	1.812738000	1.010923000	6	1.335130000	0.711294000	2.446068000				
6	-1.742567000	-1.765287000	-2.185759000	1	-0.091029000	0.521148000	2.959529000	6	-0.893132000	-0.281309000	2.018028000				
1	0.855716000	-3.551581000	0.681537000	1	1.162961000	1.497954000	1.954545000	6	-1.661685000	-1.050313000	0.971133000				
1	2.040643000	-3.638436000	-0.602649000	1	0.972095000	2.418070000	2.567290000	1	1.586248000	-0.273561000	1.314281000				
1	-0.388152000	-3.988980000	-1.380721000	1	2.468356000	2.193970000	1.370000000	7	-1.926780000	-1.439705000	-1.301689000				
1	0.532179000	-2.322770000	-2.239120000	8	3.106172000	2.611855000	0.459372000	6	-2.983897000	-2.320139000	-1.076794000				
1	-2.187166000	-3.023919000	-0.004012000	1	3.650181000	2.220328000	-0.278177000	6	-3.365215000	-2.579534000	0.241396000				
1	-2.744566000	-1.721702000	0.054819000	1	2.442031000	2.910682000	-0.278177000	6	-2.692028000	-1.974571000	1.532412000				
1	-0.588843000	-3.023261000	1.768428000	1	-1.568420000	0.197923000	2.796255000	26	0.616319000	0.236849000	-0.567127000				
1	-2.026318000	-2.161847000	2.275974000	8	4.451184000	0.728276000	-0.674328000	6	3.181060000	1.838730000	-0.697436000				
1	-2.785590000	-0.781231000	1.641042000	1	-4.232026000	-2.459295000	-0.410126000	6	1.474955000	-2.516740000	-1.874931000				
1	-2.428157000	-3.893525000	-0.825970000	1	3.987655000	0.632445000	-1.525912000	6	0.650440000	-1.957865000	-2.457162000				
1	1.037801000	-0.159976000	2.892639000	1	1.128146000	3.058306000	-1.077085000	4	4.513142000	0.045563000	0.316181000				
1	0.578506000	-1.841102000	3.211192000	1	0.612323000	2.594606000	-0.349957000	1	-2.739078000	-0.216891000	-0.104877000				
1	-1.900480000	-0.124623000	2.944985000	1	0.843729000	3.987193000	-1.017531000	1	3.451917000	-1.067614000	-0.1478327000				
1	-1.558100000	-0.322275000	-0.212976000	$I_{\alpha}(O)(OH_2)(G = -2488.075554)$											
1	-3.691643000	2.544081000	-2.023279000	7	-1.632091000	-1.750577000	-0.350736000	1	0.428375000	-2.267692000	2.351744000				
1	-4.826141000	2.640634000	0.217121000	1	-1.763969000	-1.249456000	-0.523310000	1	1.580624000	-2.466348000	1.194099000				
1	-3.747298000	1.486834000	2.168923000	7	-1.118858000	-3.104423000	0.031087000	1	3.059401000	1.976411000	2.046188000				
1	2.444448000	-1.763969000	-0.602649000	6	-0.269622000	-2.994953000	1.283717000	1	0.652090000	1.362590000	2.996717000				
1	3.124920000	-0.300673000	-0.562297000	6	-0.761676000	-1.905743000	1.191495000	1	1.977607000	0.220580000	3.186139000				
1	3.689567000	-1.994403000	-2.994075000	6	-2.474441000	-0.944146000	-0.410126000	1	-1.045860000	-1.957865000	-2.457162000				
1	-1.104765000	-1.409183000	-2.995342000	6	1.652430000	-2.232727000	-1.566670000	1	-1.573961000	-1.229219000	-0.205243000				
1	-2.198043000	-0.042077000	-0.596582000	6	-0.728487000	-1.115728000	-1.546256000	1	-3.479371000	-2.799142000	-1.914354000				
8	0.577498000	0.194746000	-2.085896000	6	-1.737315000	-1.584410000	-1.821050000	1	-4.171395000	-3.273960000	0.456983000				
1	-2.198043000	0.420077000	-0.596582000	6	0.420077000	-1.429565000	0.225916000	1	-2.952147000	-2.110693000	-0.840556000				
1	1.130973500	0.419070000	-2.034710000	6	1.486594000	0.04670000	-2.066218000	1	3.391291000	1.303313000	-1.629786000				
8	2.475054000	1.935547000	-2.209030000	6	2.202075000	0.757774000	-0.948846000	1	2.482905000	2.652613000	-0.904827000				
1	2.349790000	1.422431000	-1.956083000	7	1.578050000	0.749936000	0.244950000	1	4.121997000	-2.528749000	-0.302093000				
1	2.424615000	2.649787000	-1.498487000	6	2.077016000	1.447933000	1.281513000	1	1.823939000	-1.957865000	-2.457162000				
1	-1.191654000	-1.942466000	-0.319746000	6	3.352197000	-1.183527000	-3.487650000	1	2.008693000	-3.479441000	-1.737398000				
1	1.586967000	3.742530000	0.098945000	6	3.924616000	2.170240000	-0.061079000	1	0.403147000	-2.708690000	-1.889625000				
1	2.963894000	3.163190000	0.395421000	6	3.395073000	1.449553000	-1.130029000	1	-1.213770000	-0.764817000	1.988909000				
1	0.322680000	-0.513448000	-2.658427000	26	-0.242458000	-2.626933000	0.316153000	8	0.672800000	0.327184000	-2.840556000				
1	-0.193482000	1.492466000	-0.704101000	6	-2.950680000	-1.901892000	0.285299000	7	0.034713000	0.559250000	-0.794314000				
1	-0.608663000	3.454376000	-0.126085000	6	1.283476000	-1.167125000	2.567606000	1	0.022240000	1.061382000	-0.915030000				
1	0.227761000	2.439658000	0.666212000	1	-0.568895000	-3.527829000	-0.804724000	8	-1.023902000	2.278781000	-1.843727000				
1	3.486185000	1.606455000	1.320012000	1	-1.968926000	-3.697026000	0.225916000	1	-0.796260000	1.317894000	-2.457162000				
1	-1.893145000	-0.941392000	-1.458997000	1	-2.950680000	-1.901892000	0.285299000	1	0.347137000	0.559250000	-0.794314000				
1	2.629934000	1.270889000	1.020613000	1	-0.914693000	-2.729428000	2.125638000	8	-3.051306000	2.807333000	-0.274570000				
				1	2.307644000	-3.243613000	0.639363000	1	-3.592705000	1.948133000	-0.808601000				
				1	2.718691000	-1.521590000	0.575527000	1	-2.424724000	2.466348000	-1.194099000				
				1	1.223177000	-1.429565000	-1.470844400	1	1.532037000	0.752155000	-3.008710000				
				1	2.602384000	-2.123574000	-1.691200000	8	-4.423864000	0.671056000	0.171688000				
				1	-2.260150000	-0.642767000	-1.991087000	1	-4.223717000	0.062377000	-0.559474000				
				1	-2.338871000	-2.402308000	-2.235061000	1	-3.999410000	0.243470000	0.939600000				
				1	-0.388341000	-0.988341000	-3.487650000	8	-1.133786000	-0.943766000	-1.937666000				
				1	-0.092295000	-2.548657000	-2.877240000	1	-0.590613000	2.702391000	0.601055000				
				1	-0.624583000	-0.261027000	-2.847200000	1	-0.897847000	3.985553000	1.456197000				
				1	1.511073000	1.401835000	2.050190000								
				1	3.430130000	3.430130000	-2.470837000								
				1	4.851434000	2.723995000	-0.181676000	$H_{2O}(G = -281.005305)$	1	0.000000000	0.135290000	0.000000000			
				1	3.884971000	1.421815000	-2.097286000	7	0.000000000	0.135290000	0.000000000				
				1	-2.852393000	-1.606022000	1.368236000	1	-0.223016000	-1.229261000	0.000000000				
				1	-3.281321000	-0.328132000	0.000000000	8	-0.016714000	0.000000000	0.000000000				
				1	-3.676218000	-2.233963000	-0.091267000	8	-1.155825000	0.518379000	0.000000000				
				1	0.461866000	1.283727000	3.240775000	1	0.671231000	-1.638074000	0.000000000				
				1	1.783903000	-2.577752000	2.919868000	1							
				1	2.001275000	3.430130000	2.518367000								
				1	0.768253000	-0.748572000	-2.498716000								
				8	-0.958610000	3.322530000	2.161001000								
				8	-2.952588000	0.916400000	-0.540873000								
				1	-1.229474000										

8	-3.804310000	0.707663000	1.358365000	1	-1.992261000	0.737984000	-0.854630000	8	-1.165340000	1.547182000	1.000804000
1	-3.332406000	1.428619000	1.833193000	1	-1.136457000	-0.922996000	-1.041212000	1	-1.146352000	0.855506000	1.510372000
1	-4.122991000	0.141121000	2.084095000	8	0.631612000	2.209287000	-0.321998000	8	-1.254629000	-0.804430000	2.130488000
$HNO_2 \cdot H_2O$ (G = -357.475332)											
8	2.407274000	-0.084381000	-0.016932000	8	1.088372000	-0.515670000	-1.363051000	8	-2.256826000	0.855359000	-1.259961000
1	2.359161000	0.625611000	-0.683125000	8	-0.591296000	-1.609513000	-0.430898000	1	-1.925045000	-0.072500000	-1.193899000
1	0.955942000	-0.625770000	-0.009917000	8	1.378995000	-1.637394000	0.488039000	8	1.050746000	1.980061000	-0.181969000
1	2.459357000	0.402334000	0.825599000	8	2.768814000	0.930109000	0.918050000	1	0.848460000	1.389633000	-0.3936215000
7	-0.842620000	0.065319000	0.000391000	1	2.471359000	0.001860000	0.871031000	1	1.801273000	1.489216000	0.250948000
8	-0.349280000	1.187517000	0.002779000	1	3.286714000	1.030337000	0.100940000	1	-1.620968000	1.269241000	-1.870567000
8	-0.010230000	-1.002713000	-0.007297000	$NO_2 \cdot H_2O$ (G = -357.465910)							
8	-2.032279000	-0.207849000	0.004539000	8	2.372219000	-0.086175000	-0.004986000	8	0.561740000	-0.447284000	-1.638462000
$HNO_2 \cdot 2H_2O$ (G = -433.93745)											
8	-2.104421000	-1.275367000	-0.336304000	1	2.397237000	0.613306000	-0.695944000	8	-1.011480000	-1.515202000	-0.561039000
1	-1.925384000	-1.216817000	-1.290862000	1	1.390763000	-0.479470000	-0.202035000	1	3.557373000	0.427854000	-0.166197000
1	-1.211339000	-1.372934000	0.047529000	1	2.465758000	0.384200000	0.852535000	8	1.036261000	-1.590306000	0.167257000
8	-1.693746000	1.333385000	0.234245000	7	-0.826016000	0.024602000	-0.002796000	8	3.026632000	0.301836000	0.638741000
8	-2.052399000	0.423014000	0.039820000	8	-0.322978000	1.168169000	-0.007950000	1	2.415981000	-0.431935000	0.393571000
1	-0.306122000	1.111393000	-0.201423000	8	-2.056668000	-0.159858000	0.021711000	1	2.415981000	-0.431935000	0.393571000
1	-1.628315000	1.354359000	1.206028000	$NO_2 \cdot H_2O(H_2O)$ (G = -433.935561)							
7	1.228633000	-0.071132000	0.061697000	8	-2.097096000	-1.189966000	-0.192439000	8	1.036261000	-1.590306000	0.167257000
8	0.533311000	-0.719282000	0.846872000	1	-1.2121307000	-1.123176000	-0.0045287000	8	0.561740000	-0.447284000	-1.638462000
8	0.682685000	0.982273000	-0.566287000	8	-1.796672000	1.264826000	0.148191000	8	1.036261000	-1.590306000	0.167257000
8	2.397562000	-0.296146000	-0.207647000	1	-2.097443000	0.254134000	-0.004167000	8	1.036261000	-1.590306000	0.167257000
$HNO_2 \cdot 3H_2O$ (G = -510.401983)											
8	-2.067821000	-0.631859000	1.253525000	1	-0.768036000	1.200712000	0.009127000	8	1.036261000	-1.590306000	0.167257000
1	-1.186933000	-0.851737000	1.549646000	1	-1.941160000	-1.460698000	1.036190000	8	1.036261000	-1.590306000	0.167257000
1	-1.982181000	-0.3182736000	-0.953216000	7	1.271520000	-0.039458000	0.016020000	8	1.036261000	-1.590306000	0.167257000
8	-1.156886000	-1.209785000	-1.222753000	8	0.574524000	-0.980677000	0.479920000	8	1.036261000	-1.590306000	0.167257000
1	-1.711630000	-1.072173000	-0.404359000	8	0.721076000	1.059679000	-0.341152000	8	1.036261000	-1.590306000	0.167257000
1	0.132772000	-1.134690000	-0.521852000	8	2.503175000	-1.156964000	-0.097045000	8	1.036261000	-1.590306000	0.167257000
8	-1.661756000	1.779168000	0.020278000	$NO_2 \cdot H_2O(H_2O)_2$ (G = -510.400734)							
1	-2.232835000	1.517765000	-0.722568000	8	-2.265330000	0.077718000	-0.667290000	8	1.036261000	-1.590306000	0.167257000
1	-0.778051000	1.469044000	-0.259741000	1	-2.112129000	0.118233000	-1.632161000	8	1.036261000	-1.590306000	0.167257000
1	-1.214997000	-0.356052000	-1.688373000	1	-1.822531000	-0.817506000	-0.324483000	8	1.036261000	-1.590306000	0.167257000
7	1.570455000	0.073548000	0.016778000	1	-1.010346000	2.037431000	0.358558000	8	1.036261000	-1.590306000	0.167257000
8	1.043860000	0.929832000	-0.698453000	1	-1.735717000	0.889094000	-0.242649000	8	1.036261000	-1.590306000	0.167257000
8	0.995569000	-1.136721000	0.099680000	1	-0.062801000	1.841853000	0.135543000	8	1.036261000	-1.590306000	0.167257000
8	2.592110000	0.218696000	0.666034000	8	-1.158722000	-2.042078000	0.190642000	8	1.036261000	-1.590306000	0.167257000
$HNO_2 \cdot 4H_2O$ (G = -586.862461)											
8	-0.124179000	2.005766000	-0.617086000	8	-1.670067000	-2.203590000	0.977351000	8	1.036261000	-1.590306000	0.167257000
1	-1.572771000	1.407099000	-0.976072000	1	-0.337447000	-1.629687000	0.561326000	8	1.036261000	-1.590306000	0.167257000
8	2.212740000	0.539974000	-1.090738000	7	1.434744000	-0.024831000	0.000808000	8	1.036261000	-1.590306000	0.167257000
1	2.629639000	1.149785000	-0.458560000	8	0.735561000	-0.294970000	1.024870000	8	1.036261000	-1.590306000	0.167257000
1	2.105874000	-0.276673000	-0.572524000	8	-1.496574000	1.175602000	-0.400052000	8	1.036261000	-1.590306000	0.167257000
1	-1.575190000	1.2201047000	-0.665320000	8	2.046474000	-0.392612000	-0.605946000	8	1.036261000	-1.590306000	0.167257000
8	0.619029000	1.199501000	1.935815000	$NO_2 \cdot H_2O(H_2O)_3$ (G = -586.869837)							
1	0.045110000	1.914783000	0.351398000	8	0.534247000	1.878385000	-0.372706000	8	1.036261000	-1.590306000	0.167257000
1	1.388635000	0.796438000	1.496419000	1	1.206020000	1.189668000	-0.745603000	8	1.036261000	-1.590306000	0.167257000
8	-2.386821000	0.613505000	-0.532646000	8	2.220298000	0.037742000	-1.096112000	8	1.036261000	-1.590306000	0.167257000
1	-2.936321000	1.104051000	0.104369000	1	3.043283000	0.324862000	-0.662533000	8	1.036261000	-1.590306000	0.167257000
1	-1.720926000	-0.424629000	0.237505000	1	1.868022000	-0.659460000	-0.495301000	8	1.036261000	-1.590306000	0.167257000
1	-0.043263000	0.484444000	1.906088000	1	-0.394624000	1.640424000	-0.751815000	8	1.036261000	-1.590306000	0.167257000
7	-0.058386000	-1.381702000	-0.012572000	8	0.328299000	1.032617000	2.070059000	8	1.036261000	-1.590306000	0.167257000
8	-1.067180000	-1.032099000	0.812956000	1	0.467251000	1.644212000	0.630214000	8	1.036261000	-1.590306000	0.167257000
8	0.972102000	-1.747043000	0.543740000	1	-0.596169000	0.113472000	1.830641000	8	1.036261000	-1.590306000	0.167257000
8	-0.232903000	-1.290133000	-1.218952000	8	-1.863701000	1.200545000	-1.119889000	8	1.036261000	-1.590306000	0.167257000
$HNO_2 \cdot 5H_2O$ (G = -663.327817)											
8	-1.886324000	1.610075000	0.539656000	8	-2.418539000	1.845421000	-0.646796000	8	1.036261000	-1.590306000	0.167257000
1	-1.793883000	0.849068000	1.165305000	1	-1.936974000	0.388484000	-0.573251000	8	1.036261000	-1.590306000	0.167257000
8	-1.658895000	-0.688633000	2.089116000	1	-0.640032000	0.945224000	2.134695000	8	1.036261000	-1.590306000	0.167257000
1	-2.597529000	-0.932435000	2.018587000	1	-0.380873000	-1.320445000	0.101792000	8	1.036261000	-1.590306000	0.167257000
1	-1.249994000	-1.166836000	1.341359000	8	-1.424091000	-0.905511000	0.678997000	8	1.036261000	-1.590306000	0.167257000
1	-0.949563000	1.894129000	0.373382000	8	0.703626000	-1.407906000	0.769386000	8	1.036261000	-1.590306000	0.167257000
8	-1.911099000	0.103079000	-1.640746000	8	-0.389236000	-1.609022000	-1.109034000	8	1.036261000	-1.590306000	0.167257000
$NO_2 \cdot H_2O(H_2O)_4$ (G = -663.334535)											

SI.3 – References

- (1) Kasapbasi, E. E.; Whangbo, M.H. *Inorg. Chem.* **2012**, *51*, 10850-10855.
- (2) Bell, R. P. (1973), *The Proton in Chemistry* (2nd ed.), Ithaca, NY: Cornell University Press.