Oxidation of olefins with H_2O_2 catalysed by salts of Group III metals (Ga, In, Sc, Y and La): epoxidation versus hydroperoxidation

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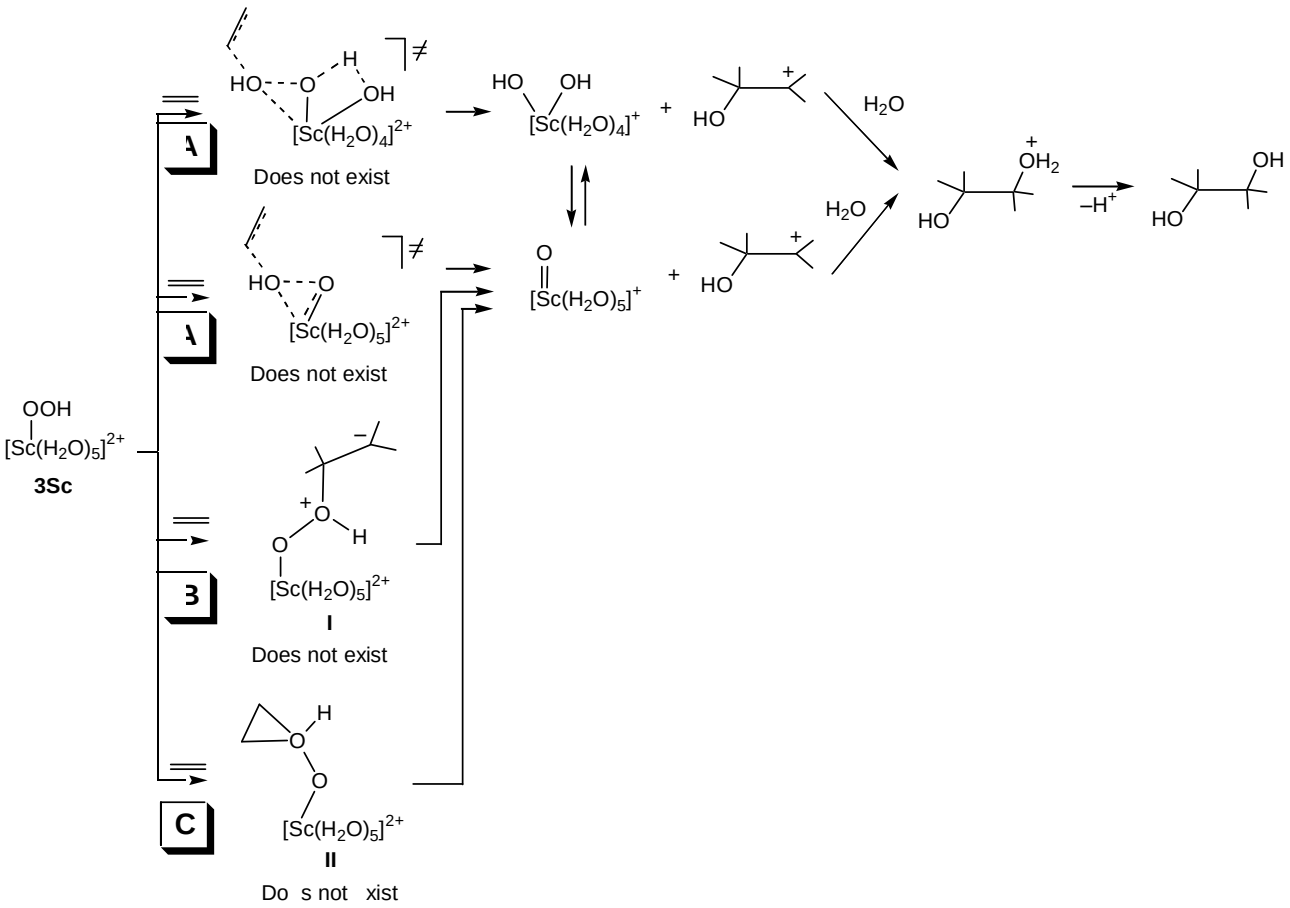
Supplementary Information

Non-radical pathways of the direct *trans*-diol formation

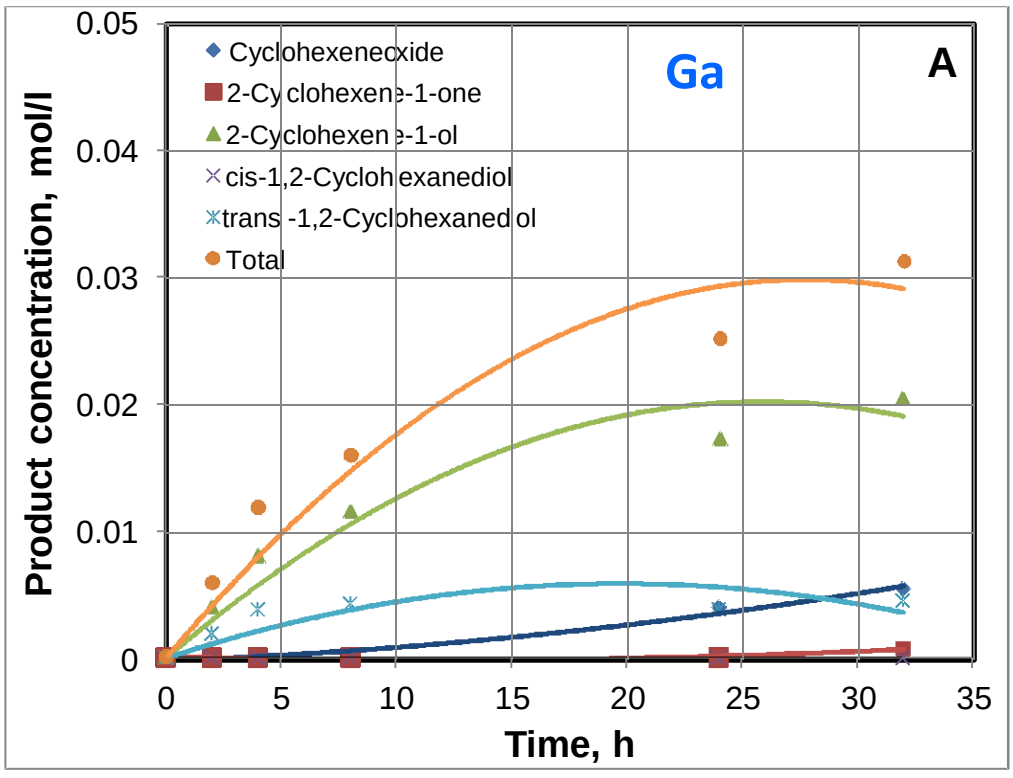
The possibility of a direct non-radical formation of *trans*-diol (*i.e.* that not including the generation of epoxide) was investigated for M = Sc. First, the concerted transfer of the OH group from **3Sc** to ethylene molecule was considered (Scheme S1A). However, no transition state for this process was located. All attempts led to **TS3Sc** of the Mechanism II (Scheme 5). Second, the stepwise mechanism of the OH group transfer via intermediate **I** (Scheme S1B) was also searched. However, all attempts to locate this intermediate (in both singlet and triplet spin states) also failed. In one of the attempts of the **I** optimization, the system $[Sc(H_2O)_5(=O)]^+ + HOCH_2CH_2^+$ was formed at the triplet spin state. Meanwhile, the calculated energy of its formation from **1Sc** and C_2H_4 is 30.5 kcal/mol what is higher than the activation energy of the epoxidation via **TS1Sc** (28.2 kcal/mol). Third, intermediate **II** of the mechanism involving the olefin addition at the O(H) atoms in **3Sc** followed by the OO and CO bond cleavages (Scheme S1C) was also not found: the geometry optimization led to $[Sc(H_2O)_5(=O)]^+$ and protonated epoxide. Thus, examined non-radical mechanisms of the direct formation of *trans*-diol may be ruled out.

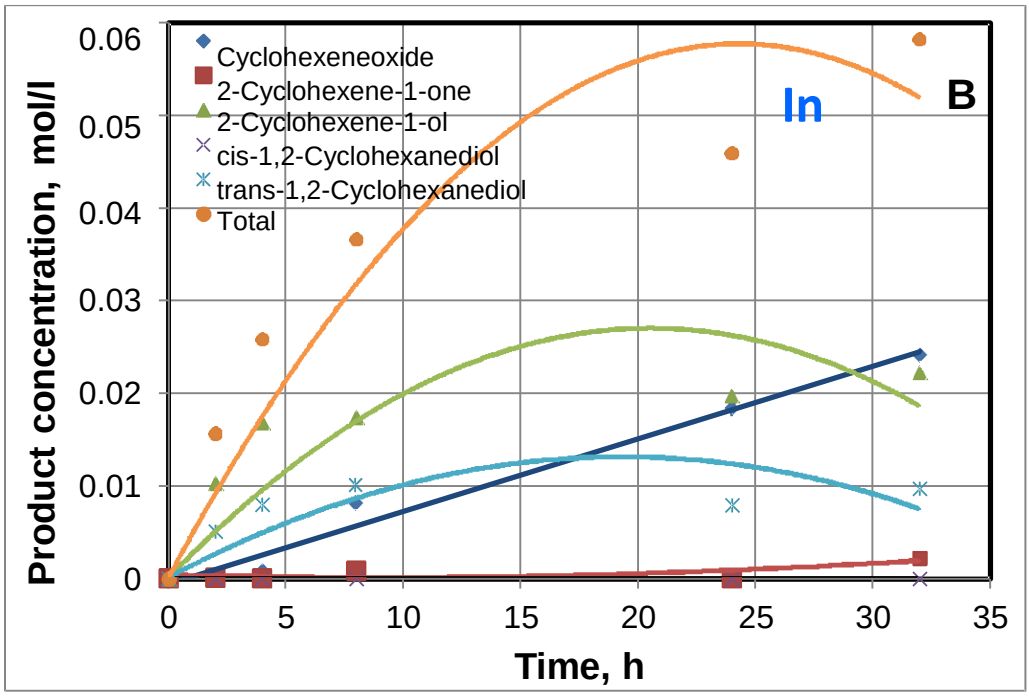
Mechanism based on the formation of the M^V species

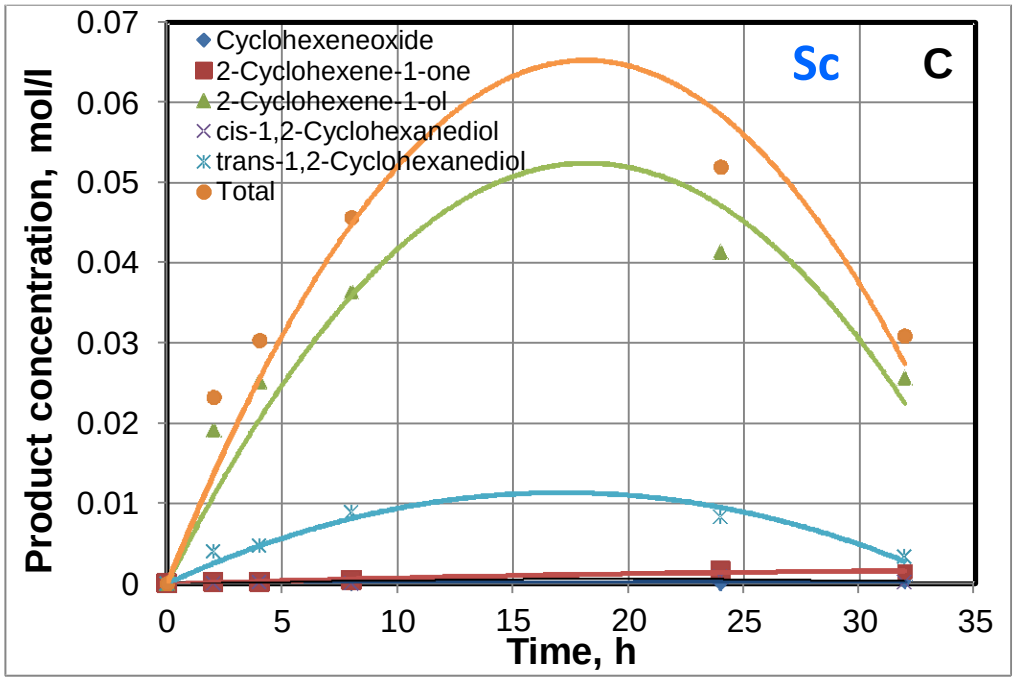
One of the popular mechanisms proposed for the hydrocarbon oxidations catalysed by iron based systems includes the formation of the Fe^V=O ferryl complexes which play the role of an oxidant. For the systems under study, attempts of the calculations of similar M^V complexes $[M(H_2O)_4(OH)(=O)](H_2O)^{2+}$ (M = Ga, Sc) were undertaken at both singlet and triplet spin states for both *trans*- and *cis*-isomeric configurations. At the singlet spin state, no minima were found for these structures, all attempts led to the M^{III} peroxo species. At the triplet spin state, the minima were found. However, analysis of the spin electron density distribution indicated that two unpaired electrons are centred at the O and OH ligands (*ca.* 1.5 and 0.5 e, respectively). Thus, the formation of these triplet complexes corresponds to the oxidation of oxygen atoms rather than that of the metal atoms. Additionally, the energy of formation of these complexes relative to the initial **1Ga** and **1Sc** complexes are 31.2–55.7 kcal/mol, and these values are higher than the overall activation barrier of both hydroperoxidation (25.1 and 27.8 kcal/mol) and epoxidation (27.1–29.6 kcal/mol). Thus, a mechanism based on the M^V species may be completely ruled out.

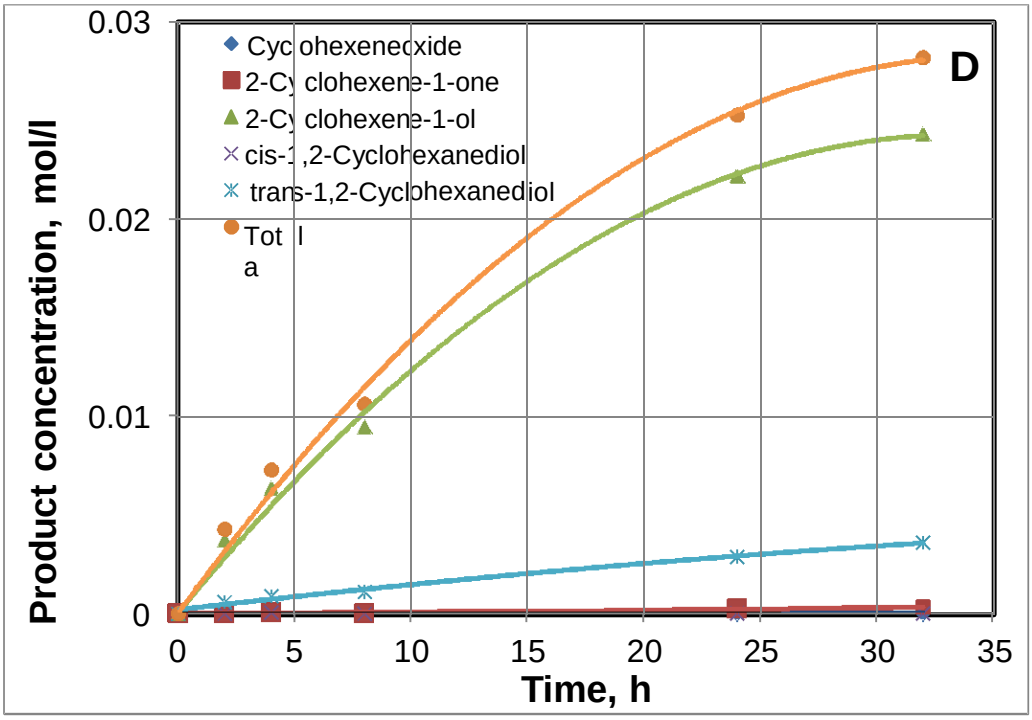


Scheme S1 Considered non-radical mechanisms of the direct *trans*-diol formation.




Product concentration, mol/l
Time, h
Cyclohexeneoxide
2-Cyclohexene-1-one
2-Cyclohexene-1-ol
cis-1,2-Cyclohexanediol
trans-1,2-Cyclohexanediol
Total
In
B
0.06
0.05
0.04
0.03
0.02
0.01
0
0
5
10
15
20
25
30
35


Product concentration, mol/l
Time, h
Cyclohexeneoxide
2-Cyclohexene-1-one
2-Cyclohexene-1-ol
cis-1,2-Cyclohexanediol
trans-1,2-Cyclohexanediol
Total
Sc
C
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
5
10
15
20
25
30
35



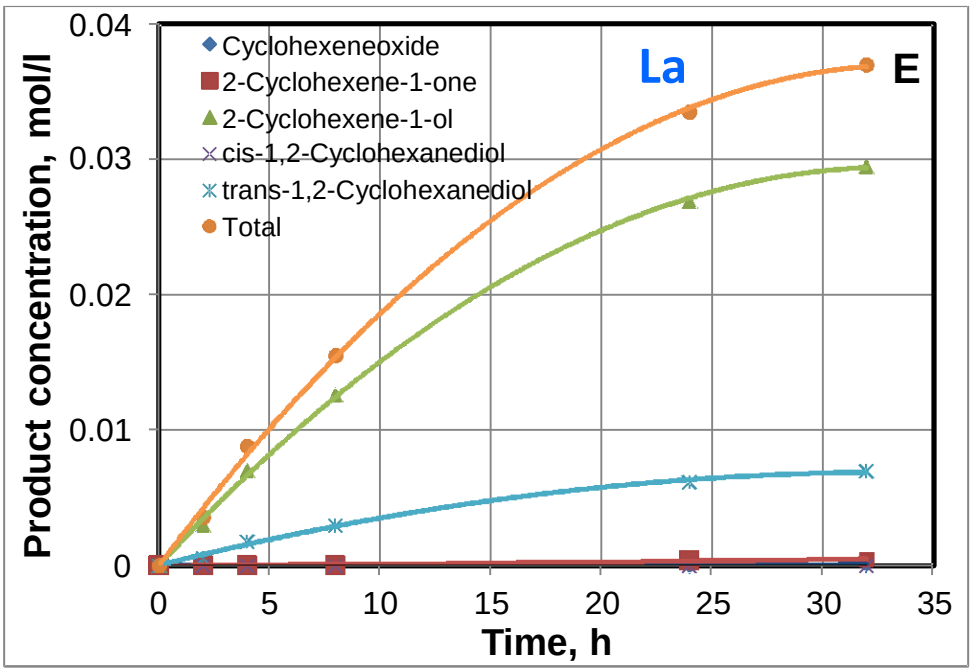


Fig. S1 Accumulation of reaction products with time in the cyclohexene (initial concentration 0.25 M) oxidation with H_2O_2 (1.2 M) catalyzed by $M(NO_3)_3$ (1.0×10^{-3} M) [M = Ga (**A**), In (**B**), Sc (**C**), Y (**D**), La (**E**)] in acetonitrile (contains H_2O, 2.3 M) at 70 °C. Concentrations of the products were measured after addition of PPh_3 to a sample of the reaction solution. The phosphine reduces remained H_2O_2 and transforms the initial product cyclohexenyl hydroperoxide into 2-cyclohexen-1-ol.

Table S1 Synchronicity of the Mechanism I based on **TS1M** and **TS2M**

TS1M	S_y	**TS2M**	S_y
TS1Ga	0.75	**TS2Ga**	0.73
TS1In	0.80	**TS2In**	0.78
TS1Sc	0.89	**TS2Sc**	0.87
TS1Y	0.85	**TS2Y**	0.88
TS1La	0.76	**TS2La**	0.84

Table S2 Calculated Gibbs free energies of activation and reaction (in kcal/mol)

Reaction	$\Delta G_s^{\neq}$	ΔG
Formation of active catalytic species		
[Ga(H O)](H O_2)$^{3+}$ (**1Ga**) [Ga(H_2O)$_5$(H O_2)](H_2O)$^{3+}$ (**2Ga**)	13.5	4.7
[In(H_2O)$_6$](H_2O_2)$^{3+}$ (**1In**) → [In(H_2O)$_5$(H O_2)](H O)$^{3+}$ (**2In**)	13.7	5.1
[Sc(H O)](H O_2)$^{3+}$ (**1Sc**) → [Sc(H_2O) (H_2O_2)](H_2O)$^{3+}$ (**2Sc**)	8.2[a]	3.4
[Y(H_2O)$_8$](H_2O)$^{3+}$ (**1Y**) [Y(H_2O)$_7$(H_2O)](H_2O)$^{3+}$ (**2Y**)	7.8[a]	2.3
[La(H_2O)$_9$](H_2O_2)$^{3+}$ (**1La**) → [La(H O) (H_2O_2)](H_2O)$^{3+}$ (**2La**)	5.3[a]	3.2
[Ga(H O) (H_2O_2)](H_2O)$^{3+}$ (**2Ga**) + H O → [Ga(H O) (OOH)](H O)$^{2+}$ (**3Ga**) + H_3O^+		0.6
[In(H_2O)$_5$(H_2O_2)](H_2O)$^{3+}$ (**2In**) + H_2O → [In(H_2O) (OOH)](H O)$^{2+}$ (**3In**) + H_3O		2.2
[Sc(H O) (H_2O_2)](H_2O)$^{3+}$ (**2Sc**) + H_2O [Sc(H_2O)$_5$(OOH)](H O)$^{2+}$ (**3Sc**) + H O$^+$		7.0
[Y(H_2O)$_7$(H O_2)](H O)$^{3+}$ (**2Y**) + H O → [Y(H_2O)$_7$(OOH)](H_2O)$^{2+}$ (**3Y**) + H_3O^+		7.3
[La(H_2O)$_8$(H_2O)](H_2O)$^{3+}$ (**2La**) + H O → [La(H_2O)$_8$(OOH)](H_2O)$^{2+}$ (**3La**) + H_3O		4.0
Mechanism I		
[Ga(H O) (OOH)]$^{2+}$ (**3Ga**) + C H_4 → [Ga(H O) (OOH)](C H)$^{2+}$ (**3Ga**•C_2H)		6.4
[Ga(H O) (OOH)](C_2H_4)$^{2+}$ (**3Ga**•C_2H) → [Ga(H O) (OH)(OC_2H_4)](H_2O)$^{2+}$ (**7Ga**), via **TS1Ga**	24.7	58.1
[Ga(H O) (OOH)]$^{2+}$ (**3Ga**) → [Ga(H_2O) (OOH)](H_2O)$^{2+}$ (**4Ga**)		4.1
[Ga(H O) (OOH)](H O)$^{2+}$ (**4Ga**) + C_2H_4 [Ga(H_2O)$_4$(OOH)](H_2O)(C_2H)$^{2+}$ (**4Ga**•C_2H_4)		4.7
[Ga(H_2O)$_4$(OOH)](H_2O)(C_2H_4)$^{2+}$ (**4Ga**•C_2H_4) → [Ga(H_2O)$_4$(OH)(OC_2H_4)](H_2O)$^{2+}$ (**7Ga**), via **TS2Ga**	14.5	–60.5
[Ga(H O) (OH)(OC_2H_4)](H_2O)$^{2+}$ (**7Ga**) + H O → [Ga(H_2O)$_5$(OH)](H_2O)$^{2+}$ (**9Ga**) + OC_2H_4		4.9
[In(H_2O)$_5$(OOH)]$^{2+}$ (**3In**) + C_2H_4 [In(H O) (OOH)](C_2H_4)$^{2+}$ (**3In**•C_2H_4)		5.6
[In(H_2O)$_5$(OOH)](C_2H_4)$^{2+}$ (**3In**•C H_4) → [In(H O)$_4$(OH)(OC_2H_4)](H O)$^{2+}$ (**7In**) via **TS1In**	21.4	57.7
[In(H_2O)$_5$(OOH)]$^{2+}$ (**3In**) [In(H O) (OOH)](H O)$^{2+}$ (**4In**)		9.1
[In(H_2O)$_4$(OOH)](H_2O)$^{2+}$ (**4In**) + C_2H_4 → [In(H_2O)$_4$(OOH)(C H_4)](H_2O)$^{2+}$ (**5In**)		6.2
[In(H_2O)$_4$(OOH)(C H_4)](H_2O)$^{2+}$ (**5In**) → [In(H_2O)$_4$(OH)(OC_2H_4)](H_2O)$^{2+}$ (**7In**), via **TS2In**	5.9	67.5
[In(H_2O)$_4$(OH)(OC H_4)](H_2O)$^{2+}$ (**7In**) + H_2O → [In(H_2O)$_5$(OH)](H_2O)$^{2+}$ (**9In**) + OC_2H		4.4
[Sc(H O) (OOH)]$^{2+}$ (**3Sc**) + C_2H → [Sc(H_2O)$_5$(OOH)](C_2H_4)$^{2+}$ (**3Sc**•C H_4)		0.6
[Sc(H O) (OOH)](C_2H_4)$^{2+}$ (**3Sc**•C_2H_4) → [Sc(H_2O)$_5$(OH)(OC_2H_4)]$^{2+}$ (**6Sc**), via **TS1Sc**	17.2	52.7
[Sc(H O) (OH)(OC_2H)]$^{2+}$ (**6Sc**) + H_2O → [Sc(H O) (OH)](H_2O)$^{2+}$ (**9Sc**) + OC H_4		6.7
[Sc(H O) (OOH)]$^{2+}$ (**3Sc**) → [Sc(H O)$_4$(OOH)](H O)$^{2+}$ (**4Sc**)		3.8
[Sc(H O) (OOH)](H_2O)$^{2+}$ (**4Sc**) + C H_4 → [Sc(H O) (OOH)(C_2H)](H_2O)$^{2+}$ (**5Sc**)		7.2
[Sc(H O) (OOH)(C_2H)](H_2O)$^{2+}$ (**5Sc**) → [Sc(H_2O)$_4$(OH)(OC_2H)](H_2O)$^{2+}$ (**7Sc**), via **TS2Sc**	9.8	65.3
[Sc(H O) (OH)(OC_2H)](H_2O)$^{2+}$ (**7Sc**) + H_2O → [Sc(H_2O)$_5$(OH)](H_2O)$^{2+}$ (**9Sc**) + OC_2H_4		4.5
[Y(H_2O)$_7$(OOH)]$^{2+}$ (**3Y**) + C H_4 → [Y(H_2O)$_7$(OOH)](C_2H_4)$^{2+}$ (**3Y**•C_2H_4)		7.9
[Y(H_2O)$_7$(OOH)](C_2H_4)$^{2+}$ (**3Y**•C_2H_4) → [Y(H_2O)$_7$(OH)(OC H_4)](H_2O)$^{2+}$ (**6Y**), via **TS1Y**	17.0	55.4
[Y(H_2O)$_7$(OH)(OC H_4)](H_2O)$^{2+}$ (**6Y**) + H_2O → [Y(H_2O)$_7$(OH)](H_2O)$^{2+}$ (**9Y**) + OC_2H_4		3.3
[Y(H_2O)$_7$(OOH)]$^{2+}$ (**3Y**) → [Y(H_2O)$_6$(OOH)](H_2O)$^{2+}$ (**4Y**)		2.6
[Y(H_2O)$_6$(OOH)](H_2O)$^{2+}$ (**4Y**) + C_2H_4 [Y(H O)$_6$(OOH)](H O)(C H_4)$^{2+}$ (**4Y**•C_2H)		5.0
[Y(H_2O)$_6$(OOH)](H_2O)(C_2H)$^{2+}$ (**4Y**•C H_4)→ [Y(H_2O)$_6$(OH)(OC H_4)](H_2O)$^{2+}$ (**7Y**), via **TS2Y**	16.2	55.1

$[La(H_2O)_8(OOH)]^{2+}$ (**3La**) + C H_4 → $[La(H_2O)_8(OOH)](C_2H_4)^{2+}$ (**3La•**C_2H_4)		8.6
$[La(H_2O)_8(OOH)](C_2H$ $)^{2+}$ (**3La•**C_2H_4) → $[La(H_2O)_8(OH)](OC_2H_4)^{2+}$ (**9La•**C H_4O), via **TS1La**	18.8	51.5
$[La(H_2O)_8(OH)](OC_2H$ $)^{2+}$ (**9La•**C_2H_4O) + H_2O $[La(H_2O)$ $(OH)](H$ $O)^{2+}$ (**9La**) + OC_2H_4		5.1
$[La(H_2O)_8(OOH)]^{2+}$ (**3La**) → $[La(H_2O)_7(OOH)](H_2O)^{2+}$ (**4La**)		2.0
$[La(H_2O)_7(OOH)](H$ $O)^{2+}$ (**4La**) + C_2H_4 → [La(H $O)$ $(OOH)](H_2O)(C_2H_4)^{2+}$ (**4La•**C_2H_4)		4.7
$[La(H_2O)_7(OOH)](H$ $O)(C$ $H_4)^{2+}$ (**4La•**C_2H) → [La(H $O)_6(OH)(OC$ $H_4)](H$ $O)$ $^{2+}$ (**8La**)	17.1	52.5
$[La(H_2O)_6(OH)(OC_2H_4)](H$ $O)$ $^{2+}$ (**8La**) + H O → $[La(H_2O)_8(OH)](H_2O)^{2+}$ (**9La**) + OC H_4		2.1
Mechanism I with cyclohexene (Cy)		
[Ga(H $O)$ $(OOH)](H$ $O)^{2+}$ (**4Ga**) + Cy **TS2Ga**	20.2	
$[In(H_2O)_4(OOH)](H_2O)^{2+}$ (**4In**) + Cy → **TS2In**	13.7	
[Sc(H $O)$ $(OOH)]^{2+}$ (**5In**) + Cy → **TS1Sc**	16.7	
$[Y(H_2O)_6(OOH)](H_2O)^{2+}$ (**4In**) + Cy → **TS2Y**	20.2	
$[La(H_2O)_7(OOH)](H$ $O)^{2+}$ (**4In**) + Cy → **TS2La**	21.9	
Mechanism II		
[Ga(H $O)$ $(OOH)]^{2+}$ (**3Ga**) + C H_4 → [Ga(H $O)$ $(OH)]^{2+}$ (**9Ga**) + C H_4O, via **TS3Ga**	34.4	50.8
$[Ga(H_2O)$ $(OOH)](H_2O)^{2+}$ (**4Ga**) + C H → $[Ga(H_2O)$ $(OH)](H_2O)^{2+}$ (**10Ga**) + C_2H_4O, via **TS4Ga**	30.1	48.9
[Ga(H $O)$ $(OH)](H_2O)^{2+}$ (**10Ga**) → $[Ga(H_2O)_5(OH)]^{2+}$ (**9Ga**)		6.1
$[In(H_2O)_5(OOH)]^{2+}$ (**3In**) + C_2H_4 $[In(H$ $O)$ $(OH)]^{2+}$ (**9In**) + C_2H_4O, via **TS3In**	38.6	49.9
$[In(H_2O)_4(OOH)](H_2O)^{2+}$ (**4In**) + C_2H_4 → $[In(H_2O)_4(OH)](H_2O)^{2+}$ (**10In**) + C_2H_4O, via **TS4In**	33.6	48.8
$[In(H_2O)_4(OH)](H_2O)^{2+}$ (**10Y**) [In(H $O)$ $(OH)]^{2+}$ (**9In**)		10.3
[Sc(H $O)$ $(OOH)]^{2+}$ (**3Sc**) + C_2H → $[Sc(H_2O)_5(OH)]^{2+}$ (**9Sc**) + C H_4O, via **TS3Sc**	28.6	53.9
[Sc(H $O)$ $(OOH)](H_2O)^{2+}$ (**4Sc**) + C H_4 → [Sc(H $O)$ $(OH)](H_2O)^{2+}$ (**10Sc**) + C_2H_4O, via **TS4Sc**	29.8	48.6
[Sc(H $O)$ $(OH)](H_2O)^{2+}$ (**10Sc**) → [Sc(H $O)$ $(OH)]^{2+}$ (**9Sc**)		9.1
$[Y(H_2O)_7(OOH)]^{2+}$ (**3Y**) + C H_4 → $[Y(H_2O)_7(OH)]^{2+}$ (**9Y**) + C_2H_4O, via **TS3Y**	42.5	47.7
$[Y(H_2O)_6(OOH)](H_2O)^{2+}$ (**4Y**) + C_2H_4 $[Y(H$ $O)_6(OH)](H_2O)^{2+}$ (**10Y**) + C_2H O, via **TS4Y**	41.2	50.8
$[Y(H_2O)_6(OH)](H_2O)^{2+}$ (**10Y**) → $[Y(H_2O)_7(OH)]^{2+}$ (**9Y**)		0.5
$[La(H_2O)_7(OOH)](H$ $O)^{2+}$ (**4La**) + C_2H_4 → [La(H $O)$ $(OH)](H_2O)^{2+}$ (**10La**) + C H_4O, via **TS4La**	40.9	48.6
Mechanism III		
[Ga(H $O)$ $(OO)](H$ $O)$ (**12Ga**) + C H_4 → [Ga(H $O)(OH)_2(C$ $H_4O)](H$ $O)$ $^{+}$ (**15Ga**), via **TS5Ga**	23.2	78.5
$[In(H_2O)_4(OO)](H_2O)$ (**12In**) + C_2H_4 $[In(H$ $O)$ $(OH)_2(C_2H_4O)](H_2O)^{+}$ (**16In**), via **TS5In**	25.4	76.3
[Sc(H $O)$ $(OO)]$ (**11Sc**) → $[Sc(H_2O)_4(OO)](H_2O)^{+}$ (**12Sc**)		2.1
$[Sc(H_2O)$ $(OO)](H_2O)^{+}$ (**12Sc**) + C_2H_4 → $[Sc(H_2O)_4(=O)(C_2H_4O)](H_2O)^{+}$ (**18Sc**), via **TS5Sc**	32.7	22.5
[Sc(H $O)$ $(=O)(C_2H_4O)](H$ $O)$ (**18Sc**) → $[Sc(H_2O)_3(OH)_2(C_2H_4O)](H_2O)^{+}$ (**16Sc**)		33.7
$[Y(H_2O)_7(OO)]^{+}$ (**11Y**) → $[Y(H_2O)_6(OO)](H$ $O)$ (**12Y**)		0.8
$[Y(H_2O)_6(OO)](H_2O)^{+}$ (**12Y**) + C H_4 → $[Y(H_2O)_4(OH)_2(C$ H $O)](H_2O)_2^{+}$ (**17Y**), via **TS5Y**	3 .8	58.1
$[La(H_2O)_7(OO)](H$ $O)$ (**12La**) → $[La(H_2O)_5(OO)](H_2O)_3^{+}$ (**13La**)		2.5
$[La(H_2O)_5(OO)](H$ $O)_3^{+}$ (**13La**) + C H_4 → $[La(H_2O)_5(=O)(C_2H_4O)](H_2O)_3^{+}$ (**19La**), via **TS5La**	30.6	30.7
$[La(H_2O)_5(=O)(C_2H$ $O)](H_2O)_3$ (**19La**) $[La(H_2O)_5(OH)_2(C$ $H_4O)](H$ $O)$ $^{+}$ (**17La**)		21.4
Mechanism IV		
$[Ga(H_2O)_3(OOH)_2](H_2O)^{+}$ (**20Ga**) + C_2H_4 $[Ga(H_2O)_3(OH)(OOH)(C_2H_4O)](H_2O)^{+}$ (**22Ga**), via **TS6Ga**	25.8	37.2
$[In(H_2O)$ $(OOH)_2](H_2O)$ (**20In**) + C_2H → $[In(H_2O)_3(OH)(OOH)(C_2H$ $O)](H_2O)^{+}$ (**22In**), via **TS6In**	18.9	53.6
$[Sc(H_2O)_3(OOH)_2](H_2O)^{+}$ (**20Sc**) + C_2H_4 $[Sc(H_2O)_3(OH)(OOH)(C$ $H_4O)](H_2O)^{+}$ (**22Sc**), via **TS6Sc**	18.6	49.0
$[Y(H_2O)$ $(OOH)_2](H_2O)$ (**20Y**) + C_2H_4 $[Y(H_2O)_5(OH)(OOH)(C$ H $O)](H_2O)^{+}$ (**22Y**), via **TS6Y**	24.2	40.1
$[La(H_2O)_6(OOH)_2](H_2O)^{+}$ (**20La**) + C_2H_4 → $[La(H$ $O)_6(OH)(OOH)(C$ H $O)](H_2O)^{+}$ (**22La**), via **TS6La**	28.0	38.1
Mimoun Mechanism		
[Ga(H $O)$ $(OOH)]^{2+}$ (**3Ga**) + C H_4 → *cis*-$[Ga(H_2O)_4(OOH)(C$ $H_4)](H_2O)^{2+}$ (**5Ga**)		11.0
cis-$[Ga(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (**5Ga**) → $[Ga(H$ $O)_3(OOH)(C$ $H_4)](H$ $O)$ $^{2+}$ (**27Ga**)		2.9
cis-$[Ga(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ (**27Ga**) → $[Ga(H_2O)_3\{CH_2CH_2OO(H)\}](H_2O)_2^{2+}$ (**24Ga**), via **TS8Ga**	23.7	18.4
[Ga(H $O)$ $\{CH_2CH_2OO(H)\}](H$ $O)$ $^{2+}$ (**24Ga**) $[Ga(H_2O)_4\{CH$ CH $OO(H)\}](H_2O)^{2+}$ (**23Ga**)		3.6
$[In(H_2O)_5(OOH)]^{2+}$ (**3In**) + C_2H_4 *cis*-$[In(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$(**5In**)		12.4

cis-[In(H_2O)$_4$(OOH)(C_2H)](H_2O)$^{2+}$ (**5In**) → [In(H_2O)$_3$(OOH)(C H_4)](H_2O)$_2^{2+}$ (**27In**)		8.9
[In(H_2O)$_3${CH_2CH_2OO(H)}](H_2O)$_2^{2+}$ (**24In**) → [In(H_2O)$_4${CH_2CH_2OO(H)}](H_2O)$^{2+}$ (**23In**)		3.5
[Sc(H O) (OOH)]$^{2+}$ + (**3Sc**) + C_2H *cis*-[Sc(H_2O)$_4$(OOH)(C_2H_4)](H_2O)$^{2+}$(**5Sc**)		12.0
cis-[Sc(H_2O) (OOH)(C H_4)](H_2O)$^{2+}$(**5Sc**) → [Sc(H O)$_4${CH_2CH_2OO(H)}](H O)$^{2+}$ (**23Sc**), via **TS7Sc**	19.7	17.0
cis-[Sc(H_2O)$_4$(OOH)(C_2H_4)](H O)$^{2+}$ (**5Sc**) [Sc(H_2O)$_3$(OOH)(C_2H_4)](H_2O)$_2^{2+}$ (**27Sc**)		6.1
cis-[Sc(H_2O) (OOH)(C_2H_4)](H_2O)$_2^{2+}$ (**27Sc**) [Sc(H_2O)$_3${CH_2CH_2OO(H)}](H_2O)$_2^{2+}$ (**24Sc**), via **TS8Sc**	18.8	17.7
[Sc(H O) {CH_2CH_2OO(H)}](H_2O)$_2^{2+}$ (**24Sc**) → [Sc(H_2O)$_4${CH CH OO(H)}](H_2O)$^{2+}$ (**23Sc**)		6.8
[Y(H_2O)$_7$(OOH)]$^{2+}$ (**3Y**) + C H_4 → [Y(H_2O)$_6$(OOH)](H_2O)(C_2H)$^{2+}$(**4Y**•C_2H_4)		6.5
[Y(H_2O) (OOH)](H_2O)(C_2H_4)$^{2+}$ (**4Y**•C H_4) [Y(H O)$_6${CH_2CH_2OO(H)}](H$_2$O)$^{2+}$ (**23Y**), via **TS7Y**	28.5	24.7
[Y(H_2O)$_6$(OOH)](H_2O)(C_2H)$^{2+}$ (**4Y**•C H_4) [Y(H_2O) (OOH)(C_2H_4)](H O) $^{2+}$ (**27Y**)		7.5
[Y(H_2O)$_5$(OOH)(C H_4)](H_2O)$_2^{2+}$ (**27Y**) → [Y(H_2O)$_5${CH CH_2OO(H)}](H O) $^{2+}$ (**24Y**), via **TS8Y**	20.4	19.6
[Y(H_2O)$_5${CH_2CH_2OO(H)}](H_2O)$_2^{2+}$ (**24Y**) [Y(H O) {CH_2CH_2OO(H)}](H O)$^{2+}$ (**23Y**)		2.5
[La(H_2O)$_8$(OOH)]$^{2+}$ (**3La**) + C H_4 → [La(H_2O)$_7$(OOH)](H_2O)(C H_4)$^{2+}$(**4La**•C_2H_4)		7.2
[La(H_2O)$_7$(OOH)](H_2O)(C_2H_4)$^{2+}$ (**4La**•C_2H_4) → [La(H_2O)$_7${CH_2CH_2OO(H)}](H_2O)$^{2+}$ (**23La**), via **TS7La**	29.2	25.3
[La(H_2O)$_7$(OOH)](H O)(C H_4)$^{2+}$ (**4La**•C_2H) → [La(H O)$_6$(OOH)(C H_4)](H O) $^{2+}$ (**27La**)		6.4
[La(H_2O) (OOH)(C H)](H_2O)$_2^{2+}$ (**27La**) → [La(H_2O)$_6${CH$_2$CH OO(H)}](H_2O)$_2^{2+}$ (**24La**), via **TS8La**	20.6	19.8
[La(H_2O)$_6${CH_2CH_2OO(H)}](H_2O)$_2^{2+}$ (**24La**) → [La(H O) {CH_2CH_2OO(H)}](H O)$^{2+}$ (**23La**)		0.8
[2+2]-Cycloaddition Mechanism		
[Ga(H O) (OOH)]$^{2+}$ (**3Ga**) + C H_4 → *cis*-[Ga(H_2O)$_4$(OOH)(C H_4)](H_2O)$^{2+}$ (**5Ga**)		13.5
cis-[Ga(H_2O)$_4$(OOH)(C H)](H O)$^{2+}$ (**5Ga**) → [Ga(H_2O)$_4${CH_2CH_2O(OH)}](H_2O)$^{2+}$ (**28Ga**), via **TS9Ga**	1.5	16.1
[Ga(H_2O)$_4${CH_2CH_2O(OH)}](H_2O)$^{2+}$ (**28Ga**) → [Ga(H_2O)$_3$(OH)(CH_2CH_2O)](H_2O)$_2^{2+}$ (**8Ga**), via **TS10Ga**	27.9	48.0
[In(H_2O)$_5$(OOH)]$^{2+}$ (**3In**) + C_2H_4 *cis*-[In(H_2O)$_4$(OOH)(C_2H_4)](H_2O)$^{2+}$ (**5In**)		15.3
cis-[In(H_2O)$_4$(OOH)(C_2H_4)](H O)$^{2+}$ (**5In**) → [In(H_2O)$_4${CH_2CH_2O(OH)}](H_2O)$^{2+}$ (**28In**), via **TS9In**	4.1	4.8
[In(H_2O) {CH_2CH_2O(OH)}](H_2O)$^{2+}$ (**28In**) [In(H_2O)$_4$(OH)(CH_2CH_2O)](H_2O)$^{2+}$(**7In**), via **TS10In**	15.8	62.7
cis-[Sc(H_2O) (OOH)(C H_4)](H_2O)$^{2+}$ (**5Sc**) [Sc(H_2O)$_4${CH_2CH_2O(OH)}](H_2O)$^{2+}$(**28Sc**), via **TS9Sc**	23.0	17.0
[Sc(H_2O)$_4${CH_2CH O(OH)}](H_2O)$^{2+}$ (**28Sc**) → [Sc(H O)$_4$(OH)(CH CH_2O)](H O)$^{2+}$ (**7Sc**), via **TS10Sc**	6.0	84.8
[Y(H_2O)$_7$(OOH)]$^{2+}$ (**3Y**) + C_2H_4 → [Y(H_2O)$_6$(OOH)(C_2H_4)](H O)$^{2+}$ (**5Y**)		13.8
[Y(H_2O)$_6$(OOH)(C H_4)](H_2O)$^{2+}$ (**5Y**) [Y(H O) {CH_2CH O(OH)}](H O)$^{2+}$ (**28Y**) , via **TS9Y**	18.5	17.4
[Y(H_2O)$_6${CH_2CH_2O(OH)}](H_2O)$^{2+}$ (**28Y**) → [Y(H_2O)$_5$(OH)(CH_2CH_2O)](H_2O)$_2^{2+}$ (**8Y**), via **TS10Y**	2.8	75.1
[La(H_2O)$_8$(OOH)]$^{2+}$ (**3La**) + C H_4 → [La(H_2O)$_7$(OOH)](H_2O)(C H_4)$^{2+}$ (**4La**•C_2H)		9.3
[La(H_2O)$_7$(OOH)](H_2O)(C_2H_4)$^{2+}$(**4La**•C_2H_4) → [La(H O) {CH_2CH O(OH)}](H_2O)$^{2+}$ (**28La**), via **TS9La**	26.7	24.4
[La(H_2O)$_7${CH_2CH_2O(OH)}](H_2O)$^{2+}$ (**28La**) [La(H_2O)$_6$(OH)(CH_2CH_2O)](H_2O)$_2^{2+}$(**8La**), via **TS10La**	0.9	77.5

[a] Taken from Ref. 26.

Table S3 Calculated total energies and enthalpies (in Hartree) in gas phase (E_g and H_g) and CH_3CN solution (E_s and H_s). Values calculated for the H_2O solution are given in parentheses. For some structures, energies of several possible isomers are indicated

Structure	E	E	H_g	H
H_2O_2	-151.603684	-151.610747 (-151.621984)	-151.573050	-151.580113 (-151.591350)
H_2O	-76.459175	-76.463390 (-76.469649)	-76.434118	-76.438333 (-76.444592)
H_3O^+	-76.731723	-76.863488 (-76.901181)	-76.693575	-76.825340 (-76.863033)
C_2H_4	-78.616478	-78.612889	-78.561721	-78.558132
CH CH_2O	-153.837903	-153.840406	-153.776677	-153.779180
$[Ga(H_2O)_5(OOH)]^{2+}$ (**3Ga**)	-2457.677660	-2457.947600	-2457.515972	-2457.785912
$[Ga(H_2O)_5(OOH)](C_2H)^{2+}$ (**3Ga**•C_2H_4)	-2536.316393	-2536.562419	-2536.098302	-2536.344328
TS1Ga	-2536.275748	-2536.524885	-2536.060105	-2536.309242
$[Ga(H_2O)_4(OOH)](H_2O)^{2+}$ (**4Ga**)	-2457.680654	-2457.936952	-2457.521095	-2457.777393
$[Ga(H_2O)_4(OOH)](H_2O)(C_2H_4)^{2+}$ (**4Ga**•C_2H_4)	-2536.321296	-2536.555454	-2536.103528	-2536.337686
TS2Ga	-2536.289241	-2536.531368	-2536.074135	-2536.316262
$[Ga(H_2O)_4(OH)(Epox)](H_2O)^{2+}$ (**7Ga**)	-2536.417466	-2536.658930	-2536.197666	-2536.439130
$[Ga(H_2O)_5(OH)]^{2+}$ (**9Ga**)	-2382.526162	-2382.802034	-2382.369481	-2382.645353
$[Ga(H_2O)_5(OH)](H_2O)^{2+}$ (**9Ga**)	-2459.032858	-2459.289841	-2458.848075	-2459.105058
TS3Ga	-2536.278555	-2536.516978	-2536.062029	-2536.300452
TS4Ga	-2536.286971	-2536.514013	-2536.071683	-2536.298725
$[Ga(H_2O)_4(OH)](H_2O)^{2+}$ (**10Ga**)	-2382.524005	-2382.789213	-2382.369263	-2382.634471
$[In(H_2O)\ (OOH)]^{2+}$ (**3In**)	-534.766340	-535.032255	-534.605275	-534.871190
$[In(H_2O)\ (OOH)](C_2H_4)^{2+}$ (**3In**•C H_4)	-613.404166	-613.647957	-613.186817	-613.430608
TS1In	-613.369853	-613.615915	-613.154430	-613.400492
$[In(H_2O)\ (OOH)](H\ O)^{2+}$ (**4In**)	-534.760994	-535.017959	-534.599842	-534.856807
	-534.754322	-535.011058	-534.595104	-534.851840
$[In(H_2O)\ (OOH)(C_2H)](H_2O)^{2+}$ (**4In**•C_2H_4)	-613.394869	-613.635525	-613.176636	-613.417292
TS2In	-613.379375	-613.622347	-613.163491	-613.406463
	-613.376990	-613.617455	-613.162269	-613.402734
$[In(H_2O)\ (OH)(Epox)](H_2O)^{2+}$ (**7In**)	-613.503955	-613.742364	-613.285227	-613.523636
$[In(H_2O)\ (OH)]^{2+}$ (**9In**)	-459.616930	-459.886462	-459.460917	-459.730449
$[In(H_2O)\ (OH)](H_2O)^{2+}$ (**9In**)	-536.121520	-536.374183	-535.937344	-536.190007
TS3In	-613.359047	-613.594946	-613.143293	-613.379192
TS4In	-613.358810	-613.589182	-613.142532	-613.372904
$[In(H_2O)\ (OH)](H_2O)^{2+}$ (**10In**)	-459.609401	-459.867031	-459.454722	-459.712352
$[Sc(H_2O)_5(OOH)]^{2+}$ (**3Sc**)	-1293.700306	-1293.956781	-1293.539005	-1293.795480
$[Sc(H_2O)_5(OOH)](C\ H_4)^{2+}$ (**3Sc**•C_2H_4)	-1372.337892	-1372.580358	-1372.120132	-1372.362598
TS1Sc	-1372.310258	-1372.552844	-1372.094528	-1372.337114
$[Sc(H_2O)_5(OH)(Epox)]^{2+}$ (**6Sc**)	-1372.431989	-1372.668227	-1372.212291	-1372.448529
	-1372.425174		-1372.205850	
	-1372.432041		-1372.212277	
	-1372.430389		-1372.210607	
	-1372.429319		-1372.209613	
	-1372.432158		-1372.212415	
	-1372.430508		-1372.210800	
$[Sc(H_2O)_5(OH)]^{2+}$ (**9Sc**)	-1218.558769	-1218.817787	-1218.402671	-1218.661689
$[Sc(H_2O)_5(OH)](H\ O)^{2+}$ (**9Sc**)	-1295.061331	-1295.304100	-1294.876781	-1295.119550
$[Sc(H_2O)_4(OOH)](H_2O)^{2+}$ (**4Sc**)	-1293.695822	-1293.949208	-1293.535480	-1293.788866
	-1293.694364		-1293.532554	
	-1293.698377		-1293.536513	
	-1293.691126		-1293.529612	
$[Sc(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (**4Sc**•C H_4)	-1372.326309	-1372.563850	-1372.108543	-1372.346084
TS2Sc	-1372.312900	-1372.545364	-1372.097920	-1372.330384
cis-$[Sc(H_2O)_4(OH)(Epox)](H_2O)^{2+}$ (*cis*-**7Sc**)	-1372.441680	-1372.668581	-1372.222583	-1372.449484
trans-$[Sc(H_2O)\ (OH)(Epox)](H_2O)^{2+}$ (*trans*-**7Sc**)	-1372.441728		-1372.222635	
$[Sc(H_2O)_4(OH)](H\ O)^{2+}$ (**10Sc**)	-1218.549096	-1218.799917	-1218.394243	-1218.645064
	-1218.553930		-1218.397227	
TS3Sc	-1372.307820	-1372.534094	-1372.091652	-1372.317926
TS4Sc	-1372.306117	-1372.527115	-1372.089509	-1372.310507
$[Y(H_2O)\ (OOH)]^{2+}$ (**3Y**)	-724.326280	-724.563696	-724.109760	-724.347176

$[Y(H_2O)\ (OOH)](C_2H_4)^{2+}$ (**3Y**•C_2H_4)	-802.950553	-803.174523	-802.678692	-802.902662
TS1Y	-802.923149	-803.147367	-802.652560	-802.876778
$[Y(H_2O)\ (OH)]^{2+}$ (**9Y**)	-649.174743	-649.412282	-648.963673	-649.201212
$[Y(H_2O)\ (OH)](H_2O)^{2+}$ (**9Y**)	-725.670039	-725.894589	-725.430596	-725.655146
$[Y(H_2O)\ (OOH)](H\ O)^{2+}$ (**4Y**)	-724.331102	-724.559717	-724.114287	-724.342902
	-724.329308		-724.112355	
$[Y(H_2O)\ (OOH)](H\ O)(C_2H\ )^{2+}$ (**4Y**•C_2H_4)	-802.957921	-803.175037	-802.684680	-802.901796
TS2Y	-802.933494	-803.150045	-802.662294	-802.878845
$[Y(H_2O)\ (OH)(Epox)](H_2O)^{2+}$ (**7Y**)	-803.053473	-803.266199	-802.778335	-802.991061
	-803.049070		-802.773852	
	-803.053428		-802.778157	
	-803.051558		-802.776478	
$[Y(H_2O)\ (OH)](H_2O)^{2+}$ (**10Y**)	-649.183963	-649.414230	-648.972164	-649.202431
	-649.182226		-648.970574	
	-649.183238		-648.971537	
	-649.181469		-648.970912	
TS3Y	-802.909432	-803.117528	-802.638723	-802.846819
TS4Y	-802.916766	-803.115929	-802.645589	-802.844752
$[La(H_2O)_8(OOH)]^{2+}$ (**3La**)	-794.078998	-794.299351	-793.835481	-794.055834
$[La(H_2O)_8(OOH)](C_2H_4)^{2+}$ (**3La**•C_2H_4)	-872.698977	-872.907388	-872.398692	-872.607103
TS1La	-872.671388	-872.880517	-872.373455	-872.582584
$[La(H_2O)_8(OH)](Epox)^{2+}$ (**9La**•C_2H_4O)	-872.794553	-872.995082	-872.492432	-872.692961
$[La(H_2O)_8(OH)]^{2+}$ (**9La**)	-718.922716	-719.145035	-718.684538	-718.906857
$[La(H_2O)_8(OH)](H_2O)^{2+}$ (**9La**)	-795.415526	-795.626322	-795.149061	-795.359857
$[La(H_2O)_7(OOH)](H_2O)^{2+}$ (**4La**)	-794.084617	-794.297235	-793.840490	-794.053108
$[La(H_2O)_7(OOH)](H_2O)(C_2H_4)^{2+}$ (**4La**•C_2H_4)	-872.707338	-872.909742	-872.407170	-872.609574
TS2La	-872.682330	-872.884802	-872.384153	-872.586625
$[La(H_2O)_6(OH)(Epox)](H_2O)_2^{2+}$ (**8La**)	-872.802608	-872.999619	-872.500288	-872.697299
$[La(H_2O)_7(OH)(Epox)](H_2O)^{2+}$ (**7La**)	-872.797427	-872.997618	-872.495457	-872.695648
	-872.796869		-872.494613	
	-872.795189		-872.492880	
	-872.796837		-872.494783	
	-872.795992		-872.493952	
	-872.795315		-872.493348	
	-872.797295		-872.494976	
$[La(H_2O)_7(OH)](H_2O)^{2+}$ (**10La**)	-718.931092	-719.145660	-718.692415	-718.906983
TS4La	-872.658267	-872.854151	-872.360262	-872.556146
cis-$[Ga(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (*cis*-**5Ga**)	-2536.315387	-2536.556602	-2536.096853	-2536.338068
trans-$[Ga(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (*trans*-**5Ga**)	-2536.312057		-2536.092649	
$[Ga(H_2O)_4(CH_2CH_2OO(H))](H_2O)^{2+}$ (**23Ga**)	-2536.331703	-2536.578706	-2536.111466	-2536.358469
	-2536.312542		-2536.092683	
$[Ga(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ (**27Ga**)	-2536.320441	-2536.549363	-2536.102669	-2536.331591
	-2536.314202		-2536.097077	
	-2536.320946		-2536.102965	
TS8Ga	-2536.280332	-2536.515593	-2536.062790	-2536.298051
$[Ga(H_2O)_3(CH_2CH_2OO(H))](H_2O)_2^{2+}$ (**24Ga**)	-2536.348196	-2536.585539	-2536.127639	-2536.364982
$[Ga(H_2O)_3(CH_2CH_2O(H)O)](H_2O)_2^{2+}$ (**26Ga**)	-2536.328954		-2536.108776	
cis-$[In(H_2O)_4(OOH)(C_2H\ )](H_2O)^{2+}$ (*cis*-**5In**)	-613.401807	-613.639758	-613.183639	-613.421590
trans-$[In(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (*trans*-**5In**)	-613.397570		-613.179001	
$[In(H_2O)\ (CH_2CH_2OO(H))](H_2O)^{2+}$ (**23In**)	-613.405375	-613.649801	-613.185968	-613.430394
$[In(H_2O)\ (CH_2CH_2O(H)O)](H_2O)^{2+}$ (**25In**)	-613.385868		-613.166809	
$[In(H_2O)\ (OOH)(C_2H\ )](H_2O)^{2+}$ (**27In**)	-613.394696	-613.621427	-613.177453	-613.404184
	-613.389025	-613.623325	-613.171077	-613.405377
	-613.388690		-613.171208	
$[In(H_2O)\ (CH_2CH_2OO(H))](H_2O)_2^{2+}$ (**24In**)	-613.411656	-613.646055	-613.191615	-613.426014
$[In(H_2O)\ (CH_2CH_2O(H)O)](H_2O)_2^{2+}$ (**26In**)	-613.392098		-613.172453	
cis-$[Sc(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (*cis*-**5Sc**)	-1372.332780	-1372.564863	-1372.114201	-1372.346284
trans-$[Sc(H_2O)\ (OOH)(C_2H\ )](H_2O)^{2+}$ (*trans*-**5Sc**)	-1372.331399		-1372.112699	
TS7Sc	-1372.295993	-1372.534239	-1372.079316	-1372.317562
$[Sc(H_2O)_4(CH_2CH_2OO(H))](H_2O)^{2+}$ (**23Sc**)	-1372.297910	-1372.540115	-1372.079178	-1372.321383
$[Sc(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ (**27Sc**)	-1372.329540	-1372.556936	-1372.110808	-1372.338204
	-1372.322025		-1372.104046	
	-1372.328984	-1372.556957	-1372.109748	-1372.337721
TS8Sc	-1372.297643	-1372.526703	-1372.080678	-1372.309738
$[Sc(H_2O)_3(CH_2CH_2OO(H))](H_2O)_2^{2+}$ (**24Sc**)	-1372.299485	-1372.529114	-1372.081361	-1372.310990
$[Y(H_2O)\ (OOH)](H\ O)(C_2H\ )^{2+}$ (**4Y**•C_2H_4)	-802.959842	-803.175902	-802.686488	-802.902548

[Y(H_2O) (OOH)(C_2H)](H_2O)$^{2+}$ (**5Y**)	-802.949787	-803.167047	-802.675437	-802.892697
[Y(H_2O) (CH_2CH_2OO(H))](H O)$^{2+}$ (**23Y**)	-802.916865	-803.143329	-802.642620	-802.869084
[Y(H_2O) (OOH)(C_2H)](H_2O) $^{2+}$ (**27Y**)	-802.955325	-803.166268	-802.681220	-802.892163
	-802.954541		-802.680065	
	-802.958499		-802.684044	
	-802.956302		-802.681728	
	-802.957416		-802.683037	
	-802.954083		-802.679739	
	-802.960350	-803.166589	-802.685710	-802.891949
	-802.954670		-802.680170	
	-802.955327		-802.681223	
	-802.951958		-802.677731	
TS7Y	-802.912028	-803.136234	-802.639531	-802.863737
TS8Y	-802.921958	-803.137069	-802.649033	-802.864144
[Y(H_2O) (CH_2CH_2OO(H))](H $O)_2^{2+}$ (**24Y**)	-802.924335	-803.139749	-802.649847	-802.865261
	-802.924159		-802.649549	
[La(H_2O)$_7$(OOH)](H_2O)(C_2H_4)$^{2+}$ (**4La•**C_2H_4)	-872.707171	-872.908614	-872.406842	-872.608285
[La(H_2O)$_7$(OOH)(C_2H_4)](H_2O)$^{2+}$ (**5La**)	-872.704240	-872.906856	-872.403312	-872.605928
	-872.702673	-872.907008	-872.401656	-872.605991
[La(H_2O)$_7$(CH_2CH OO(H))](H_2O)$^{2+}$ (**23La**)	-872.664128	-872.876425	-872.362842	-872.575139
[La(H_2O)$_6$(OOH)(C_2H_4)](H_2O)$_2^{2+}$ (**27La**)	-872.710455	-872.906744	-872.408637	-872.604926
	-872.708311	-872.903565	-872.406576	-872.601830
	-872.704159		-872.402520	
	-872.707852		-872.405988	
TS8La	-872.668867	-872.872979	-872.368883	-872.572995
[La(H_2O)$_6$(CH_2CH OO(H))](H_2O)$_2^{2+}$ (**24La**)	-872.670943	-872.874883	-872.369486	-872.573426
TS7La	-872.656228	-872.868327	-872.356778	-872.568877
cis-[Ga(H_2O)$_4$(OOH)(C_2H_4)](H_2O)$^{2+}$ (*cis*-**5Ga**)	-2536.310247	-2536.55129	-2536.092303	-2536.333346
TS9Ga	-2536.311963	-2536.552685	-2536.094075	-2536.334797
[Ga(H_2O)$_4${CH_2CH_2O(OH)}](H_2O)$^{2+}$ (**28Ga**)	-2536.342796	-2536.583081	-2536.122116	-2536.362401
TS10Ga	-2536.297052	-2536.533367	-2536.081476	-2536.317791
8Ga	-2536.423419	-2536.654676	-2536.204195	-2536.435452
cis-[In(H_2O)$_4$(OOH)(C_2H)](H_2O)$^{2+}$ (*cis*-**5In**)	-613.392589	-613.633426	-613.175582	-613.416419
TS9In	-613.390053	-613.629181	-613.172849	-613.411977
[In(H_2O) {CH_2CH_2O(OH)}](H_2O)$^{2+}$ (**28In**)	-613.407146	-613.646423	-613.186814	-613.426091
TS10In	-613.378675	-613.616648	-613.165213	-613.403186
7In	-613.50967	-613.744769	-613.289564	-613.524663
TS9Sc	-1372.296016	-1372.530957	-1372.078802	-1372.313743
[Sc(H_2O)$_4${CH_2CH_2O(OH)}](H O)$^{2+}$ (**28Sc**)	-1372.303889	-1372.541115	-1372.084462	-1372.321688
TS10Sc	-1372.290404	-1372.527774	-1372.075325	-1372.312695
7Sc	-1372.445301	-1372.672917	-1372.225305	-1372.452921
[Y(H_2O) (OOH)(C_2H)](H_2O)$^{2+}$ (**5Y**)	-802.950259	-803.167855	-802.676158	-802.893754
TS9Y	-802.920255	-803.14113	-802.64747	-802.868345
[Y(H_2O) {CH_2CH_2O(OH)}](H_2O)$^{2+}$ (**28Y**)	-802.923194	-803.142983	-802.648906	-802.868695
TS10Y	-802.917562	-803.138729	-802.645071	-802.866238
[Y(H_2O) (OH)(CH_2CH O)](H $O)_2^{2+}$ (**8Y**)	-803.054263	-803.261463	-802.779072	-802.986272
[La(H_2O)$_7$(OOH)](H_2O)(C_2H_4)$^{2+}$ (**4La•**C_2H_4)	-872.706493	-872.906405	-872.406159	-872.606071
TS9La	-872.659844	-872.870272	-872.360311	-872.570739
[La(H_2O)$_7${CH_2CH_2O(OH)}](H_2O)$^{2+}$ (**28La**)	-872.664957	-872.874553	-872.363783	-872.573379
TS10La	-872.672581	-872.873226	-872.372705	-872.573350
[La(H_2O)$_6$(OH)(CH_2CH_2O)](H_2O)$_2^{2+}$ (**8La**)	-872.799411	-872.997265	-872.497313	-872.695167
[Ga(H_2O)$_3$(OOH)$_2$](H O)$^{+}$ (**20Ga**)	-2532.620198	-2532.687369	-2532.466251	-2532.533422
TS6Ga	-2611.211540	-2611.272741	-2611.002756	-2611.063957
[Ga(H_2O)$_3$(OOH)(OH)(Epox)](H_2O)$^{+}$ (**22Ga**)	-2611.319508	-2611.379738	-2611.105941	-2611.166171
[In(H_2O) (OOH)$_2$](H_2O)$^{+}$ (**20In**)	-609.687279	-609.752570	-609.534422	-609.599713
TS6In	-688.290300	-688.349784	-688.082246	-688.141730
[In(H_2O) (OOH)(OH)(Epox)](H_2O)$^{+}$ (**22In**)	-688.413160	-688.473307	-688.201069	-688.261216
[Sc(H_2O)$_3$(OOH)](H_2O)$^{+}$ (**20Sc**)	-1368.616194	-1368.681516	-1368.462438	-1368.527760
TS6Sc	-1447.218791	-1447.273005	-1447.011112	-1447.065326
[Sc(H_2O)$_3$(OOH)(OH)(Epox)](H_2O)$^{+}$ (**22Sc**)	-1447.333297	-1447.385984	-1447.121516	-1447.174203
[Y(H_2O) (OOH)$_2$](H_2O)$^{+}$ (**20Y**)	-799.213073	-799.274321	-799.004126	-799.065374
TS6Y	-877.810291	-877.862966	-877.546028	-877.598703
[Y(H_2O) (OOH)(OH)(Epox)](H_2O)$^{+}$ (**22Y**)	-877.920260	-877.968277	-877.652715	-877.700732
[La(H_2O)$_6$(OOH)$_2$](H_2O)$^{+}$ (**20La**)	-868.953881	-869.008536	-868.717773	-868.772428
TS6La	-947.540926	-947.588066	-947.249664	-947.296804
[La(H_2O)$_6$(OOH)(OH)(Epox)](H_2O)$^{+}$ (**22La**)	-947.653219	-947.697146	-947.358279	-947.402206

$[Ga(H_2O)_4O_2](H_2O)^+$ (**12Ga**)	-2457.408757	-2457.492632	-2457.259567	-2457.343442
TS5Ga	-2536.002996	-2536.077159	-2535.798632	-2535.872795
$[Ga(H_2O)(OH)_2(C_2H_4O)](H_2O)_3^+$ (**15Ga**)	-2536.190052	-2536.241028	-2535.982562	-2536.033538
$[In(H_2O)\ O_2](H_2O)^+$ (**12In**)	-534.471083	-534.563296	-534.323474	-534.415687
TS5In	-613.068934	-613.144704	-612.867209	-612.942979
$[In(H_2O)\ (OH)\ (C\ H_4O)](H_2O)^+$ (**16In**)	-613.254606	-613.312797	-613.047763	-613.105954
$[Sc(H_2O)_5(OO)]^+$ (**11Sc**)	-1293.447809	-1293.527183	-1293.299364	-1293.378738
$[Sc(H_2O)_4O\ ](H_2O)^+$ (**12Sc**)	-1293.444801	-1293.524953	-1293.295841	-1293.375993
TS5Sc	-1372.029252	-1372.096913	-1371.825252	-1371.892913
$[Sc(H_2O)_4(=O)(C_2H_4O)](H_2O)^+$ (**18Sc**)	-1372.127582	-1372.190266	-1371.919402	-1371.982086
$[Sc(H_2O)_3(OH)_2(C_2H_4O)](H_2O)^+$ (**16Sc**)	-1372.187279	-1372.241909	-1371.980744	-1372.035374
$[Y(H_2O)\ O_2]^+$ (**11Y**)	-724.032080	-724.101979	-723.829697	-723.899596
$[Y(H_2O)\ O_2](H\ O)^+$ (**12Y**)	-724.036147	-724.105710	-723.833304	-723.902867
TS5Y	-802.623787	-802.680232	-802.365927	-802.422372
$[Y(H_2O)\ (OH)_2(C_2H_4O)](H_2O)_2^+$ (**17Y**)	-802.778476	-802.825178	-802.516988	-802.563690
$[La(H_2O)_7O_2](H_2O)^+$ (**12La**)	-793.768640	-793.826652	-793.538905	-793.596917
$[La(H_2O)_5O_2](H_2O)_3^+$ (**13La**)	-793.777998	-793.835625	-793.547077	-793.604704
TS5La	-872.364366	-872.412372	-872.078448	-872.126454
$[La(H_2O)_5(=O)(C_2H\ O)](H\ O)_3^+$ (**19La**)	-872.464603	-872.510380	-872.177425	-872.223202
$[La(H_2O)_5(OH)\ (C\ H_4O)](H_2O)^+$ (**17La**)	-872.500463	-872.543511	-872.211931	-872.254979
Cyclohexene	-234.716166	-234.715068	-234.564085	-234.562987
TS $[Ga(H_2O)\ (\underline{O}OH)](H_2O)^{2+}$ + Cyclohexene	-2692.398897	-2692.632344	-2692.087108	-2692.320555
TS $[In(H_2O)_4(\underline{O}OH)](H_2O)^{2+}$ + Cyclohexene	-769.486619	-769.722429	-769.173718	-769.409528
TS $[Sc(H_2O)_5(\underline{O}OH)]^{2+}$ + Cyclohexene	-1528.425525	-1528.657964	-1528.11298	-1528.345419
TS $[Y(H_2O)\ (\underline{O}OH)](H\ O)^{2+}$ + Cyclohexene	-959.043141	-959.253053	-958.675118	-958.885030
TS $[La(H_2O)_7(\underline{O}OH)](H_2O)^{2+}$ + Cyclohexene	-1028.79075	-1028.98718	-1028.395711	-1028.592141

Table S4 Calculated entropies (in cal/mol•K) and Gibbs free energies (in Hartree) in gas phase (S_g and G_g) and CH_3CN solution (S_s and G_s). Values calculated for the H_2O solution are given in parentheses. For some structures, energies of several possible isomers are indicated

Structure	S_g	S_s	G_g	G_s
H_2O_2	55.77	39.41 (30.37)	-151.599550	-151.598839 (-151.605782)
H_2O	45.09	31.19 (24.61)	-76.455541	-76.453151 (-76.456283)
H_3O^+	48.44	33.77 (26.42)	-76.716591	-76.841384 (-76.875584)
C_2H_4	55.07	38.87	-78.587886	-78.576601
CH CH_2O	57.96	41.10	-153.804215	-153.798707
$[Ga(H_2O)_5(OOH)]^{2+}$ (**3Ga**)	122.32	90.65	-2457.574092	-2457.828985
$[Ga(H_2O)_5(OOH)](C_2H)^{2+}$ (**3Ga**•C_2H_4)	144.33	107.60	-2536.166878	-2536.395454
(**TS1Ga**	132.84	98.76	-2536.123223	-2536.356164
$[Ga(H_2O)_4(OOH)](H_2O)^{2+}$ (**4Ga**)	127.55	94.68	-2457.581699	-2457.822379
$[Ga(H_2O)_4(OOH)](H_2O)(C_2H_4)^{2+}$ (**4Ga**•C_2H_4)	151.83	113.38	-2536.175668	-2536.391556
TS2Ga	147.38	109.95	-2536.144160	-2536.368503
$[Ga(H_2O)_4(OH)(Epox)](H_2O)^{2+}$ (**7Ga**)	138.16	102.85	-2536.263309	-2536.487998
$[Ga(H_2O)_5(OH)]^{2+}$ (**9Ga**)	120.69	89.40	-2382.426824	-2382.687830
$[Ga(H_2O)_5(OH)](H_2O)^{2+}$ (**9Ga**)	128.14	95.13	-2458.908956	-2459.150259
TS3Ga	142.33	106.06	-2536.129655	-2536.350846
TS4Ga	147.31	109.90	-2536.141673	-2536.350941
$[Ga(H_2O)_4(OH)](H_2O)^{2+}$ (**10Ga**)	124.00	91.95	-2382.428179	-2382.678158
$[In(H_2O)\ (OOH)]^{2+}$ (**3In**)	127.36	94.54	-534.665786	-534.916107
$[In(H_2O)\ (OOH)](C_2H_4)^{2+}$ (**3In**•C H_4)	150.15	112.09	-613.258160	-613.483864
TS1In	139.28	103.71	-613.220606	-613.449770
$[In(H_2O)\ (OOH)](H\ O)^{2+}$ (**4In**)	126.82	94.12	-534.660096	-534.901526
	133.04	98.91	-534.658316	-534.898835
$[In(H_2O)\ (OOH)(C_2H)](H_2O)^{2+}$ (**4In**•C_2H_4)	143.73	107.14	-613.244925	-613.468197
TS2In	147.57	110.10	-613.233608	-613.458774
	153.48	114.65	-613.235194	-613.457207
$[In(H_2O)\ (OH)(Epox)](H_2O)^{2+}$ (**7In**)	147.07	109.71	-613.355104	-613.575764
$[In(H_2O)\ (OH)]^{2+}$ (**9In**)	122.37	90.69	-459.519059	-459.773540
$[In(H_2O)\ (OH)](H_2O)^{2+}$ (**9In**)	133.61	99.35	-536.000827	-536.237210
TS3In	146.89	109.57	-613.213086	-613.431254
TS4In	145.68	108.64	-613.211749	-613.424523
$[In(H_2O)\ (OH)](H_2O)^{2+}$ (**10In**)	126.93	94.21	-459.515033	-459.757113
$[Sc(H_2O)_5(OOH)]^{2+}$ (**3Sc**)	129.50	96.18	-1293.600535	-1293.841180
$[Sc(H_2O)_5(OOH)](C\ H_4)^{2+}$ (**3Sc**•C_2H_4)	152.78	114.11	-1372.192724	-1372.416816
TS1Sc	147.60	110.12	-1372.164657	-1372.389436
$[Sc(H_2O)_5(OH)(Epox)]^{2+}$ (**6Sc**)	147.59	110.11	-1372.282417	-1372.500847
	152.38		-1372.278253	
	145.62		-1372.281465	
	145.67		-1372.279817	
	148.08		-1372.279968	
	144.97		-1372.281293	
	148.54		-1372.281374	
$[Sc(H_2O)_5(OH)]^{2+}$ (**9Sc**)	122.71	90.96	-1218.460972	-1218.704905
$[Sc(H_2O)_5(OH)](H\ O)^{2+}$ (**9Sc**)	131.57	97.78	-1294.939295	-1295.166008
$[Sc(H_2O)_4(OOH)](H_2O)^{2+}$ (**4Sc**)	131.08	97.40	-1293.597761	-1293.835144
	126.38		-1293.592601	
	125.17		-1293.595987	
	131.21		-1293.591952	
$[Sc(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (**4Sc**•C H_4)	152.66	114.02	-1372.181078	-1372.400258
TS2Sc	152.86	114.17	-1372.170547	-1372.384630
cis-$[Sc(H_2O)_4(OH)(Epox)](H_2O)^{2+}$ (*cis*-**7Sc**)	154.46	115.40	-1372.295974	-1372.504315
trans-$[Sc(H_2O)\ (OH)(Epox)](H_2O)^{2+}$ (*trans*-**7Sc**)	152.09		-1372.294900	
$[Sc(H_2O)_4(OH)](H\ O)^{2+}$ (**10Sc**)	128.74	95.60	-1218.455410	-1218.690486
	119.61		-1218.454055	
TS3Sc	153.08	114.34	-1372.164385	-1372.372253
TS4Sc	151.36	113.02	-1372.161426	-1372.364204
$[Y(H_2O)\ (OOH)]^{2+}$ (**3Y**)	154.08	115.11	-724.182966	-724.401868

$[Y(H_2O)\ (OOH)](C_2H_4)^{2+}$ (**3Y**•C_2H_4)	177.39	133.05	-802.762974	-802.965881
TS1Y	173.92	130.39	-802.735195	-802.938729
$[Y(H_2O)\ (OH)]^{2+}$ (**9Y**)	153.75	114.86	-649.036724	-649.255784
$[Y(H_2O)\ (OH)](H_2O)^{2+}$ (**9Y**)	164.94	123.47	-725.508964	-725.713812
$[Y(H_2O)\ (OOH)](H\ O)^{2+}$ (**4Y**)	154.43	115.38	-724.187663	-724.397722
	154.67		-724.185841	
$[Y(H_2O)\ (OOH)](H\ O)(C_2H\ )^{2+}$ (**4Y**•C_2H_4)	180.86	135.73	-802.770611	-802.966285
TS2Y	173.14	129.79	-802.744560	-802.940511
$[Y(H_2O)\ (OH)(Epox)](H_2O)^{2+}$ (**7Y**)	177.00	132.76	-802.862434	-803.054139
	175.95		-802.857454	
	174.69		-802.861157	
	176.79		-802.860474	
$[Y(H_2O)\ (OH)](H_2O)^{2+}$ pentagbipiram1 (**10Y**)	152.40	113.82	-649.044574	-649.256509
	154.00		-649.043745	
	152.93		-649.044198	
	147.43		-649.040958	
TS3Y	179.33	134.55	-802.723927	-802.910749
TS4Y	179.22	134.47	-802.730742	-802.908642
$[La(H_2O)_8(OOH)]^{2+}$ (**3La**)	173.30	129.91	-793.917821	-794.117558
$[La(H_2O)_8(OOH)](C_2H_4)^{2+}$ (**3La**•C_2H_4)	204.93	154.27	-872.496062	-872.680400
TS1La	190.26	142.96	-872.463851	-872.650511
$[La(H_2O)_8(OH)](Epox)^{2+}$ (**9La**•C_2H_4O)	194.40	146.15	-872.584796	-872.762403
$[La(H_2O)_8(OH)]^{2+}$ (**9La**)	172.90	129.60	-718.766690	-718.968435
$[La(H_2O)_8(OH)](H_2O)^{2+}$ (**9La**)	182.55	137.03	-795.235797	-795.424966
$[La(H_2O)_7(OOH)](H_2O)^{2+}$ (**4La**)	172.25	129.10	-793.922331	-794.114448
$[La(H_2O)_7(OOH)](H_2O)(C_2H_4)^{2+}$ (**4La**•C_2H_4)	206.93	155.80	-872.505490	-872.683602
TS2La	195.15	146.73	-872.476874	-872.656343
$[La(H_2O)_6(OH)(Epox)](H_2O)_2^{2+}$ (**8La**)	195.63	147.11	-872.593239	-872.767194
$[La(H_2O)_7(OH)(Epox)](H_2O)^{2+}$ (**7La**)	196.15	147.50	-872.588656	-872.765732
	194.19		-872.586878	
	192.23		-872.584215	
	196.95		-872.588359	
	186.93		-872.582769	
	190.40		-872.583814	
	193.06		-872.586704	
$[La(H_2O)_7(OH)](H_2O)^{2+}$ (**10La**)	176.17	132.12	-718.776120	-718.969757
TS4La	195.01	146.63	-872.452916	-872.625813
cis-$[Ga(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (*cis*-**5Ga**)	141.28	105.25	-2536.163980	-2536.388077
trans-$[Ga(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (*trans*-**5Ga**)	138.49		-2536.158449	
$[Ga(H_2O)_4(CH_2CH_2OO(H))](H_2O)^{2+}$ (**23Ga**)	137.48	102.33	-2536.176788	-2536.407088
	140.35		-2536.159367	
$[Ga(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ (**27Ga**)	146.50	109.27	-2536.172276	-2536.383510
	143.50		-2536.165259	
	144.27		-2536.171513	
TS8Ga	134.95	100.38	-2536.126908	-2536.345745
$[Ga(H_2O)_3(CH_2CH_2OO(H))](H_2O)_2^{2+}$ (**24Ga**)	135.28	100.63	-2536.191913	-2536.412796
$[Ga(H_2O)_3(CH_2CH_2O(H)O)](H_2O)_2^{2+}$ (**26Ga**)	138.59		-2536.174625	
cis-$[In(H_2O)_4(OOH)(C_2H\ )](H_2O)^{2+}$ (*cis*-**5In**)	144.97	108.10	-613.252521	-613.472949
trans-$[In(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (*trans*-**5In**)	145.17		-613.247974	
$[In(H_2O)\ (CH_2CH_2OO(H))](H_2O)^{2+}$ (**23In**)	142.60	106.27	-613.253723	-613.480886
$[In(H_2O)\ (CH_2CH_2O(H)O)](H_2O)^{2+}$ (**25In**)	145.16		-613.235777	
$[In(H_2O)\ (OOH)(C_2H\ )](H_2O)^{2+}$ (**27In**)	153.76	114.86	-613.250511	-613.458759
	147.72	110.21	-613.241264	-613.457743
	154.90		-613.244804	
$[In(H_2O)\ (CH_2CH_2OO(H))](H_2O)_2^{2+}$ (**24In**)	139.38	103.79	-613.257838	-613.475328
$[In(H_2O)\ (CH_2CH_2O(H)O)](H_2O)_2^{2+}$ (**26In**)	142.69		-613.240248	
cis-$[Sc(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (*cis*-**5Sc**)	147.81	110.28	-1372.184432	-1372.398682
trans-$[Sc(H_2O)\ (OOH)(C_2H\ )](H_2O)^{2+}$ (*trans*-**5Sc**)	147.96		-1372.183001	
TS7Sc	140.51	104.66	-1372.146079	-1372.367290
$[Sc(H_2O)_4(CH_2CH_2OO(H))](H_2O)^{2+}$ (**23Sc**)	141.78	105.64	-1372.146541	-1372.371575
$[Sc(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ (**27Sc**)	147.45	110.00	-1372.180868	-1372.390471
	151.76		-1372.176151	
	144.82	107.98	-1372.178558	-1372.389026
TS8Sc	139.21	103.66	-1372.146819	-1372.358990
$[Sc(H_2O)_3(CH_2CH_2OO(H))](H_2O)_2^{2+}$ (**24Sc**)	140.75	104.85	-1372.148237	-1372.360806
$[Y(H_2O)\ (OOH)](H\ O)(C_2H\ )^{2+}$ (**4Y**•C_2H_4)	183.62	137.86	-802.773730	-802.968048

$[Y(H_2O)\ (OOH)(C_2H\ )](H_2O)^{2+}$ (**5Y**)	172.85	129.56	-802.757562	-802.954256
$[Y(H_2O)\ (CH_2CH_2OO(H))](H\ O)^{2+}$ (**23Y**)	167.57	125.50	-802.722238	-802.928712
$[Y(H_2O)\ (OOH)(C_2H\ )](H_2O)^{2+}$ (**27Y**)	179.19	134.44	-802.766359	-802.956042
	180.24		-802.765703	
	175.83		-802.767586	
	175.50		-802.765116	
	174.90		-802.766138	
	179.08		-802.764824	
	172.73	129.47	-802.767780	-802.953465
	175.67		-802.763639	
	179.13		-802.766332	
	177.99		-802.762301	
TS7Y	165.46	123.87	-802.718147	-802.922593
TS8Y	166.71	124.84	-802.728243	-802.923457
$[Y(H_2O)\ (CH_2CH_2OO(H))](H\ O)_2^{2+}$ (**24Y**)	167.33	125.31	-802.729350	-802.924801
	166.67		-802.728737	
$[La(H_2O)_7(OOH)](H_2O)(C_2H_4)^{2+}$ (**4La•**C_2H_4)	208.13	156.73	-872.505730	-872.682752
$[La(H_2O)_7(OOH)(C_2H_4)](H_2O)^{2+}$ (**5La**)	197.05	148.20	-872.496937	-872.676341
	193.94	145.80	-872.493803	-872.675266
$[La(H_2O)_7(CH_2CH\ OO(H))](H_2O)^{2+}$ (**23La**)	188.36	141.51	-872.452340	-872.642373
$[La(H_2O)_6(OOH)(C_2H_4)](H_2O)_2^{2+}$ (**27La**)	195.04	146.65	-872.501307	-872.674604
	197.87	148.83	-872.500589	-872.672543
	198.76		-872.496955	
	196.20		-872.499209	
TS8La	186.98	140.44	-872.457725	-872.639724
$[La(H_2O)_6(CH_2CH\ OO(H))](H_2O)_2^{2+}$ (**24La**)	189.45	142.34	-872.459499	-872.641059
TS7La	188.86	141.89	-872.446509	-872.636294
cis-$[Ga(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (**5Ga**)	143.39	106.88	-2536.160435	-2536.384129
TS9Ga	133.03	98.90	-2536.157279	-2536.381788
$[Ga(H_2O)_4\{CH_2CH_2O(OH)\}](H_2O)^{2+}$ (**28Ga**)	134.14	99.76	-2536.185852	-2536.409799
TS10Ga	134.64	100.14	-2536.145448	-2536.365371
8Ga	143.37	106.87	-2536.272317	-2536.486228
cis-$[In(H_2O)_4(OOH)(C_2H\ )](H_2O)^{2+}$ (**5In**)	146.54	109.31	-613.245209	-613.468354
TS9In	140.90	104.96	-613.239793	-613.461847
$[In(H_2O)\ \{CH_2CH_2O(OH)\}](H_2O)^{2+}$ (**28In**)	140.90	104.96	-613.253759	-613.475961
TS10In	134.79	100.26	-613.229257	-613.450821
7In	144.41	107.66	-613.358177	-613.575817
TS9Sc	136.65	101.69	-1372.143731	-1372.362059
$[Sc(H_2O)_4\{CH_2CH_2O(OH)\}](H\ O)^{2+}$ (**28Sc**)	136.32	101.43	-1372.14923	-1372.369881
TS10Sc	134.58	100.10	-1372.139269	-1372.360254
7Sc	146.78	109.49	-1372.295044	-1372.504942
$[Y(H_2O)\ (OOH)(C_2H\ )](H_2O)^{2+}$ (**5Y**)	175.98	131.98	-802.759773	-802.956460
TS9Y	164.67	123.26	-802.72571	-802.926912
$[Y(H_2O)\ \{CH_2CH_2O(OH)\}](H_2O)^{2+}$ (**28Y**)	168.50	126.21	-802.728966	-802.928663
TS10Y	162.89	121.89	-802.722464	-802.924154
$[Y(H_2O)\ (OH)(CH_2CH\ O)](H\ O)_2^{2+}$ (**8Y**)	174.13	130.55	-802.861807	-803.048300
$[La(H_2O)_7(OOH)](H_2O)(C_2H_4)^{2+}$ (**4La•**C_2H_4)	204.72	154.10	-872.503428	-872.679290
TS9La	185.17	139.05	-872.448293	-872.636806
$[La(H_2O)_7\{CH_2CH_2O(OH)\}](H_2O)^{2+}$ (**28La**)	187.868	141.13	-872.453045	-872.640433
TS10La	184.15	138.26	-872.460200	-872.639044
$[La(H_2O)_6(OH)(CH_2CH_2O)](H_2O)_2^{2+}$ (**8La**)	192.57	144.75	-872.588808	-872.763941
$[Ga(H_2O)_3(OOH)_2](H\ O)^{+}$ (**20Ga**)	135.73	100.98	-2532.530738	-2532.581401
TS6Ga	149.36	111.48	-2611.073723	-2611.116923
$[Ga(H_2O)_3(OOH)(OH)(Epox)](H_2O)^{+}$ (**22Ga**)	144.14	107.46	-2611.174425	-2611.217227
$[In(H_2O)\ (OOH)_2](H_2O)^{+}$ (**20In**)	142.31	106.05	-609.602040	-609.650101
TS6In	154.64	115.54	-688.155719	-688.196626
$[In(H_2O)\ (OOH)(OH)(Epox)](H_2O)^{+}$ (**22In**)	143.87	107.25	-688.269428	-688.312173
$[Sc(H_2O)_3(OOH)\ ](H_2O)^{+}$ (**20Sc**)	133.24	99.07	-1368.525746	-1368.574829
TS6Sc	158.84	118.78	-1447.086582	-1447.121760
$[Sc(H_2O)_3(OOH)(OH)(Epox)](H_2O)^{+}$ (**22Sc**)	155.86	116.48	-1447.195570	-1447.229547
$[Y(H_2O)\ (OOH)_2](H_2O)^{+}$ (**20Y**)	158.17	118.26	-799.079279	-799.121563
TS6Y	171.03	128.16	-877.627289	-877.659597
$[Y(H_2O)\ (OOH)(OH)(Epox)](H_2O)^{+}$ (**22Y**)	172.32	129.15	-877.734588	-877.762098
$[La(H_2O)_6(OOH)_2](H_2O)^{+}$ (**20La**)	169.16	126.72	-868.798148	-868.832637
TS6La	189.99	142.76	-947.339935	-947.364634
$[La(H_2O)_6(OOH)(OH)(Epox)](H_2O)^{+}$ (**22La**)	189.72	142.55	-947.448420	-947.469937

$[Ga(H_2O)_4O_2](H_2O)^+$ (**12Ga**)	116.49	86.17	-2457.314916	-2457.384382
TS5Ga	144.73	107.91	-2535.867397	-2535.924067
$[Ga(H_2O)(OH)_2(C_2H_4O)](H_2O)_3^+$ (**15Ga**)	148.10	110.50	-2536.052928	-2536.086042
$[In(H_2O)\ O_2](H_2O)^+$ (**12In**)	127.85	94.91	-534.384219	-534.460783
TS5In	152.05	113.55	-612.939450	-612.996929
$[In(H_2O)\ (OH)\ (C\ H_4O)](H_2O)^+$ (**16In**)	149.54	111.62	-613.118816	-613.158987
$[Sc(H_2O)_5(OO)]^+$ (**11Sc**)	132.04	98.14	-1293.362099	-1293.425366
$[Sc(H_2O)_4O\ ](H_2O)^+$ (**12Sc**)	130.56	97.00	-1293.357876	-1293.422081
TS5Sc	151.30	112.97	-1371.897139	-1371.946588
$[Sc(H_2O)_4(=O)(C_2H_4O)](H_2O)^+$ (**18Sc**)	147.87	110.33	-1371.989662	-1372.034508
$[Sc(H_2O)_3(OH)_2(C_2H_4O)](H_2O)^+$ (**16Sc**)	148.89	111.12	-1372.051487	-1372.088168
$[Y(H_2O)\ O_2]^+$ (**11Y**)	152.81	114.13	-723.902303	-723.953824
$[Y(H_2O)\ O_2](H\ O)^+$ (**12Y**)	147.39	109.96	-723.903333	-723.955112
TS5Y	165.09	123.58	-802.444365	-802.481091
$[Y(H_2O)\ (OH)_2(C_2H_4O)](H_2O)_2^+$ (**17Y**)	170.09	127.44	-802.597803	-802.624239
$[La(H_2O)_7O_2](H_2O)^+$ (**12La**)	174.47	130.81	-793.621799	-793.659069
$[La(H_2O)_5O_2](H_2O)_3^+$ (**13La**)	163.90	122.67	-793.624952	-793.662989
TS5La	180.38	135.36	-872.164154	-872.190768
$[La(H_2O)_5(=O)(C_2H\ O)](H\ O)_3^+$ (**19La**)	183.18	137.52	-872.264461	-872.288542
$[La(H_2O)_5(OH)\ (C\ H_4O)](H_2O)^+$ (**17La**)	189.45	142.34	-872.301944	-872.322611
Cyclohexene	73.89	53.36	-234.599192	-234.588342
TS $[Ga(H_2O)\ (\underline{O}OH)](H_2O)^{2+}$ + Cyclohexene	162.99	121.97	-2692.16455	-2692.378507
TS $[In(H_2O)_4(\underline{O}OH)](H_2O)^{2+}$ + Cyclohexene	164.702	123.29	-769.251973	-769.468106
TS $[Sc(H_2O)_5(\underline{O}OH)]^{2+}$ + Cyclohexene	161.73	121.00	-1528.189822	-1528.402910
TS $[Y(H_2O)\ (\underline{O}OH)](H\ O)^{2+}$ + Cyclohexene	192.759	144.89	-958.766704	-958.953873
TS $[La(H_2O)_7(\underline{O}OH)](H_2O)^{2+}$ + Cyclohexene	211.839	159.58	-1028.496362	-1028.667965

Table S5 Cartesian atomic coordinates (in Å) of the calculated structures. Nuclear charges are indicated in the first column

$[Ga(H_2O)_5(OOH)]^{2+}$ (**3Ga**)

31	-0.166038	-0.029415	0.001885
8	-1.142297	0.006712	1.816476
8	0.884359	0.186202	-1.733689
8	1.307807	-0.713538	0.869008
8	-1.891125	0.557496	-0.887839
8	0.101133	2.009849	0.231004
8	-0.807645	-1.950986	-0.443372
1	-0.631941	-0.304031	2.583189
1	-2.075419	0.091520	2.065094
1	1.828722	0.005600	-1.526174
1	0.689778	-0.026353	-2.658086
8	2.477990	-0.064277	0.271420
1	-2.420812	0.058016	-1.529145
1	-2.099844	1.502234	-0.974428
1	-0.088090	-2.599415	-0.353732
1	-1.634863	-2.403856	-0.215630
1	0.783082	2.446872	-0.305632
1	0.151980	2.390061	1.123150
1	3.202804	-0.500452	0.748880

$[Ga(H_2O)_5(OOH)](C_2H_4)^{2+}$ (**3Ga**•C_2H_4)

31	-0.553253	-0.184463	-0.010145
8	-0.729960	0.740495	-1.849690
8	-0.743293	-1.355420	1.686767
8	-2.438431	0.517061	0.509428
8	1.197634	-1.067197	-0.360898
8	0.168223	1.330213	0.775990
8	-1.471739	-1.778760	-0.922490
1	-0.730509	1.702692	-1.664435
1	-0.145041	0.588828	-2.607723
1	0.041986	-1.698209	2.142257
1	-1.359360	-1.038796	2.367800
1	-3.315845	0.336391	0.141750
1	-2.364151	1.473822	0.700763
8	-0.640022	2.441029	0.245678
1	-1.768550	-2.565368	-0.438442
1	-1.894156	-1.762714	-1.795303
1	-0.199514	3.205816	0.651275
6	3.822336	0.024180	0.730206
6	3.996767	0.143138	-0.591782
1	3.425528	0.840333	1.326173
1	4.147737	-0.862453	1.266206
1	4.469338	-0.640617	-1.176344
1	3.752786	1.062285	-1.115716
1	1.339970	-1.926492	-0.783877
1	2.096712	-0.620440	-0.208700

TS1Ga

31	-0.405478	-0.092978	-0.008135
8	-1.297931	1.053225	-1.417043

8 -0.102964 -1.453532 1.541960
8 -0.925155 1.143866 1.512700
8 -0.152498 -1.691600 -1.307280
8 1.268796 0.798495 -0.152682
8 -2.348628 -0.927904 0.080183
1 -0.741300 1.889538 -1.268776
1 -1.343926 0.858219 -2.363977
1 0.328204 -2.319083 1.487390
1 0.031782 -1.092919 2.432812
1 -1.811437 1.382230 1.820969
1 -0.437743 1.973162 1.222911
8 0.338953 2.414277 -0.195722
1 -2.674276 -1.516805 0.777430
1 -3.103379 -0.463935 -0.314477
1 1.113466 2.970549 -0.360244
6 3.029131 0.014366 0.468203
6 2.836476 -0.937604 -0.490940
1 3.559226 0.929876 0.242428
1 2.861803 -0.194157 1.517828
1 2.481580 -1.929997 -0.234343
1 3.139087 -0.758564 -1.516419
1 -0.872464 -2.251268 -1.637416
1 0.600947 -1.749709 -1.914428

$[Ga(H_2O)_4(OOH)](H_2O)^{2+}$ (**4Ga**)

31 -0.289505 -0.217044 -0.031591
8 -1.423255 -1.631563 -0.842062
8 -0.927999 0.940379 -1.581191
8 -0.154686 -1.523215 1.582510
8 -0.782804 0.994004 1.224472
8 1.468443 -0.599528 -0.660675
8 -1.180305 2.250789 0.602277
1 -1.713954 -2.417726 -0.350371
1 -2.066757 -1.430340 -1.542269
1 -0.511395 1.151154 -2.430338
1 -1.268926 1.768120 -1.164830
1 0.587374 -2.106657 1.804517
1 -0.525537 -1.181137 2.414635
1 1.642794 -1.226165 -1.378566
1 2.377447 -0.082220 -0.381246
1 -1.728552 2.645947 1.300784
8 3.512442 0.576863 0.003711
1 4.237798 0.167850 0.496409
1 3.849678 1.377713 -0.421733

$[Ga(H_2O)_4(OOH)](H_2O)(C_2H_4)^{2+}$ (**4Ga**•C_2H_4)

31 0.258635 0.044862 0.300297
8 3.634582 -1.085760 -0.957099
8 -1.126949 -1.089906 -0.451993
8 1.224425 0.293182 -1.454833
8 -0.491939 -0.245550 2.216304
8 -0.037423 1.804013 0.632994
8 1.707396 -1.155153 0.822248
1 4.457992 -0.598801 -0.793673

1 3.896032 -1.876975 -1.454248
1 -2.112425 -0.816028 -0.520466
1 -0.931712 -1.673348 -1.202746
1 2.130149 -0.050582 -1.605808
1 1.198486 1.251366 -1.664549
8 0.631924 2.601861 -0.391021
1 1.830837 -1.472038 1.729681
1 2.549359 -1.236798 0.280361
1 0.218657 3.469551 -0.252835
1 -0.593440 0.557354 2.754947
1 -1.120463 -0.912230 2.532106
6 -4.148836 -1.025442 -0.495766
6 -3.813845 0.144707 -1.056176
1 -3.663071 0.238021 -2.127694
1 -3.772150 1.062176 -0.476547
1 -4.389332 -1.103430 0.560222
1 -4.276642 -1.926043 -1.089104

TS2Ga

31 0.147095 0.198257 0.081670
8 3.965959 -0.729552 -0.441885
8 -0.504313 2.005822 0.716752
8 0.120372 -0.262813 2.111392
8 -0.084514 0.971273 -1.827252
8 -1.097540 -1.132617 -0.226163
8 2.008885 0.718468 0.114175
1 4.655134 -0.488163 -1.075651
1 4.323828 -1.427607 0.122941
1 -0.915050 2.652449 0.121308
1 -0.875994 2.113545 1.607087
1 0.869604 -0.285922 2.726090
1 -0.417729 -1.057850 2.267301
8 0.449013 -1.786593 -0.274625
1 2.306720 1.583148 0.430356
1 2.829595 0.104448 -0.104735
1 0.397734 -2.272064 -1.112783
1 0.595453 1.299316 -2.435401
1 -0.797510 0.562393 -2.344638
6 -3.505196 -0.002867 -0.757737
6 -3.518457 -0.896300 0.244287
1 -3.607963 -0.585079 1.280062
1 -3.532469 -1.961660 0.053175
1 -3.515045 -0.322983 -1.794288
1 -3.597238 1.063162 -0.571057

$[Ga(H_2O)_4(OH)(Epox)](H_2O)^{2+}$ (**7Ga**)

31 -0.501813 0.104361 -0.078681
8 0.122189 1.166019 -1.409978
8 -1.400020 -0.868196 1.538353
8 0.551076 1.055223 1.325472
8 -1.798095 -1.215554 -1.107308
8 0.774928 -1.464014 -0.200088
8 -2.188877 1.339489 0.074427
1 2.026898 2.379001 -0.841901

1 -0.001634 0.918678 -2.332170
1 -2.001568 -1.613880 1.393003
1 -0.992300 -0.967559 2.411182
1 0.143123 1.631222 1.986479
1 1.341592 1.567185 0.893933
8 2.407198 2.124374 0.012134
1 -2.900436 1.415726 0.726495
1 -2.154980 2.144012 -0.466308
1 3.105501 2.751241 0.243264
6 2.179528 -1.469729 -0.694359
6 1.886972 -1.968936 0.647709
1 2.321974 -2.168607 -1.509436
1 2.600404 -0.478305 -0.810456
1 2.106221 -1.339564 1.501884
1 1.812323 -3.035062 0.824638
1 -2.557567 -0.902557 -1.621919
1 -1.439560 -2.003454 -1.543757

$[Ga(H_2O)_5(OH)]^{2+}$ (**9Ga**)

31 -0.000090 -0.006185 -0.135600
8 0.016286 -2.005955 0.445057
8 -0.016532 2.094572 -0.075690
8 -2.075940 -0.007713 -0.033145
8 2.075698 0.024688 -0.034055
8 0.002878 -0.422549 -1.871105
8 -0.001473 0.240849 1.883133
1 -0.753339 -2.545480 0.199715
1 0.796247 -2.531958 0.203019
1 -0.802428 2.605734 -0.327695
1 0.760856 2.618125 -0.328628
1 -2.721439 0.080264 0.684931
1 -2.542016 -0.212422 -0.860614
1 2.720220 0.124276 0.683379
1 2.544474 -0.172089 -0.861923
1 -0.008129 1.089114 2.352768
1 0.003939 -0.494784 2.515707
1 -0.002933 0.239803 -2.570629

$[Ga(H_2O)_5(OH)](H_2O)^{2+}$ (**9Ga**)

31 0.452571 0.000024 0.111044
8 0.573549 -2.085003 -0.063123
8 0.572640 2.085002 -0.064675
8 1.501533 0.001214 1.566145
8 -0.986284 -0.000878 -1.279576
8 1.737232 -0.000361 -1.545356
8 -1.122705 0.000093 1.391137
1 -0.007883 -2.730739 -0.490724
1 0.992609 -2.508264 0.703742
1 -0.008798 2.730520 -0.492586
1 0.991969 2.508685 0.701813
1 2.463273 0.000486 1.531910
1 -0.825224 -0.000952 -2.233469
1 -1.960990 -0.000752 -1.065798
1 2.260541 -0.785327 -1.770389

1 2.260008 0.784746 -1.771131
1 -2.084078 0.000279 1.220661
1 -0.915158 0.000691 2.337993
8 -3.423095 -0.000056 -0.203381
1 -4.009494 0.770043 -0.262275
1 -4.009445 -0.770255 -0.261480

TS3Ga

31 0.851205 -0.028383 -0.033318
8 2.077227 0.564906 -1.633741
8 -0.400140 -0.189357 1.619465
8 -0.460521 -0.426481 -1.170566
8 2.476041 0.144223 1.190585
8 0.797372 2.040794 0.369057
8 1.456993 -2.076149 -0.066258
1 1.616971 0.421937 -2.477346
1 3.033167 0.564105 -1.789549
1 -1.265177 -0.390366 1.190949
1 -0.314039 -0.683597 2.446565
1 2.895338 -0.558600 1.708286
1 2.712638 1.006080 1.566908
1 0.092909 2.384840 0.938994
1 0.892628 2.647765 -0.381405
1 0.774531 -2.504645 -0.610143
1 2.288459 -2.553617 -0.205787
8 -2.181299 -0.115896 -0.393765
1 -2.363924 -0.761542 -1.093920
6 -4.039727 0.692215 -0.309852
6 -4.289824 -0.478698 0.357721
1 -4.256761 0.796215 -1.366118
1 -3.805220 1.601772 0.227692
1 -4.195526 -0.544922 1.435199
1 -4.641414 -1.362972 -0.162875

TS4Ga

31 -0.718849 -0.430973 0.017314
8 -1.498342 -2.008558 -0.961250
8 -1.999571 -1.154235 1.576704
8 0.557559 -0.301265 -1.613312
8 0.581974 -0.395712 1.201697
8 -1.996270 0.880310 -0.595886
1 -1.024142 -2.412799 -1.705322
1 -1.965164 -2.700280 -0.465057
1 -2.874696 -0.858952 1.869454
1 -1.449661 -1.282771 2.368476
1 0.530553 0.259279 -2.401453
1 1.433367 -0.212243 -1.163991
1 -2.745300 0.652272 -1.164426
1 -2.032101 1.891523 -0.334232
8 2.245303 0.038680 0.447861
1 2.527445 -0.662621 1.056898
8 -2.070138 3.300072 0.016046
1 -1.996723 4.027689 -0.615632
1 -2.438076 3.659733 0.834012

6 4.412891 -0.045081 -0.323532
6 4.029107 1.049799 0.403261
1 4.327177 -0.066431 -1.403726
1 4.867413 -0.908255 0.151086
1 4.226862 1.118796 1.466078
1 3.681240 1.952570 -0.082163

$[Ga(H_2O)_4(OH)](H_2O)^{2+}$ (**10Ga**)

31 -0.307400 0.076237 0.018258
8 0.566907 1.606954 0.084774
8 -0.833835 -1.180948 -1.418123
8 1.306770 -1.010142 0.172699
1 0.127183 2.462462 0.025625
1 -1.619067 -1.089909 -1.982113
1 -0.179087 -1.763446 -1.838925
1 1.429772 -1.761168 0.769246
1 2.232811 -0.492543 0.057798
8 -2.268869 0.848676 -0.458986
1 -3.043573 0.794008 0.122445
1 -2.390845 1.632176 -1.019455
8 -1.201810 -0.668726 1.665801
1 -1.618156 -1.538934 1.781639
1 -1.063930 -0.270466 2.542740
8 3.416231 0.228961 -0.137812
1 3.468669 1.180415 0.019399
1 4.302460 -0.114118 -0.311209

$[In(H_2O)_5(OOH)]^{2+}$ (**3In**)

49 -0.162930 -0.029241 -0.020972
8 -1.105500 -0.579733 1.830953
8 0.981316 0.792700 -1.605239
8 1.476389 -0.776504 0.745132
8 -2.015267 0.535890 -0.868161
8 -0.227099 1.995293 0.733620
8 -0.432323 -1.978441 -0.889322
1 -0.502620 -0.946263 2.500739
1 -2.014219 -0.769903 2.109150
1 1.927520 0.644386 -1.368188
1 0.895084 0.992224 -2.547683
8 2.577930 0.080758 0.290520
1 -2.581343 0.085606 -1.514414
1 -2.383375 1.422857 -0.723270
1 0.363967 -2.518945 -0.743217
1 -1.109400 -2.547765 -1.284410
1 0.354791 2.682513 0.370070
1 -0.360358 2.206441 1.671525
1 3.349929 -0.378038 0.657314

$[In(H_2O)_5(OOH)](C_2H_4)^{2+}$ (**3In**•C_2H_4)

49 -0.482111 -0.176402 -0.018677
8 -0.694575 0.857612 -1.889959
8 -0.612223 -1.396711 1.759578
8 -2.373514 0.629581 0.619238
8 1.334340 -1.133990 -0.423595
8 0.316973 1.451628 0.746676

8 -1.520091 -1.805727 -0.928127
1 -0.644709 1.814121 -1.681303
1 -0.377795 0.723580 -2.794253
1 0.137391 -1.875930 2.145546
1 -1.182880 -1.122209 2.495455
1 -3.311245 0.455351 0.457951
1 -2.250339 1.586329 0.789080
8 -0.549877 2.529201 0.222563
1 -1.757764 -2.625249 -0.466865
1 -1.961627 -1.813216 -1.791592
1 -0.119415 3.316525 0.591947
6 3.816572 0.204674 0.725916
6 4.183807 0.009593 -0.546444
1 3.319630 1.116868 1.042100
1 4.072057 -0.510498 1.502112
1 4.747340 -0.868427 -0.847508
1 4.005054 0.759048 -1.311502
1 1.509033 -1.962612 -0.892572
1 2.228193 -0.688340 -0.251246

TS1In

49 -0.353058 -0.074568 -0.008218
8 -1.180797 1.141425 -1.540589
8 -0.151998 -1.478301 1.641564
8 -0.889278 1.242638 1.569220
8 -0.140694 -1.767595 -1.332937
8 1.430717 0.826910 -0.127627
8 -2.408205 -0.817950 0.030784
1 -0.624297 1.960834 -1.396420
1 -1.354830 1.020195 -2.483611
1 0.162288 -2.394346 1.637349
1 -0.039395 -1.132213 2.541110
1 -1.706973 1.501117 2.015134
1 -0.376105 2.054751 1.298317
8 0.487187 2.391837 -0.164261
1 -2.798232 -1.424452 0.677687
1 -3.132875 -0.342124 -0.403860
1 1.262314 2.956385 -0.287804
6 3.221425 0.028375 0.325546
6 2.850087 -1.086891 -0.364500
1 3.763253 0.826593 -0.163329
1 3.190903 0.059042 1.407327
1 2.492552 -1.971781 0.151566
1 3.032421 -1.159415 -1.431478
1 -0.846061 -2.322844 -1.698796
1 0.670335 -1.938551 -1.835983

$[In(H_2O)_4(OOH)](H_2O)^{2+}$ axial monodentate (**4In**)

49 -0.175756 -0.057705 0.034521
8 -1.188487 -1.040067 -1.489731
8 -0.538588 -0.875572 1.942123
8 1.176792 1.532121 0.001298
8 -1.662798 1.181451 0.224796
8 1.533528 -1.202253 -0.206091

8 -2.848417 0.537399 -0.354614
1 -1.066752 -1.671682 -2.212516
1 -2.098083 -0.646441 -1.506369
1 -1.320526 -0.528332 2.407087
1 -0.113667 -1.536558 2.511017
1 2.156070 1.483485 -0.064543
1 0.880378 2.457100 0.010427
1 1.617950 -2.157147 -0.347671
1 2.441500 -0.778097 -0.250594
1 -3.457814 1.289096 -0.433206
8 3.662901 0.373662 -0.265039
1 4.177459 0.488691 -1.080331
1 4.316064 0.373490 0.453223

$[In(H_2O)_4(OOH)](H_2O)^{2+}$ equatorial bidentate (**4In**)

49 -0.367592 -0.040501 0.001496
8 -1.760957 -1.513008 -0.608590
8 -0.613773 0.765342 -1.971002
8 -0.497906 -0.911908 1.957792
8 -1.090055 1.634580 0.694260
8 1.354982 -1.017781 -0.433563
8 0.401143 1.922427 0.606299
1 -2.204617 -2.149546 -0.025026
1 -2.272856 -1.464090 -1.432531
1 -0.176979 0.625325 -2.824798
1 -0.979728 1.667649 -1.964729
1 -0.006870 -1.615916 2.408385
1 -0.935495 -0.368897 2.635711
1 1.409548 -1.885455 -0.858784
1 2.334434 -0.660792 -0.293787
1 0.554083 2.568522 1.313882
8 3.680680 -0.189606 -0.098138
1 4.302918 -0.550901 0.547845
1 4.194631 0.298278 -0.755953

$[In(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (**5In**)

49 0.296583 -0.172316 0.042970
8 -3.114310 -0.049873 -0.750898
8 1.206936 -2.092572 -0.277488
8 1.184765 -0.278194 2.029392
8 -0.718813 -0.387164 -1.823496
8 -0.391811 1.606436 0.522994
8 -1.326962 -1.381721 0.730946
1 -4.022906 -0.172714 -1.060832
1 -3.066704 0.794928 -0.259956
1 0.656186 -2.891827 -0.292104
1 2.101319 -2.340701 -0.555483
1 1.737023 -0.907173 2.517112
1 1.056165 0.509197 2.582498
8 -1.772951 1.586589 1.011491
1 -1.500229 -1.538995 1.670606
1 -2.189697 -1.125922 0.311331
1 -1.848562 2.481432 1.377698
1 -1.692335 -0.204477 -1.771617

1 -0.454845 -0.510827 -2.744606
6 2.369876 0.755979 -0.980128
6 1.866892 2.012080 -0.930414
1 2.020703 2.658951 -0.073324
1 1.295418 2.433914 -1.750785
1 2.345039 0.198433 -1.914852
1 3.075437 0.422916 -0.221500

TS2In

49 0.027508 -0.415974 0.001822
8 -1.742208 0.082088 -0.657020
8 -1.355619 -1.452196 -1.219498
1 -1.769170 -1.436932 -2.093728
8 1.114021 -2.238015 -0.053235
1 2.007988 -2.480206 0.228925
1 0.729361 -2.990616 -0.530931
8 -0.958169 -1.121689 1.781842
1 -0.786835 -1.850070 2.397257
1 -1.921599 -1.006159 1.716045
8 1.261068 0.470802 -1.478812
1 0.983143 0.587787 -2.399324
1 2.038841 1.043762 -1.298081
8 1.398691 0.493828 1.290947
1 1.256097 0.635547 2.238387
1 2.133567 1.082663 0.972039
8 3.197082 1.904122 -0.124289
1 4.135741 1.659813 -0.142072
1 3.186276 2.874220 -0.130726
6 -1.766683 2.474035 0.558082
6 -2.803318 2.145991 -0.232989
1 -1.796577 2.299716 1.629577
1 -0.923561 3.039162 0.171788
1 -2.823534 2.412848 -1.282273
1 -3.696551 1.679488 0.163814

TS2In

49 0.110575 0.172089 0.023592
8 4.079976 -0.850351 -0.204465
8 -0.463416 2.213604 0.238331
8 -0.019130 0.143131 2.175898
8 -0.048220 0.507775 -2.097911
8 -1.205786 -1.282219 -0.021944
8 2.095287 0.687489 0.005033
1 4.744094 -0.801014 -0.904785
1 4.451865 -1.389674 0.505810
1 -0.760453 2.789649 -0.483364
1 -0.814493 2.576565 1.067001
1 0.625364 0.328057 2.875243
1 -0.592247 -0.579007 2.486462
8 0.341931 -1.907341 0.089321
1 2.438269 1.579844 0.150826
1 2.902024 0.041563 -0.073954
1 0.295300 -2.642739 -0.537874
1 0.609439 0.789557 -2.751569

1 -0.744075 0.017987 -2.565924
6 -3.484448 0.216337 -0.159956
6 -3.591405 -1.122080 -0.139222
1 -3.706333 -1.669514 0.787925
1 -3.650732 -1.703130 -1.051401
1 -3.476914 0.768905 -1.095016
1 -3.529292 0.798329 0.755604

$[In(H_2O)_4(OH)(Epox)](H_2O)^{2+}$ (**7In**)

49 0.105482 0.147625 -0.008575
8 3.564583 -0.998532 -0.197644
8 -0.567515 1.845550 1.167502
8 0.155517 -0.999173 1.832878
8 -0.112187 1.553206 -1.641713
8 -1.963004 -0.165813 -0.357934
8 2.021876 0.927108 0.181459
1 4.480068 -1.129172 -0.473635
1 2.995195 -1.654291 -0.629562
1 -0.800447 2.689225 0.751833
1 -0.758084 1.925793 2.113049
1 0.344703 -0.879166 2.774118
1 0.492541 -1.872780 1.564596
8 0.809809 -1.506634 -0.722674
1 2.362523 1.664755 0.701851
1 2.775592 0.233645 0.014968
1 0.499424 -1.988750 -1.492831
1 0.660893 1.908331 -2.107427
1 -0.866670 1.588288 -2.248468
6 -3.218728 -0.466523 0.368115
6 -2.783998 -1.350131 -0.711656
1 -2.313176 -2.295514 -0.469789
1 -3.237684 -1.264052 -1.691549
1 -3.991883 0.269395 0.183349
1 -3.067903 -0.775120 1.395892

$[In(H_2O)_5(OH)]^{2+}$ (**9In**)

49 -0.036480 -0.003071 -0.070004
8 0.311745 -2.128512 -0.156634
8 -0.054458 2.149665 -0.007472
8 -1.217810 -0.008681 -1.558422
8 0.940608 0.004261 1.824312
8 1.999910 0.196730 -0.790632
8 -1.911972 -0.197381 0.940741
1 -0.199476 -2.605997 -0.831522
1 0.655488 -2.783025 0.470162
1 -0.646047 2.551512 -0.666312
1 0.162686 2.826922 0.650720
1 -1.098543 -0.021660 -2.510120
1 0.559514 -0.054279 2.714262
1 1.901853 0.094398 1.922106
1 -2.580406 -0.215322 0.230074
1 -2.359026 -0.266802 1.795365
1 2.352006 1.024467 -1.155602
1 2.495274 -0.528372 -1.204102

$[In(H_2O)_5(OH)](H_2O)^{2+}$ (**9In**)

49	-0.392236	-0.004927	-0.078194
8	-0.552347	-2.133255	0.299981
8	-0.531959	2.158238	-0.192054
8	-1.465541	-0.227830	-1.630606
8	1.145873	0.158525	1.337259
8	-1.725621	0.196922	1.630433
8	1.255735	-0.159704	-1.405014
1	-0.074217	-2.794716	0.820443
1	-1.039181	-2.593302	-0.404214
1	-0.038675	2.897371	0.192456
1	-0.996592	2.486194	-0.979436
1	-2.408918	-0.169232	-1.792176
1	1.057564	0.260964	2.294818
1	2.110307	0.122239	1.085308
1	-2.228183	-0.547324	1.996141
1	-2.223882	1.004120	1.830918
1	2.218948	-0.155260	-1.253540
1	1.046639	-0.280793	-2.344149
8	3.561247	0.006322	0.196163
1	4.153344	0.772972	0.155800
1	4.143320	-0.755577	0.339857

TS3In

49	-0.765969	-0.034009	0.000865
8	-1.950392	0.139683	1.825897
8	0.591944	0.254584	-1.639561
8	0.655492	-0.715005	1.071794
8	-2.469107	0.370876	-1.197599
8	-0.812023	2.157054	0.088997
8	-1.249367	-2.140719	-0.337142
1	-1.405396	-0.153314	2.576743
1	-2.881528	0.089837	2.086650
1	1.458439	-0.011625	-1.243777
1	0.609958	0.149457	-2.599935
1	-3.028332	-0.233997	-1.706700
1	-2.777984	1.275778	-1.357317
1	-0.176271	2.703554	-0.396969
1	-1.006526	2.613500	0.922044
1	-0.539418	-2.591460	0.155351
1	-1.888501	-2.802281	-0.638019
8	2.382393	-0.164900	0.329076
1	2.498301	-0.965812	0.864567
6	4.173655	0.616327	0.486421
6	4.477973	-0.328953	-0.464244
1	3.948525	1.636358	0.203818
1	4.378607	0.442435	1.535634
1	4.830080	-1.316217	-0.186644
1	4.411258	-0.106600	-1.522581

TS4In

49	-0.461831	0.243050	-0.103575
8	-1.282042	2.204948	-0.132294
8	-2.171242	-0.238383	-1.334024

8 0.995759 0.907796 1.313866
8 0.904539 -0.343477 -1.261337
8 -1.619861 -0.608098 1.408683
1 -0.818536 3.015366 0.128268
1 -2.047587 2.460713 -0.669492
1 -2.949653 -0.747290 -1.020073
1 -1.991980 -0.481608 -2.256577
1 1.161976 1.339471 2.161999
1 1.842851 0.611341 0.886900
1 -1.351065 -0.787689 2.320535
1 -2.492742 -1.048494 1.224989
8 2.608226 -0.418859 -0.342632
1 2.801546 -0.142477 -1.253024
8 -3.883630 -1.614488 0.383613
1 -3.997897 -2.573566 0.294876
1 -4.756308 -1.273644 0.633751
6 4.785831 -0.068474 0.190669
6 4.285157 -1.344854 0.092938
1 4.781585 0.468783 1.131689
1 5.234732 0.429376 -0.661801
1 4.418470 -1.932232 -0.807222
1 3.954379 -1.883038 0.971685

$[In(H_2O)_4(OH)](H_2O)^{2+}$ (**10In**)

49 0.337442 0.009872 0.106896
8 1.820923 0.404851 -1.332070
8 0.769513 -2.042893 -0.345936
8 0.304904 2.161450 0.374546
8 -1.399274 0.120288 -0.947490
8 0.733719 -0.601316 1.838860
1 2.165704 1.275812 -1.586505
1 2.451149 -0.267056 -1.640414
1 0.563851 -2.714311 -1.012104
1 0.995411 -2.487572 0.492296
1 -0.316794 2.805448 0.000601
1 0.751128 2.592997 1.122012
1 -1.473157 0.133141 -1.912826
1 -2.366229 -0.010931 -0.548500
1 0.643066 -0.200607 2.706657
8 -3.666488 -0.178412 0.029134
1 -4.347078 0.508229 0.056226
1 -4.108077 -1.030636 0.148306

$[Sc(H_2O)_5(OOH)]^{2+}$ (**3Sc**)

21 0.212349 0.068042 0.028783
8 1.223998 0.486084 1.961629
8 -0.989057 -0.666631 -1.634172
8 -1.478949 0.532749 0.673633
8 2.067613 -0.513325 -1.152443
8 0.337830 -2.057575 0.695727
8 0.598556 2.111349 -0.724246
1 0.709680 0.793064 2.725852
1 2.158660 0.569508 2.204430
1 -1.950031 -0.557586 -1.477889

1 -0.852353 -0.995122 -2.533624
8 -2.735870 0.025414 0.247625
1 2.489932 -0.086431 -1.912902
1 2.525343 -1.359553 -1.032341
1 -0.138716 2.739862 -0.777461
1 1.403956 2.615437 -0.912388
1 -0.195834 -2.768282 0.308159
1 0.571508 -2.348825 1.589977
1 -3.374440 0.624540 0.671705

$[Sc(H_2O)_5(OOH)](C_2H_4)^{2+}$ (**3Sc•**C_2H_4)

21 -0.682577 -0.002327 0.011252
8 -2.878509 -0.321683 0.376456
8 1.176428 1.083502 -0.279799
8 -0.968561 -0.764514 -2.049318
8 -0.723093 0.980422 2.005172
8 0.584538 -1.441706 0.208048
8 -1.496222 1.969302 -0.897707
1 -3.246207 -1.186293 0.613861
1 -3.627477 0.260796 0.185845
1 2.088052 0.681792 -0.178535
1 1.299259 1.951907 -0.686862
1 -1.716265 -0.788658 -2.663096
1 -0.340485 -1.444136 -2.341037
8 -0.636428 -2.041598 0.757703
1 -1.736816 2.774369 -0.416204
1 -1.556400 2.191159 -1.838416
1 -0.351468 -2.378317 1.625124
6 3.888470 -0.418340 -0.543322
6 4.145111 0.419834 0.466383
1 3.517568 -1.423258 -0.367325
1 4.112159 -0.151593 -1.571798
1 4.584983 1.397924 0.297202
1 3.997758 0.125263 1.500916
1 -1.414259 0.939509 2.682348
1 0.057014 1.379644 2.418880

TS1Sc

21 -0.489258 0.083589 -0.047445
8 -1.982064 0.354354 -1.729504
8 0.233826 -1.027870 1.808876
8 -1.418219 1.343498 1.538725
8 0.142221 -1.719716 -1.188479
8 1.302137 0.881047 -0.305776
8 -2.215093 -1.366472 0.523164
1 -2.206702 1.242648 -2.042849
1 -2.305002 -0.264666 -2.399126
1 0.901334 -1.728044 1.811901
1 0.330969 -0.556246 2.649193
1 -2.146479 1.244760 2.166902
1 -1.176215 2.282847 1.499989
8 -0.022562 2.000521 -0.569073
1 -2.176318 -1.985114 1.266190
1 -3.133638 -1.346752 0.220022

1 0.358797 2.431113 -1.347729
6 3.371474 0.378402 0.379591
6 3.207072 -0.687466 -0.433831
1 3.708154 1.332567 -0.002635
1 3.281670 0.295125 1.456473
1 2.988844 -1.674175 -0.036759
1 3.402999 -0.610945 -1.497895
1 -0.307086 -2.563701 -1.337526
1 0.959863 -1.723290 -1.707833

$[Sc(H_2O)_5(OH)(Epox)]^{2+}$ cappedtrigonalprismatic2 (**6Sc**)

21 0.559828 -0.126466 0.025562
8 1.577726 0.059812 -1.960552
8 -0.167352 -0.495914 2.122406
8 -0.278720 -2.041237 -0.833571
8 0.075296 2.044555 -0.751119
8 1.914151 1.428393 1.057116
1 2.302725 -0.536200 -2.193549
1 1.438091 0.660058 -2.704294
1 0.423222 -1.009064 2.691672
1 -0.945860 -0.267705 2.645556
1 0.267754 -2.831875 -0.729471
1 -0.966635 -2.243466 -1.480306
1 0.736456 2.748994 -0.786647
1 -0.728302 2.384109 -1.164618
1 2.777558 1.077311 1.316378
1 1.735594 2.189226 1.626102
8 1.956502 -1.251492 0.484536
1 2.677536 -1.848171 0.703553
8 -1.721265 0.159719 -0.229318
6 -3.001936 -0.533665 -0.060958
6 -2.937563 0.918497 0.096191
1 -3.402218 -0.944740 -0.981047
1 -3.054236 -1.170867 0.814268
1 -3.289729 1.552701 -0.710048
1 -2.942064 1.355813 1.088261

$[Sc(H_2O)_5(OH)(Epox)]^{2+}$ cappedtrigonalprismatic3 (**6Sc**)

21 0.413951 -0.021583 -0.122297
8 0.542698 0.612088 2.085895
8 0.263415 -0.230752 -1.935242
8 2.327244 -1.445401 -0.360173
8 -0.038399 -2.073288 0.736112
8 2.320812 1.240527 0.013307
8 -0.172304 2.207287 -0.357619
1 -0.059322 0.392184 2.809850
1 1.321086 1.028345 2.481210
1 0.172038 -0.307989 -2.889331
1 2.534745 -1.718650 -1.265081
1 2.980328 -1.858630 0.221446
1 0.473579 -2.861171 0.512246
1 -0.820375 -2.361794 1.223870
1 2.314764 2.189898 -0.169314
1 3.188911 0.901892 -0.242759

1 -0.520693 2.825224 0.299216
1 -0.348622 2.583441 -1.231120
8 -1.768780 -0.104367 0.334241
6 -2.989798 0.596764 -0.089386
6 -2.886166 -0.846519 -0.285035
1 -3.566485 0.987028 0.740973
1 -2.853123 1.251946 -0.941084
1 -3.392211 -1.513827 0.403265
1 -2.659299 -1.234876 -1.270793

$[Sc(H_2O)_5(OH)(Epox)]^{2+}$ cappedtrigonalprismatic6 or 12 (**6Sc**)

21 0.440801 0.089634 0.165238
8 0.031062 -2.050450 0.898946
8 -0.285253 2.349490 0.110440
8 0.533243 0.521158 1.948455
8 1.912021 1.391198 -0.997422
8 2.488745 -0.966980 0.189504
8 0.486473 -1.094795 -1.833658
1 -0.211814 -2.857576 0.426215
1 -0.101920 -2.210350 1.843532
1 -0.371960 2.724431 0.998055
1 -0.772892 2.921243 -0.497431
1 0.741035 0.632190 2.880842
1 1.894306 2.349812 -0.870707
1 2.511873 1.202149 -1.730917
1 3.305694 -0.466256 0.323683
1 2.589695 -1.791742 0.684498
1 1.246043 -1.583694 -2.178775
1 -0.179388 -1.072030 -2.534111
8 -1.688159 -0.035305 -0.394349
6 -2.978664 0.555685 -0.006964
6 -2.891571 -0.876469 -0.285773
1 -3.016518 0.893348 1.022041
1 -3.388940 1.220070 -0.758417
1 -2.869010 -1.575026 0.541980
1 -3.236665 -1.258706 -1.239381

$[Sc(H_2O)_5(OH)(Epox)]^{2+}$ cappedtrigonalprismatic8 (**6Sc**)

21 -0.589808 0.090562 0.014273
8 -0.536362 -0.694337 -2.125581
8 -0.023458 1.719844 1.548303
8 -0.114382 -0.903548 1.997629
8 -1.466174 -2.110216 0.118391
8 -2.362886 0.556659 0.065135
1 0.217544 -0.676767 -2.729281
1 -1.326286 -0.862962 -2.657696
1 0.284267 2.571819 1.208646
1 -0.612111 1.923419 2.289255
1 -0.531867 -1.743570 2.233154
1 0.322365 -0.548823 2.782882
1 -2.432423 -2.133133 0.171687
1 -1.191206 -2.922924 -0.327751
1 -3.262638 0.889181 0.136777
8 -0.169327 2.044969 -1.158325

1 -0.940256 2.578861 -1.398724
1 0.512196 2.228346 -1.818640
8 1.616377 -0.143636 -0.401390
6 2.937701 0.280587 0.096566
6 2.694871 -1.129864 -0.191084
1 3.490170 0.883056 -0.614964
1 2.932867 0.625338 1.124025
1 3.068353 -1.560442 -1.112686
1 2.509251 -1.815401 0.627380

$[Sc(H_2O)_5(OH)(Epox)]^{2+}$ cappedtrigonalprismatic10 (**6Sc**)

21 -0.366069 -0.000049 -0.104838
8 -2.090484 1.480606 -0.649468
8 0.116506 -2.081065 0.696816
8 -2.087986 -1.484159 -0.650026
8 -1.364266 0.002938 1.972746
8 0.116542 2.083157 0.691402
1 -2.208944 1.647150 -1.595267
1 -2.938973 1.666363 -0.224581
1 0.899755 -2.379720 1.177674
1 -0.344547 -2.862922 0.363256
1 -2.202378 -1.652216 -1.596073
1 -2.937384 -1.672150 -0.227961
1 -1.482162 0.779602 2.536623
1 -1.484662 -0.772517 2.537754
1 -0.345784 2.863938 0.357077
1 0.900797 2.383506 1.169551
8 0.001021 -0.001683 -1.905678
1 0.208618 0.005206 -2.844368
8 1.805360 0.000463 0.390974
6 2.935242 0.729353 -0.216787
6 2.934761 -0.730204 -0.215657
1 2.677669 1.255882 -1.128188
1 3.537978 1.261294 0.510417
1 2.676754 -1.257999 -1.126202
1 3.537123 -1.261347 0.512431

$[Sc(H_2O)_5(OH)(Epox)]^{2+}$ pentagbipiram1 (**6Sc**)

21 -0.416036 -0.010233 0.130535
8 0.064341 -2.157613 -0.425715
8 0.226259 2.105056 -0.423916
8 -0.388785 -0.021605 1.959100
8 -2.346581 -1.354670 0.269352
8 -2.205724 1.547704 0.319556
1 0.965710 -2.504253 -0.444581
1 -0.534488 -2.886597 -0.213898
1 -0.381156 2.827707 -0.211757
1 1.110817 2.481321 -0.509322
1 -0.287433 -0.050258 2.915022
1 -3.087963 -1.497131 -0.334584
1 -2.678563 -1.521256 1.162837
1 -2.978114 1.712062 -0.238676
1 -2.486280 1.710122 1.231693
8 -0.804765 -0.011389 -2.126880

1 -0.789381 0.752989 -2.719198
1 -0.789790 -0.801562 -2.684777
8 1.815860 -0.165531 -0.015161
6 3.154221 0.128771 -0.546472
6 2.972101 -0.086067 0.889523
1 3.559786 -0.662943 -1.165639
1 3.277329 1.136636 -0.927574
1 3.245611 -1.038003 1.329211
1 2.947895 0.764224 1.561011

$[Sc(H_2O)_5(OH)(Epox)]^{2+}$ pentagbipiram2 (**6Sc**)

21 0.584641 0.000120 -0.020638
8 0.953220 -0.037393 2.308823
8 0.452835 -1.434321 -1.857157
8 0.263289 -2.121203 0.709587
8 0.452845 1.494451 -1.810806
8 2.408737 0.001840 -0.209075
8 0.265029 2.097745 0.776400
8 -1.635552 0.001569 -0.114419
6 -2.883665 0.728657 0.166576
6 -2.884225 -0.733207 0.143145
1 0.404827 -0.050177 3.105020
1 1.877172 -0.040711 2.597017
1 1.287000 -1.648339 -2.299014
1 -0.249132 -1.563378 -2.508865
1 0.257808 -2.859672 0.085785
1 0.553048 -2.461445 1.565791
1 -0.250044 1.646475 -2.456555
1 1.286349 1.722853 -2.246694
1 3.366836 0.002492 -0.292167
1 0.261268 2.855191 0.175759
1 0.552551 2.411262 1.643492
1 -2.880862 1.250709 1.115826
1 -3.268726 1.275885 -0.685904
1 -2.881773 -1.285351 1.075209
1 -3.269683 -1.252522 -0.726440

$[Sc(H_2O)_5(OH)]^{2+}$ (**9Sc**)

21 -0.100371 -0.000107 -0.148074
8 0.122877 -2.201301 -0.103079
8 0.119608 2.201435 -0.103305
8 -0.808150 -0.000677 -1.818569
8 0.723001 0.000662 1.999360
8 2.100123 0.001488 -0.579104
8 -2.114769 -0.001441 0.760885
1 -0.195227 -2.741389 -0.843074
1 0.344354 -2.809952 0.617024
1 -0.199168 2.740937 -0.843438
1 0.340004 2.810518 0.616763
1 -1.131189 -0.000911 -2.726893
1 0.308792 0.000494 2.874768
1 1.679222 0.001329 2.158334
1 -2.866466 -0.001855 0.147909
1 -2.487089 -0.001969 1.654292

1 2.585965 0.777307 -0.897759
1 2.587070 -0.773592 -0.897872

$[Sc(H_2O)_5(OH)](H_2O)^{2+}$ (**9Sc**)

21 0.547767 -0.000280 0.182192
8 0.694713 -2.204552 -0.046448
8 0.693627 2.204553 -0.041936
8 1.674185 -0.001163 1.612755
8 -1.061106 0.001774 -1.414256
8 1.951504 0.001914 -1.567161
8 -1.267166 -0.002001 1.384983
1 0.182543 -2.833351 -0.574183
1 1.215946 -2.719252 0.588033
1 0.180749 2.834172 -0.567997
1 1.214801 2.718168 0.593469
1 2.275610 -0.001652 2.364822
1 -0.948606 0.002922 -2.374400
1 -2.025376 0.001174 -1.220189
1 2.448310 -0.773557 -1.866260
1 2.447141 0.778528 -1.865204
1 -2.198401 -0.001689 1.067860
1 -1.261814 -0.003160 2.352220
8 -3.534367 -0.000063 -0.168644
1 -4.122593 0.769547 -0.198378
1 -4.122526 -0.769653 -0.200186

$[Sc(H_2O)_4(OOH)](H_2O)^{2+}$ axial monodentate (**4Sc**)

21 -0.248223 0.156580 -0.065461
8 -1.174559 -0.458683 1.771799
8 -0.571667 2.182916 -0.755980
8 1.167172 -1.012323 -1.154791
8 -1.849617 -0.468562 -0.756964
8 1.552932 0.758942 1.112616
8 -3.054544 -0.835449 -0.112181
1 -0.938627 -0.533705 2.707602
1 -2.082193 -0.807415 1.646272
1 -1.390017 2.424935 -1.220394
1 -0.022548 2.980813 -0.708382
1 2.140083 -1.023283 -0.964193
1 0.974596 -1.644143 -1.864896
1 1.668292 1.320514 1.892877
1 2.438301 0.393228 0.876247
1 -3.518170 -1.369971 -0.781095
8 3.623552 -0.610800 -0.101100
1 4.080451 -1.332990 0.358404
1 4.316359 -0.144490 -0.594954

$[Sc(H_2O)_4(OOH)](H_2O)^{2+}$ axial bidentate (**4Sc**)

21 -0.454651 0.058472 0.076049
8 -0.725030 -1.343857 1.711486
8 -0.774945 2.205676 -0.126014
8 0.994163 -0.731365 -1.311559
8 -2.373971 -0.060595 -0.042362
8 1.398924 0.666196 1.145264
8 -1.917747 -0.781122 -1.236295

1 -0.129328 -1.760295 2.351934
1 -1.618976 -1.693000 1.864007
1 -1.676416 2.550345 -0.233842
1 -0.171252 2.963763 -0.112987
1 1.973799 -0.663154 -1.194360
1 0.811287 -1.260406 -2.102134
1 1.515842 1.126711 1.989139
1 2.294885 0.457318 0.787082
1 -2.447817 -0.406080 -1.963042
8 3.502147 -0.208725 -0.393989
1 4.083255 -0.926895 -0.097890
1 4.084070 0.414110 -0.857169

$[Sc(H_2O)_4(OOH)](H_2O)^{2+}$ equatorial monodentate (**4Sc**)

21 0.508943 -0.247001 0.023692
8 1.193209 1.393145 -0.461173
8 1.232414 -0.836644 2.006048
8 -1.112297 -1.324005 -0.933384
8 2.075058 -1.401600 -1.011801
8 -1.134867 0.868848 0.847276
1 2.128087 -1.121224 2.248055
1 0.767832 -0.659297 2.839733
1 -2.061246 -1.082674 -0.762284
1 -1.096043 -2.011392 -1.615377
1 2.718150 -0.945834 -1.580951
1 2.293203 -2.346149 -1.050802
1 -1.023129 1.837819 0.830019
1 -2.091511 0.657782 0.766882
8 0.526832 2.643826 -0.547199
1 1.263132 3.270791 -0.661506
8 -3.465275 -0.313775 -0.065768
1 -4.038870 0.191575 -0.663016
1 -4.067988 -0.842742 0.479726

$[Sc(H_2O)_4(OOH)](H_2O)^{2+}$ equatorial bidentate (**4Sc**)

21 0.512480 0.024987 -0.037044
8 2.434081 0.250720 -1.081158
8 0.817648 -2.114846 -0.475558
8 0.677791 2.205763 0.299061
8 0.765532 -0.365169 1.811836
8 -1.231213 0.240531 -1.251024
8 -0.690540 -0.493642 1.661079
1 2.938083 1.066714 -1.225841
1 3.003800 -0.482983 -1.361639
1 0.566820 -2.676950 -1.224137
1 1.020396 -2.705753 0.268391
1 0.281271 2.945849 -0.185661
1 1.072385 2.576409 1.104917
1 -1.283130 0.374386 -2.208611
1 -2.196502 0.157868 -0.912560
1 -1.055330 0.041441 2.388586
8 -3.614640 0.050599 -0.357069
1 -4.266038 0.763452 -0.402910
1 -4.113117 -0.776804 -0.319933

$[Sc(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ (**5Sc**)

21 -0.175372 0.094658 0.025602
8 3.981391 -0.254261 -0.172865
8 -0.878058 2.281859 0.066813
8 -0.245191 0.319756 2.228100
8 -0.242553 0.147364 -2.191202
8 -0.398145 -1.791250 0.328365
8 1.745683 1.060676 -0.191621
1 4.661786 -0.171578 -0.854317
1 4.440424 -0.521061 0.634602
1 -0.981939 2.859170 -0.703886
1 -1.387067 2.698294 0.777733
1 0.129797 0.972386 2.836738
1 -0.417694 -0.483451 2.744691
8 1.063367 -1.642776 0.338633
1 1.921266 2.009065 -0.132661
1 2.635498 0.578791 -0.167000
1 1.369862 -2.298730 -0.311544
1 0.456441 0.493726 -2.765344
1 -0.865928 -0.328026 -2.760516
6 -3.069052 0.060990 0.088257
6 -2.962163 -1.150529 -0.475028
1 -2.814254 -2.050365 0.111548
1 -3.091535 -1.292030 -1.544305
1 -3.325586 0.934716 -0.501679
1 -3.072923 0.177572 1.169126

TS2Sc

21 0.072664 0.275530 0.020556
8 4.094269 -0.957052 -0.070602
8 -0.722423 2.369295 0.118753
8 -0.127194 0.387749 2.224541
8 0.014227 0.636953 -2.172693
8 -1.107939 -1.251372 -0.026590
8 2.179398 0.762545 0.044591
1 4.796533 -0.959671 -0.733685
1 4.411914 -1.486720 0.671758
1 -0.901054 2.958630 -0.629130
1 -1.059624 2.814579 0.910460
1 0.455043 0.767440 2.898696
1 -0.622172 -0.328791 2.651789
8 0.565246 -1.687291 0.052099
1 2.596971 1.625922 0.168387
1 2.930811 0.077583 0.008085
1 0.563009 -2.449002 -0.546146
1 0.730651 0.966324 -2.735274
1 -0.616863 0.189031 -2.756079
6 -3.350042 -0.077594 -0.111265
6 -3.370736 -1.427482 -0.100905
1 -3.446381 -1.987073 0.823106
1 -3.401068 -2.001905 -1.018565
1 -3.381266 0.479275 -1.042370
1 -3.422457 0.492096 0.809532

$[Sc(H_2O)_4(OH)(Epox)](H_2O)^{2+}$ cis (**7Sc**)

21	0.073450	-0.016864	0.000364
8	4.303245	-0.731156	-0.008619
8	-0.387629	2.256055	0.025196
8	0.046736	0.361386	2.222958
8	0.047656	0.416269	-2.213265
8	-2.054301	-0.304565	-0.001365
8	2.122495	0.680157	0.008309
1	4.838915	-0.936535	-0.784864
1	4.838137	-0.957306	0.762374
1	-0.551121	2.814482	-0.747223
1	-0.553892	2.801648	0.806141
1	0.864171	0.419945	2.738194
1	-0.631755	0.034418	2.830553
8	0.498562	-1.783690	-0.021790
1	2.413403	1.601344	0.020079
1	2.952265	0.104151	0.001623
1	0.768481	-2.706649	-0.031114
1	0.866144	0.485242	-2.725564
1	-0.629672	0.103015	-2.829354
6	-3.482128	0.057806	-0.001973
6	-3.092771	-1.352807	-0.014999
1	-3.133690	-1.930269	0.900639
1	-3.128157	-1.911872	-0.942208
1	-3.807521	0.532724	-0.920030
1	-3.812870	0.514170	0.923553

$[Sc(H_2O)_4(OH)(Epox)](H_2O)^{2+}$ trans (**7Sc**)

21	-0.123493	-0.513676	-0.000874
8	0.063090	-0.689275	2.213458
8	0.088240	-0.718419	-2.210131
8	1.560863	0.944944	-0.004169
6	3.023495	1.111311	0.003454
6	2.160696	2.291064	-0.001161
8	-1.541576	-1.663687	-0.000674
8	-1.338718	1.256428	-0.019493
8	1.552692	-2.028894	0.019768
1	-0.598243	-1.212087	2.690237
1	0.549829	-0.173494	2.870652
1	-0.565756	-1.248921	-2.688523
1	0.580538	-0.208029	-2.867411
1	3.503437	0.796502	-0.915506
1	3.494050	0.796560	0.927266
1	1.999621	2.837882	0.920929
1	2.009361	2.837548	-0.925104
1	-2.314129	-2.236493	-0.000073
1	-2.349944	1.253140	-0.024812
1	-1.062929	2.181064	-0.032585
1	1.805759	-2.556269	-0.750853
1	1.791608	-2.549627	0.799369
8	-3.932446	1.272111	0.000189
1	-4.499620	1.410292	-0.768682
1	-4.472541	1.459213	0.778124

$[Sc(H_2O)_4(OH)](H_2O)^{2+}$ axial (**10Sc**)

21 -0.624536 0.092368 -0.002288
8 1.091866 -1.373108 0.034624
8 -1.951921 1.319171 -0.035687
8 1.011612 1.463761 -0.034174
8 -1.285134 -0.771039 1.873524
8 -1.281861 -0.866249 -1.832356
1 2.025543 -1.052552 0.026681
1 1.122265 -2.340277 0.058262
1 -2.640278 1.995278 -0.053767
1 0.914099 2.427737 -0.056804
1 1.973590 1.231313 -0.029506
1 -2.096162 -0.453104 2.302338
1 -0.889095 -1.431482 2.462017
1 -2.092276 -0.570133 -2.277694
1 -0.885630 -1.555903 -2.386157
8 3.383122 0.156703 -0.004226
1 3.970225 0.168638 -0.776344
1 3.971492 0.206840 0.765387

$[Sc(H_2O)_4(OH)](H_2O)^{2+}$ equatorial (**10Sc**)

21 0.458596 -0.000077 0.071999
8 0.723424 -2.196784 -0.081126
8 0.721141 2.196961 -0.080692
8 -1.341692 -0.000600 -1.044681
8 0.204401 -0.000395 1.850615
1 0.598096 -2.817439 -0.814903
1 0.767700 -2.729032 0.729033
1 0.593766 2.817587 -0.814142
1 0.765790 2.729095 0.729520
1 -1.471472 -0.001453 -2.004252
1 -2.286748 -0.000362 -0.624714
1 0.072387 -0.000680 2.806470
8 -3.647902 -0.000312 -0.002156
1 -4.216784 0.776711 0.077725
1 -4.216237 -0.777616 0.078865
8 2.534837 0.001278 -0.662018
1 3.103850 0.780595 -0.758012
1 3.105449 -0.776970 -0.757094

TS3Sc

21 -0.988174 0.054691 -0.070425
8 -2.134379 -0.431977 -1.937649
8 0.262222 0.096808 1.758303
8 0.581655 0.329007 -0.892675
8 -2.858941 -0.072112 1.343985
8 -1.116013 -2.188082 0.217682
8 -1.535105 2.215927 -0.188515
8 2.279729 0.126343 -0.367175
1 -1.668902 -0.384232 -2.786249
1 -3.079109 -0.493307 -2.137308
1 1.186814 0.264785 1.505363
1 0.171493 0.180010 2.716164
1 -3.325406 0.590012 1.872715

1 -3.254979 -0.923890 1.577112
1 -0.574680 -2.683720 0.848151
1 -1.338844 -2.802866 -0.495726
1 -0.865931 2.809603 -0.558981
1 -2.346194 2.732658 -0.089961
1 2.509198 0.762730 -1.063356
6 4.239972 -0.702862 -0.287395
6 4.423278 0.482597 0.360505
1 4.464238 -0.811675 -1.342005
1 3.994612 -1.607873 0.253250
1 4.298395 0.566054 1.433307
1 4.768096 1.367492 -0.163855

TS4Sc

21 -0.685423 0.507335 0.050858
8 -1.076500 2.685572 -0.069853
8 -2.445080 0.155040 -1.235384
8 0.762792 0.702338 1.704921
8 0.758840 0.218298 -0.947796
8 -1.616111 -1.136819 1.187241
1 -0.392829 3.341207 -0.273517
1 -1.917621 3.164005 -0.032757
1 -3.134310 -0.518232 -1.035709
1 -2.508393 0.377765 -2.174937
1 0.823168 0.989829 2.625603
1 1.659504 0.550692 1.354585
1 -1.237195 -1.644497 1.917287
1 -2.452756 -1.575873 0.907788
8 2.387310 -0.264295 -0.501993
1 2.702914 0.139156 -1.327737
8 -3.921746 -1.881390 -0.107540
1 -3.981365 -2.738003 -0.556998
1 -4.796343 -1.734299 0.283076
6 4.694936 -0.314379 -0.062609
6 4.137367 -1.529887 -0.314806
1 4.759003 0.082423 0.943617
1 5.155477 0.272291 -0.850779
1 4.159474 -1.968290 -1.305536
1 3.765307 -2.156572 0.485726

$[Y(H_2O)_7(OOH)]^{2+}$ (**3Y**)

39 -0.194186 0.024935 0.016856
8 -2.463529 0.821573 0.659448
8 -1.760465 -1.059830 -1.549100
8 -1.145871 -1.816796 1.312549
8 0.968649 -1.747257 -1.104217
8 0.123421 1.989552 1.413299
8 1.353998 -0.728223 1.766427
8 -0.415384 1.691772 -1.718103
8 1.724013 0.861036 -0.579078
1 -2.867280 1.680053 0.470602
1 -3.038640 0.392168 1.308015
1 -1.434061 -1.531225 -2.328360
1 -2.697107 -0.881707 -1.706059

1 -0.592846 -2.250670 1.978108
1 -1.867072 -2.425880 1.104564
1 1.899729 -1.467307 -1.224904
1 0.946050 -2.712260 -1.114979
1 -0.369262 2.561491 2.015350
1 0.983143 2.403495 1.245232
1 2.243244 -0.653155 1.362927
1 1.441943 -0.424486 2.679618
1 -1.044860 2.114207 -2.315697
1 0.481035 1.955226 -1.986747
8 2.850790 -0.039760 -0.383665
1 3.604261 0.491035 -0.685545

$[Y(H_2O)_7(OOH)](C_2H_4)^{2+}$ (**3Y**•C_2H_4)

39 0.581936 0.038051 0.001273
8 1.110291 -1.799062 -1.407843
8 -0.310230 -1.708407 -0.983452
8 -0.793260 0.734215 -1.918108
8 2.040366 1.331512 -1.500187
8 0.378499 -1.915750 1.527568
8 -1.593418 0.253629 1.019471
1 1.051508 -2.004459 -2.352555
1 -1.242394 1.494034 -2.308770
1 -1.192975 -0.076761 -2.270248
1 1.808647 1.608397 -2.396553
1 3.001809 1.232893 -1.474970
1 0.810606 -2.433765 2.217628
1 -0.026596 -2.536035 0.893626
1 -2.473964 0.167720 0.583060
1 -1.705346 -0.148445 1.891717
8 2.963094 -0.568362 0.353548
1 3.274535 -1.392048 -0.048258
1 3.574966 -0.350874 1.068693
8 0.140912 2.486715 0.346995
1 0.604014 3.235210 -0.052099
1 -0.704426 2.814331 0.683339
8 1.217676 0.810821 2.270334
1 1.363632 0.337394 3.099361
1 1.153809 1.749783 2.490405
6 -4.465368 -0.794550 -0.000663
6 -4.668645 0.524681 0.036552
1 -4.239754 -1.314653 -0.926183
1 -4.591369 -1.414468 0.881712
1 -4.622618 1.133906 -0.860923
1 -4.966965 1.030584 0.949427

TS1Y

39 0.409607 -0.014463 -0.026970
8 -0.368205 -0.700309 -1.957870
8 -1.735867 -0.272767 -0.867822
8 -0.521291 2.151170 -0.648082
8 2.145321 1.064577 -1.508082
8 -0.605488 -2.153825 0.636263
8 -0.677402 0.707223 2.060571

1 -0.841637 -0.523544 -2.777864
1 -0.371010 3.104170 -0.657035
1 -1.360549 1.956275 -1.094370
1 1.928790 1.732569 -2.172083
1 2.756011 0.447639 -1.934761
1 -0.378528 -3.090029 0.689239
1 -1.398055 -2.069150 0.074126
1 -1.413980 1.328333 2.121301
1 -0.703650 0.164929 2.859860
8 2.008362 -1.669952 -1.013451
1 1.618245 -2.102926 -1.787094
1 2.705178 -2.245497 -0.673735
8 1.904047 1.664687 1.122397
1 2.609628 2.095885 0.621382
1 1.722879 2.205509 1.901898
8 1.740308 -0.988002 1.859633
1 1.706375 -1.840738 2.311093
1 2.444230 -0.472929 2.275378
6 -3.609528 -0.550131 0.327552
6 -3.627031 0.728370 -0.107825
1 -3.986104 -1.353364 -0.292733
1 -3.327640 -0.802806 1.343259
1 -4.010888 0.980926 -1.088144
1 -3.372915 1.556959 0.545298

$[Y(H_2O)_7(OH)]^{2+}$ (**9Y**)

39 -0.045259 0.000072 -0.119164
8 -0.518099 0.005101 -2.089961
8 -1.915471 -1.622830 -0.202265
8 -1.923364 1.616109 -0.187965
8 -1.038492 -0.015365 2.153092
8 2.165399 0.004519 -1.243802
8 0.828653 2.270944 0.111715
8 0.847408 -2.264206 0.104344
8 1.709075 0.005461 1.750758
1 -0.698468 0.010138 -3.031914
1 -2.579465 -2.032152 0.366925
1 -2.224525 -1.711092 -1.115390
1 -2.592194 2.009406 0.386917
1 -2.237617 1.706829 -1.099090
1 -0.442925 -0.013232 2.914563
1 -1.938444 -0.022989 2.503433
1 2.047923 0.008844 -2.204676
1 3.114018 0.011893 -1.063048
1 0.219252 3.020030 0.164358
1 1.622066 2.591749 -0.337396
1 0.249741 -3.022266 0.162084
1 1.640302 -2.572476 -0.354447
1 2.177103 -0.768867 2.091583
1 2.167483 0.783511 2.096144

$[Y(H_2O)_7(OH)](H_2O)^{2+}$ (**9Y**)

39 0.363072 0.050960 -0.146938
8 0.890499 0.594337 -2.030646

8 -1.752106 -0.420164 -1.309368
8 -0.503120 2.365143 -0.139569
8 -1.514779 0.093412 1.454100
8 2.669679 -0.840603 -0.466597
8 1.926409 1.528632 1.056611
8 0.080325 -2.353038 -0.429379
1 1.086805 0.866444 -2.928502
1 -2.674084 -0.354181 -0.991656
1 -1.737058 -0.210067 -2.252176
1 -1.198630 2.814308 0.356515
1 -0.360380 2.859218 -0.958507
1 -1.412141 -0.103512 2.392884
1 -2.471186 0.063495 1.246118
1 2.931002 -0.640140 -1.377137
1 3.361730 -1.381587 -0.066473
1 1.722088 2.464258 1.187756
1 2.876788 1.472144 0.889569
1 -0.721047 -2.647419 -0.883296
1 0.771733 -2.996601 -0.630777
8 1.055474 -0.975560 2.076775
1 0.923562 -1.876152 2.400220
1 1.633282 -0.528913 2.709424
8 -4.053901 -0.167106 0.283966
1 -4.592978 -0.948761 0.472125
1 -4.687140 0.559601 0.197369

$[Y(H_2O)_6(OOH)](H_2O)^{2+}$ monodentate (**4Y**)

39 0.307981 -0.232847 -0.025192
8 1.765096 -2.150760 0.046801
8 -0.353320 -1.270545 2.094700
8 1.658644 0.813010 1.629028
8 -1.359291 1.330956 0.538111
8 1.106760 -0.620960 -2.284706
8 1.016567 1.539712 -0.972337
8 -1.713744 -1.299499 -0.756864
1 1.951081 -2.767045 0.768641
1 2.409823 -2.333501 -0.651984
1 -0.264212 -0.807459 2.939627
1 -0.937497 -2.023684 2.256693
1 1.788688 1.741481 1.338125
1 2.305348 0.613219 2.316782
1 -1.074668 2.251225 0.400584
1 -2.330394 1.273082 0.470582
1 0.922609 -1.176856 -3.053184
1 1.431375 0.235868 -2.614157
1 -2.581730 -0.843201 -0.639965
1 -1.876361 -2.092481 -1.283908
8 -3.881050 0.310011 -0.205007
1 -4.575130 0.047032 0.416902
1 -4.346503 0.748325 -0.932677
8 0.984860 2.700777 -0.100904
1 1.370128 3.393407 -0.660119

$[Y(H_2O)_6(OOH)](H_2O)^{2+}$ bidentate (**4Y**)

39 0.341700 0.007996 0.021960
8 1.334243 -2.260750 -0.079486
8 0.510661 -0.752520 2.314252
8 2.704324 0.482772 0.363470
8 -1.690240 0.483330 1.285226
8 1.291628 -0.108301 -2.221262
8 0.527635 2.106533 0.356366
8 -1.438190 -1.142872 -1.109689
8 -0.507750 2.093564 -0.705952
1 1.275789 -2.929006 0.617198
1 1.809866 -2.670644 -0.814591
1 -0.279177 -0.603454 2.855206
1 1.258409 -0.844377 2.919910
1 2.864671 1.431883 0.483845
1 3.527226 0.017681 0.564705
1 -1.700723 1.421513 1.530394
1 -2.593550 0.261676 0.979770
1 0.812862 -0.132418 -3.061546
1 2.185258 0.202558 -2.423840
1 -2.387479 -0.916530 -0.974205
1 -1.411160 -1.975964 -1.596784
1 -0.174437 2.746615 -1.340316
8 -3.920484 -0.355736 -0.209258
1 -4.559113 -1.006236 0.117666
1 -4.449346 0.316706 -0.663178

$[Y(H_2O)_6(OOH)](H_2O)(C_2H_4)^{2+}$ (**4Y**•C_2H_4)

39 -0.227462 0.188077 0.004441
8 0.427310 2.041316 -1.290009
8 0.001888 -0.940080 -2.121151
8 -1.172675 0.032723 2.284014
8 -2.416761 0.940271 -0.583487
8 -1.596684 -1.857191 0.180870
8 1.485565 1.028097 -1.029672
1 0.517117 2.231367 -2.235532
1 -0.452352 -1.577709 -2.685640
1 0.814148 -0.658073 -2.567760
1 -1.324523 0.795253 2.858146
1 -1.533163 -0.739996 2.736818
1 -2.658432 1.778825 -0.997199
1 -3.235041 0.412550 -0.468422
1 -1.325446 -2.776534 0.063816
1 -2.574319 -1.826341 0.115181
6 4.481531 -1.566208 -0.039696
6 4.413365 -0.257821 0.222211
1 4.841562 -2.277432 0.697077
1 4.245559 -1.965149 -1.021380
1 4.717962 0.140472 1.185233
1 4.108052 0.463181 -0.529580
8 0.276664 2.177048 1.360477
1 0.820428 2.256651 2.155276
1 0.571779 2.881907 0.761683
8 1.489874 -1.119049 0.950177

1 2.434265 -1.032811 0.651335
1 1.504209 -1.710287 1.713584
8 -4.279283 -1.090574 -0.167731
1 -4.779907 -1.419074 -0.929075
1 -4.917426 -1.068113 0.560253

TS2Y

39 -0.087056 0.150921 -0.030919
8 0.758151 0.374015 -2.068382
8 0.254937 -2.210001 -0.290406
8 -1.295386 1.835883 1.330178
8 -2.033796 0.230276 -1.406711
8 -1.929216 -0.954419 1.237611
8 1.957285 -0.182829 -0.892717
1 1.080091 -0.135529 -2.821239
1 -0.210242 -3.055118 -0.273768
1 1.118419 -2.329728 -0.716217
1 -1.336467 2.766228 1.070644
1 -2.059900 1.663125 1.894052
1 -1.973450 0.441928 -2.347187
1 -2.950427 -0.049382 -1.208052
1 -1.844304 -1.532936 2.005707
1 -2.835484 -1.069376 0.882231
6 3.579601 -1.398090 0.371485
6 3.877423 -0.098781 0.162588
1 3.186911 -1.761730 1.316459
1 3.816850 -2.152366 -0.369357
1 3.739642 0.652154 0.932133
1 4.379274 0.224159 -0.738857
8 0.668231 2.455724 -0.470005
1 1.154371 3.144188 0.000841
1 1.087582 2.356333 -1.341931
8 0.890199 0.070213 2.186850
1 1.697192 -0.390721 2.451445
1 0.647988 0.657248 2.915604
8 -4.307207 -0.899574 -0.254346
1 -4.672674 -1.702641 -0.653222
1 -5.077938 -0.384854 0.025548

$[Y(H_2O)_6(OH)(Epox)](H_2O)^{2+}$ squareantiprism 1 (**7Y**)

39 -0.034187 0.226443 -0.126598
8 -1.417626 2.223636 0.385560
8 -0.501690 0.193805 2.312584
8 0.322132 -2.159538 0.314345
8 1.225144 2.341563 -0.510683
8 2.056028 0.330514 1.339887
8 -0.833039 0.305429 -1.984702
8 1.890672 -0.527298 -1.430232
8 -2.239804 -0.759019 0.420689
6 -3.542913 -0.445930 -0.176422
6 -2.976561 -1.781087 -0.333928
1 -2.018555 2.594513 -0.274307
1 -1.706960 2.546042 1.249083
1 0.187696 0.148850 2.987968

1 -1.330105 -0.113442 2.703047
1 0.725007 -2.755362 -0.329783
1 -0.109223 -2.710399 0.979864
1 0.753694 3.184384 -0.481028
1 1.893173 2.424399 -1.203606
1 2.417097 1.213928 1.491351
1 2.828938 -0.241101 1.169530
1 -1.128499 0.386357 -2.892469
1 1.818925 -0.605796 -2.389546
1 2.789423 -0.788615 -1.147131
1 -4.323689 -0.275040 0.555417
1 -3.487113 0.239214 -1.013756
1 -3.340726 -2.594676 0.282655
1 -2.518005 -2.042960 -1.280205
8 4.189043 -1.123322 0.073288
1 4.446966 -2.031044 0.286665
1 5.025212 -0.654585 -0.060226

$[Y(H_2O)_6(OH)(Epox)](H_2O)^{2+}$ squareantiprism 2 (**7Y**)

39 -0.040255 0.001427 -0.109074
8 -0.402982 -1.313032 1.952323
8 0.442687 1.384912 1.966580
8 0.427006 2.337042 -0.866649
8 -2.061054 -1.425243 -0.298194
8 -1.995091 1.385531 0.227064
8 0.707540 -2.317220 -0.580444
8 0.149199 -0.042546 -2.144859
8 2.336221 0.173745 0.336886
6 3.526797 -0.675776 0.452322
6 3.489373 0.387071 -0.549086
1 -1.073474 -2.005394 2.012824
1 -0.124486 -1.092295 2.849718
1 -0.153300 1.930205 2.495605
1 1.346460 1.628107 2.204322
1 0.537129 2.244616 -1.824875
1 0.871418 3.146287 -0.586346
1 -2.034031 -2.148524 -0.936563
1 -2.979611 -1.087873 -0.287111
1 -2.935603 1.116812 0.176689
1 -1.926264 2.291472 -0.100708
1 0.893708 -3.130577 -0.095436
1 0.911295 -2.467110 -1.513257
1 0.061628 -0.154497 -3.092633
1 4.074953 -0.526110 1.375035
1 3.369159 -1.701805 0.143738
1 4.011929 1.317457 -0.360433
1 3.296508 0.138208 -1.586029
8 -4.433066 0.067176 -0.073683
1 -4.984976 0.243921 -0.848908
1 -5.053192 -0.069228 0.656648

$[Y(H_2O)_6(OH)(Epox)](H_2O)^{2+}$ squareantiprism 3 (**7Y**)

39 0.011437 0.297664 -0.174604
8 1.698331 2.130073 -0.170520

8 0.416276 0.694513 -2.136453
8 -0.178675 -1.930596 -1.210919
8 -1.072772 2.385367 0.478387
8 -2.322233 0.385152 -0.996917
8 0.597101 0.721893 2.260957
8 -1.442509 -1.005334 1.319786
8 2.057884 -0.836113 0.487435
6 3.398739 -0.964891 -0.098953
6 2.700695 -2.151351 0.389702
1 2.385005 2.525521 0.379808
1 1.913315 2.308641 -1.097189
1 0.516663 0.891841 -3.068807
1 -0.550353 -2.788911 -0.975807
1 -0.047554 -1.910844 -2.168220
1 -0.604205 3.229771 0.451165
1 -1.983152 2.549244 0.199313
1 -2.418524 0.553718 -1.942836
1 -3.091214 -0.140068 -0.701422
1 1.422096 0.391068 2.638526
1 0.240559 1.379869 2.871433
1 -1.262758 -1.083683 2.264361
1 -2.373763 -1.265044 1.168740
1 3.435288 -0.769782 -1.164409
1 4.179751 -0.516926 0.504172
1 2.231137 -2.819207 -0.321419
1 2.967224 -2.573040 1.351736
8 -4.093643 -1.282265 0.426886
1 -4.470186 -2.099930 0.072152
1 -4.810075 -0.875229 0.934641

$[Y(H_2O)_6(OH)(Epox)](H_2O)^{2+}$ squareantiprism 4 (**7Y**)

39 0.003511 -0.533379 -0.038753
8 -0.940450 -0.904937 2.169179
8 -2.223145 -1.415914 -0.709488
8 -0.589902 0.477457 -2.188141
8 1.604140 -1.739676 1.425252
8 0.297074 -2.374800 -0.903410
8 1.178712 1.316558 1.080193
8 2.041263 0.021905 -1.284638
8 -1.689862 1.226954 0.510903
6 -1.821516 2.661594 0.250714
6 -2.951893 1.770001 0.005642
1 -0.654348 -1.605272 2.769718
1 -1.722306 -0.485482 2.548934
1 -1.969063 -2.306864 -0.997493
1 -3.136565 -1.455146 -0.400769
1 0.096273 0.689080 -2.834404
1 -1.346375 0.130957 -2.679699
1 2.267732 -1.573253 2.105403
1 1.787261 -2.600569 1.023658
1 0.491549 -3.170081 -1.401769
1 0.881763 1.780641 1.871828
1 2.052318 1.683759 0.833251

1 2.756863 0.647757 -1.055889
1 2.431283 -0.716581 -1.769754
1 -1.808628 3.272682 1.145962
1 -1.236967 3.015035 -0.590610
1 -3.764274 1.726644 0.722159
1 -3.188256 1.483927 -1.012475
8 3.617762 2.016355 -0.107463
1 3.727522 2.869490 -0.551243
1 4.472982 1.834272 0.307327

$[Y(H_2O)_6(OH)](H_2O)^{2+}$ cappedtrigonalprismatic1 (**10Y**)

39 0.373635 -0.087854 0.121252
8 0.613239 1.629178 1.779613
8 0.382886 -1.395378 -1.903510
8 -1.637496 -1.330076 0.452752
8 -1.539437 1.238459 -0.588305
8 1.017604 -1.263710 1.631891
8 2.717101 -0.539693 -0.385322
8 1.190604 1.852021 -1.283429
1 0.270466 2.520079 1.929822
1 0.987656 1.320696 2.617882
1 1.190776 -1.812820 -2.233618
1 -0.359094 -1.852462 -2.322432
1 -1.591823 -2.083933 1.055585
1 -2.577676 -1.086775 0.326351
1 -1.501404 2.092862 -1.035227
1 -2.486220 1.006449 -0.469284
1 3.058084 -1.117092 0.314577
1 3.469925 -0.185326 -0.875357
1 1.184376 1.923876 -2.248041
1 1.772870 2.557688 -0.969483
1 1.173734 -1.821935 2.396361
8 -3.994537 0.039586 -0.086075
1 -4.600609 -0.206509 -0.799947
1 -4.562523 0.328405 0.643071

$[Y(H_2O)_6(OH)](H_2O)^{2+}$ cappedtrigonalprismatic2 (**10Y**)

39 0.360737 -0.000261 -0.137413
8 0.351357 0.061146 2.336023
8 0.783383 0.154289 -2.086619
8 -1.587006 -1.368500 -0.587031
8 -1.571804 1.358858 0.330073
8 0.894162 -2.299294 0.436684
8 2.803008 -0.268803 0.033318
8 1.056120 2.357141 -0.036768
1 -0.163134 0.664826 2.889061
1 0.742601 -0.587606 2.937059
1 -1.599502 -1.907835 -1.389502
1 -2.513351 -1.091766 -0.419102
1 -1.547155 2.321589 0.257345
1 -2.509090 1.073631 0.270155
1 1.774470 -2.685244 0.332240
1 0.268379 -3.029120 0.538423
1 3.488537 -0.146940 0.703506

1 3.235804 -0.190818 -0.829382
1 1.320222 2.719109 -0.895138
1 1.442028 2.932618 0.637106
1 0.903165 0.196128 -3.037805
8 -3.957060 -0.020720 -0.005457
1 -4.555630 0.212097 -0.730507
1 -4.533356 -0.263436 0.733858

$[Y(H_2O)_6(OH)](H_2O)^{2+}$ cappedtrigonalprismatic3 (**10Y**)

39 -0.395461 -0.078824 0.070578
8 -1.027287 1.658963 1.614831
8 -0.036869 -2.175750 -1.049039
8 1.575845 0.354388 -1.389998
8 1.575287 -0.274985 1.383799
8 -0.821788 1.931616 -1.334917
8 -2.613388 -0.256252 -0.918690
8 -1.320082 -1.189453 1.475560
1 -1.445268 1.340026 2.427145
1 -0.943235 2.618210 1.688427
1 -0.482290 -2.956555 -0.691196
1 0.543509 -2.478637 -1.758809
1 1.627268 0.513812 -2.340822
1 2.500644 0.310729 -1.060374
1 1.529650 -0.652370 2.271898
1 2.517610 -0.141385 1.152593
1 -1.697808 2.329003 -1.434807
1 -0.195294 2.544502 -1.741428
1 -3.224342 -0.728621 -0.334645
1 -3.017721 -0.234151 -1.796030
1 -1.673614 -1.768195 2.154002
8 3.955845 0.191337 0.042371
1 4.595171 -0.524334 -0.087539
1 4.488204 0.983174 0.207714

$[Y(H_2O)_6(OH)](H_2O)^{2+}$ pentagbipiram1 (**10Y**)

39 -0.333799 0.000207 -0.143961
8 -1.137562 -2.332141 -0.246516
8 -1.138575 2.332173 -0.243678
8 -2.710262 -0.000500 0.492696
8 1.600697 1.400658 0.117764
8 -0.597858 0.002447 -2.122039
8 -0.462693 -0.003288 2.319281
8 1.601147 -1.399843 0.113682
1 -1.263774 -3.072743 0.361864
1 -1.348295 -2.654082 -1.135196
1 -1.348824 2.654432 -1.132353
1 -1.264825 3.072638 0.364852
1 -3.279136 0.773074 0.380156
1 -3.278420 -0.774476 0.379130
1 1.593833 2.351491 -0.047134
1 2.536737 1.105732 0.093317
1 0.242468 -0.003868 2.980700
1 -1.297835 -0.003407 2.806679
1 2.537019 -1.104330 0.088351

1 1.594254 -2.350378 -0.052890
1 -0.683458 0.001745 -3.077719
8 3.987016 0.000055 0.023896
1 4.626465 -0.002072 0.750999
1 4.516664 0.001689 -0.786956

TS3Y

39 -0.774630 0.002572 0.010823
8 -2.254907 1.737505 -1.144575
8 -3.123602 -0.759129 0.040432
8 -1.132502 1.942394 1.476655
8 -1.134462 -0.810704 2.322692
8 -0.667056 -0.578624 -2.348257
8 0.871467 1.661487 -0.628361
8 -0.515939 -2.496013 -0.462255
8 1.010424 -0.734058 0.701787
8 2.791053 -0.189236 0.171890
1 -2.542998 1.840954 -2.060651
1 -2.519159 2.541761 -0.677944
1 -3.526964 -1.595443 0.304851
1 -3.824056 -0.227278 -0.358978
1 -0.485772 2.660696 1.482719
1 -1.406881 1.806411 2.393804
1 -0.233174 -1.097469 2.545602
1 -1.753880 -1.237895 2.926872
1 -0.380532 -0.179650 -3.178174
1 -0.555562 -1.538959 -2.425321
1 1.048311 2.370350 -1.256620
1 1.714711 1.228085 -0.375561
1 -0.851267 -3.390401 -0.326632
1 0.358569 -2.405306 -0.020833
1 2.838057 -0.472935 1.098732
6 4.815490 0.678079 0.244475
6 4.597505 -0.502555 -0.427606
1 5.117288 0.687596 1.285721
1 4.725185 1.634879 -0.254489
1 4.427353 -0.510794 -1.496047
1 4.827564 -1.457041 0.029580

TS4Y

39 0.483430 0.227526 0.048419
8 0.511691 2.653154 -0.163522
8 1.009615 0.656191 2.383430
8 -0.988202 -1.314024 1.156363
8 1.756943 -1.864555 0.018718
8 0.222256 -0.225522 -2.287652
8 -1.389617 0.911848 -0.341726
8 2.807942 0.848308 -0.429046
1 0.898886 3.524667 -0.020140
1 -0.447063 2.748367 -0.321415
1 0.434582 0.378070 3.108367
1 1.641269 1.283554 2.758175
1 -1.877506 -0.994130 0.890998
1 -1.070897 -2.124571 1.670596

1 2.733006 -1.910961 -0.047478
1 1.423037 -2.768650 -0.019157
1 0.664350 -0.548676 -3.081590
1 -0.647443 0.126732 -2.529852
1 3.570686 0.235325 -0.406049
1 3.103984 1.666761 -0.845451
8 4.501259 -1.372600 -0.232881
1 5.096905 -1.483104 0.521973
1 4.998491 -1.692492 -0.999239
8 -3.069297 -0.038637 -0.178321
1 -3.233812 0.908187 -0.038599
6 -4.789664 -0.658314 -0.792812
6 -5.058445 -0.611640 0.555692
1 -4.485963 -1.582150 -1.267135
1 -5.099763 0.142661 -1.452588
1 -5.487794 0.271096 1.015670
1 -4.880797 -1.467779 1.194420

$[La(H_2O)_8(OOH)]^{2+}$ (**3La**)

57 -0.219743 0.026150 0.019947
8 -1.979855 1.207179 -1.549009
1 -2.048083 2.163896 -1.664533
1 -2.659427 0.805770 -2.105719
8 1.875299 -1.143232 -0.266928
8 3.047748 -0.277237 -0.178831
1 3.779199 -0.886827 -0.359203
8 0.062074 -1.475886 -2.121193
1 -0.176683 -1.665261 -3.036747
1 1.000887 -1.710754 -1.986571
8 -2.338269 -1.524294 -0.457639
1 -3.188727 -1.618948 -0.009556
1 -2.215613 -2.324136 -0.986411
8 1.455683 1.526056 -1.353551
1 1.468067 1.928725 -2.230634
1 2.333274 1.110875 -1.208946
8 0.149256 -2.186524 1.370404
1 1.091809 -2.341274 1.170371
1 -0.239760 -3.014716 1.676306
8 -0.471526 2.681078 0.387912
1 0.345539 3.135428 0.136509
1 -0.953686 3.283242 0.968962
8 1.548284 0.767295 1.768211
1 2.433193 0.460595 1.489746
1 1.646594 1.292923 2.569910
8 -1.641935 0.134121 2.257803
1 -2.375813 0.663443 2.596356
1 -1.369487 -0.441986 2.985735

$[La(H_2O)_8(OOH)](C_2H_4)^{2+}$ (**3La**•C_2H_4)

8 -2.709765 0.941006 1.205756
8 -2.548841 -0.720580 -1.512178
8 -1.133030 2.239410 -1.431305
57 -0.511630 0.047057 -0.018285
8 0.336783 -2.449300 -0.424948

8 0.300384 -0.423646 2.523563
8 -1.939846 -2.099870 0.822493
8 -0.185589 2.176505 1.635415
8 1.849768 1.163478 -0.533343
8 0.276342 0.045187 -2.580107
1 -2.645585 1.581270 1.926153
1 -3.647201 0.743737 1.086655
1 -3.042478 -0.394688 -2.274549
1 -2.948661 -1.559179 -1.241646
1 -1.754886 2.968404 -1.313173
1 -0.816893 2.286653 -2.343551
1 0.961112 -2.911951 -1.001137
1 0.882725 -1.161862 2.256260
1 0.042532 -0.564879 3.442757
1 -1.342190 -2.852573 0.674298
1 -2.486133 -2.309377 1.589953
1 0.374776 1.934934 2.386634
1 -0.111399 3.133124 1.528630
1 2.101087 2.095340 -0.559800
1 2.682824 0.674019 -0.342659
1 1.219950 0.240163 -2.667901
1 0.037047 -0.534576 -3.314590
8 1.209115 -1.520531 0.320498
6 4.588746 -0.562824 -0.338184
6 4.899019 0.460628 0.460213
1 4.091429 -1.449971 0.039725
1 4.875961 -0.568154 -1.385220
1 4.676243 0.442068 1.522565
1 5.443485 1.325171 0.093895

TS1La

8 -1.933298 -1.679065 1.435185
8 -2.988095 -0.206708 -0.869196
8 -1.867482 1.580989 1.607938
57 -0.465698 0.005977 0.025620
8 0.776201 -0.009444 -2.019025
8 1.177090 -2.063013 0.419648
8 -1.079820 -1.904737 -1.829911
8 0.557015 -0.324156 2.428954
8 1.063366 2.190748 0.139266
8 -1.327066 2.298930 -1.090870
1 -1.698915 -2.139966 2.250641
1 -2.837468 -1.935981 1.214561
1 -3.816859 0.275504 -0.758215
1 -3.075898 -0.764425 -1.655088
1 -2.277061 1.487647 2.477055
1 -2.110031 2.453212 1.268439
1 1.234626 0.476367 -2.713471
1 1.849876 -1.613511 -0.153612
1 1.199847 -3.012912 0.255875
1 -0.374151 -1.708988 -2.469831
1 -1.281368 -2.846401 -1.896096
1 1.199351 -1.049233 2.415221

1 0.703743 0.189002 3.232719
1 1.425787 2.843065 0.749671
1 1.806431 1.665067 -0.254304
1 -0.562712 2.890552 -1.160727
1 -1.912883 2.496348 -1.832231
8 2.131895 0.008573 -0.853122
6 4.233893 0.059366 -0.489995
6 3.860862 0.042704 0.809572
1 4.478216 -0.850771 -1.021874
1 4.442948 0.986075 -1.008769
1 3.771059 -0.889028 1.355850
1 3.733293 0.958318 1.375447

$[La(H_2O)_8(OH)](Epox)^{2+}$ (**9La•**C_2H_4O)

8 2.106426 1.023196 1.969666
8 3.012252 0.564601 -1.143984
8 2.197731 -2.146811 0.433468
57 0.698292 0.015170 -0.036809
8 -0.353248 1.019744 -1.735660
8 -1.367751 1.058092 1.354729
8 1.261376 2.638536 -0.568494
8 0.156298 -0.933930 2.505323
8 -1.343455 -1.662619 -0.263157
8 1.004739 -1.846047 -2.003509
1 1.960256 0.699456 2.867710
1 2.799405 1.693272 2.013377
1 3.882242 0.178397 -1.298585
1 3.046655 1.495713 -1.409715
1 2.831623 -2.455142 1.092366
1 2.237357 -2.758251 -0.315429
1 -0.859662 1.044462 -2.549492
1 -2.238495 0.849601 0.942653
1 -1.418584 1.975045 1.652097
1 0.563885 2.548362 -1.258515
1 1.316579 3.557942 -0.284322
1 -0.653929 -0.503895 2.815169
1 0.260729 -1.748536 3.011871
1 -1.490070 -2.513217 0.167985
1 -2.223375 -1.222136 -0.316290
1 0.149498 -2.215420 -2.263988
1 1.461423 -1.633681 -2.828675
8 -3.520234 -0.024860 0.026882
6 -4.541378 0.524044 -0.870534
6 -4.945459 -0.210157 0.326299
1 -4.585833 1.606857 -0.875814
1 -4.584942 0.036165 -1.837265
1 -5.285170 0.333472 1.200183
1 -5.284295 -1.235695 0.236096

$[La(H_2O)_8(OH)]^{2+}$ (**9La**)

57 0.008761 0.007866 -0.033601
8 -1.636111 1.559829 1.388498
1 -2.405842 1.956835 0.958667
1 -1.566392 1.963130 2.263273

8 1.110263 -2.406876 0.197034
1 1.159379 -2.536069 -0.769203
1 1.779968 -2.965887 0.609499
8 -0.784957 -1.389570 2.103406
1 -1.454012 -1.223108 2.779807
1 -0.617614 -2.341839 2.105804
8 1.399027 0.667478 2.148742
1 2.043089 1.377535 2.268254
1 1.437572 0.129270 2.950172
8 -2.102571 -1.484915 -0.790144
1 -2.835546 -1.963390 -0.381675
1 -1.803748 -2.011932 -1.545552
8 2.545790 0.342808 -0.926039
1 2.389384 -0.214294 -1.710694
1 3.475149 0.260707 -0.678220
8 -1.902833 1.260097 -1.431715
1 -2.565889 0.657123 -1.796292
1 -1.822899 1.991270 -2.058304
8 0.478261 -1.022337 -2.002883
1 0.385378 -1.132921 -2.952546
8 0.848358 2.446356 -0.528303
1 0.554224 3.359153 -0.419622
1 1.706636 2.463091 -0.976876

$[La(H_2O)_8(OH)](H_2O)^{2+}$ (**9La**)

57 -0.298339 0.014592 0.035963
8 -2.198354 0.028375 1.330515
1 -2.817601 0.511831 1.883075
8 1.883212 1.352745 -0.520783
1 1.890879 2.317164 -0.551148
1 2.805434 1.036861 -0.585089
8 -0.865746 -2.238928 1.291689
1 -1.671188 -1.869946 1.704600
1 -0.924889 -3.201172 1.295862
8 1.891521 -1.401679 0.553976
1 2.811663 -1.142890 0.347479
1 1.922448 -2.076520 1.243096
8 0.372808 -1.643392 -1.924802
1 0.018719 -1.754132 -2.815800
1 1.018202 -2.348790 -1.791435
8 0.386297 0.813738 2.471463
1 1.199967 0.937592 2.975525
1 -0.322568 0.656173 3.110136
8 -2.662975 -0.713645 -1.155838
1 -3.072595 -0.556302 -0.277598
1 -3.127903 -1.446258 -1.577716
8 -0.524808 2.680461 0.290681
1 -0.515711 3.087013 1.167227
1 -1.118132 3.216491 -0.251418
8 -1.059777 1.205404 -2.200950
1 -0.707299 1.731501 -2.928871
1 -1.950422 0.908596 -2.443022
8 4.262558 -0.144972 -0.346520

1 4.724103 -0.469214 -1.132725
1 4.964307 0.125390 0.262491

$[La(H_2O)_7(OOH)](H_2O)^{2+}$ (**4La**)

57 -0.062372 0.009587 -0.071432
8 -2.163725 -1.032496 0.342326
8 -1.946999 1.250742 -1.429281
1 -2.151635 1.405877 -2.360037
1 -2.780833 0.982146 -0.990173
8 -0.034791 -2.020175 1.527510
1 -0.971549 -2.248671 1.655934
1 0.507844 -2.664496 1.997757
8 -1.276301 1.289652 1.787319
1 -2.207082 0.985068 1.794717
1 -1.209358 2.068431 2.352158
8 -0.772649 -1.803549 -1.789383
1 -0.521312 -2.478624 -2.431371
1 -1.672244 -2.001612 -1.471737
8 0.518428 2.469738 -0.759888
1 -0.211755 3.030084 -1.057517
1 1.303179 3.030552 -0.716904
8 2.126773 -0.614257 -1.362848
1 2.232223 -0.993948 -2.244249
1 3.029786 -0.500708 -0.997112
8 2.014567 0.479552 1.460660
1 2.949619 0.357072 1.195989
1 2.011147 0.650978 2.411085
8 -3.233864 -0.060537 0.552352
1 -4.003768 -0.625233 0.718355
8 4.422585 -0.115183 0.152977
1 4.959363 -0.860754 0.458851
1 5.059375 0.569476 -0.098092

$[La(H_2O)_7(OOH)](H_2O)(C_2H_4)^{2+}$ (**4La**•C_2H_4)

57 -0.640457 -0.022731 -0.036811
8 -1.235675 -2.296265 0.903296
8 0.226020 -2.023258 0.913759
1 -1.383384 -2.765685 1.736360
8 -0.045294 0.125538 2.543476
1 0.295632 0.687226 3.249512
1 0.369606 -0.751516 2.627244
8 -2.936789 -0.823331 -1.102302
1 -3.216174 -1.732104 -0.922993
1 -3.449198 -0.524305 -1.864130
8 -2.660494 0.914268 1.387976
1 -2.616750 0.915193 2.353576
1 -3.597573 0.877508 1.155140
8 0.176980 -1.836457 -1.729893
1 0.285443 -2.176417 -2.625025
1 0.455140 -2.522298 -1.095931
8 -0.340035 2.596510 0.170917
1 -0.976069 3.200564 0.574127
1 0.525443 3.058312 0.141497
8 -0.918882 1.176240 -2.394632

1 -0.851383 0.846360 -3.299936
1 -0.900970 2.140386 -2.455340
8 1.850701 0.560222 -0.217752
1 2.246732 1.449855 -0.185353
1 2.592224 -0.082779 -0.217616
6 3.967771 -1.938809 -0.269734
6 4.740240 -0.952066 0.188149
1 3.395827 -2.572632 0.401033
1 3.936272 -2.186623 -1.326067
1 4.827853 -0.743551 1.249754
1 5.361371 -0.360826 -0.477125
8 2.322350 3.387613 -0.023161
1 2.646312 3.891395 -0.783041
1 2.800560 3.744227 0.738587

TS2La

57 -0.190651 -0.444071 -0.005328
8 1.746857 -1.709551 0.509357
8 2.261323 -0.003362 0.269886
1 2.497662 -1.957148 1.059536
8 0.540953 0.468519 2.339532
1 0.363985 1.037359 3.097357
1 1.496163 0.500581 2.139095
8 -0.291205 -2.947016 -0.809011
1 0.573381 -3.340101 -0.616006
1 -0.853742 -3.635849 -1.181851
8 -1.407163 -1.713195 1.994111
1 -0.963656 -1.650811 2.851270
1 -1.875135 -2.558423 1.994063
8 1.213190 -0.319384 -2.222955
1 1.299482 -0.739306 -3.087198
1 2.082923 -0.340442 -1.780921
8 -2.381993 0.859526 0.773613
1 -2.911726 0.571367 1.527511
1 -2.595216 1.799149 0.603291
8 -2.269607 -0.866249 -1.628955
1 -2.384340 -1.322808 -2.471850
1 -3.095843 -0.396681 -1.456604
8 -0.376705 1.921455 -1.090229
1 -1.006875 2.647026 -0.914984
1 0.110368 2.131605 -1.896567
6 3.534644 1.601821 -0.450407
6 2.852460 2.215608 0.540501
1 4.462631 1.080091 -0.259322
1 3.245582 1.719295 -1.488513
1 3.220532 2.198786 1.559679
1 1.974062 2.816653 0.338281
8 -2.484659 3.527234 -0.134041
1 -3.198868 3.826470 -0.714426
1 -2.304799 4.276850 0.450831

$[La(H_2O)_6(OH)(Epox)](H_2O)_2^{2+}$ (**8La**)

57 -0.204603 -0.083632 0.016594
8 -1.668544 -1.825647 -0.110964

8 2.038975 -1.298815 0.236332
6 2.733564 -2.489049 0.726780
6 3.104329 -1.905150 -0.561770
8 0.094450 -0.892136 2.548407
8 -2.164157 0.883750 1.520774
8 -0.009874 -1.416460 -2.267072
8 0.469828 2.125796 1.268560
8 -1.876636 1.192374 -1.469083
8 1.415583 1.389877 -1.482323
1 -1.926380 -2.717688 0.137254
1 3.355696 -2.303788 1.594574
1 2.121077 -3.383135 0.749349
1 3.996724 -1.294330 -0.631888
1 2.756364 -2.371762 -1.475890
1 0.714574 -0.581191 3.220467
1 -0.349875 -1.663615 2.923368
1 -2.297460 0.701597 2.458615
1 -3.024289 0.709656 1.082216
1 0.117979 -1.382250 -3.222225
1 -0.750940 -2.019941 -2.087692
1 -0.208215 2.590257 1.775893
1 1.152753 2.779750 1.021822
1 -2.804182 0.889796 -1.345550
1 -1.864737 1.895433 -2.127356
1 1.844465 2.208208 -1.158244
1 1.742775 1.242026 -2.377231
8 -3.869502 -0.174669 -0.335965
1 -3.341335 -1.006509 -0.311524
1 -4.798808 -0.392719 -0.475947
8 2.405403 3.641911 -0.094804
1 2.187456 4.536591 -0.392416
1 3.327184 3.687992 0.195589

$[La(H_2O)_7(OH)(Epox)](H_2O)^{2+}$ tricappedtrigonalprism1 (**7La**)

57 0.029809 0.113553 -0.120315
8 0.201462 -2.165410 1.231156
8 -1.515527 2.408999 -0.415155
8 -0.699025 -1.928531 -1.662668
8 -0.298956 1.076859 2.370221
8 -0.620546 0.734806 -2.214233
8 2.210400 -0.237156 1.474378
8 1.094577 2.528045 0.194127
8 2.240416 -0.318637 -1.432586
8 -2.383159 -0.507242 0.615096
6 -3.755903 -0.263968 0.174178
6 -3.333519 -1.615865 0.535931
1 0.964330 -2.257196 1.816416
1 -0.303600 -2.985346 1.284105
1 -2.324009 2.882401 -0.187739
1 -1.552092 2.133201 -1.357880
1 -0.923341 -1.393140 -2.442443
1 -0.457482 -2.813517 -1.959354
1 -0.978001 0.799600 2.998634

1 -0.095697 1.999572 2.571856
1 -0.521411 1.013404 -3.127839
1 2.240905 0.186250 2.341114
1 3.131779 -0.402878 1.193532
1 0.407671 3.146779 -0.103878
1 1.952205 2.943596 0.046679
1 3.142030 -0.524451 -1.117241
1 2.270941 -0.262268 -2.395071
1 -4.342434 0.317516 0.876037
1 -3.847604 -0.000716 -0.873513
1 -3.612155 -2.020386 1.502246
1 -3.114421 -2.327081 -0.251988
8 4.582026 -0.808503 0.050714
1 5.334183 -0.201866 0.002928
1 4.972256 -1.692845 0.092339

$[La(H_2O)_7(OH)(Epox)](H_2O)^{2+}$ tricappedtrigonalprism2 (**7La**)

57 -0.032120 -0.344497 -0.023739
8 0.131631 1.233575 -2.132487
8 -1.640914 -2.260570 0.799877
8 -1.237215 -0.970917 -1.887396
8 0.996740 -2.292403 -1.572138
8 -0.769881 -0.061089 2.539620
8 2.584680 -0.233643 -0.460779
8 1.432331 -1.843662 1.640136
8 1.093085 1.875671 0.915429
8 -2.046037 1.287983 0.425308
6 -3.391127 1.386995 -0.153615
6 -2.496694 2.540408 -0.193338
1 0.604600 1.854351 -2.696682
1 -0.417384 0.637936 -2.679919
1 -2.111767 -2.811313 0.161427
1 -2.019570 -2.441737 1.668764
1 -2.051434 -1.206963 -2.337403
1 0.215857 -2.216040 -2.159940
1 1.348789 -3.187674 -1.635352
1 -0.263193 -0.222076 3.345224
1 -1.508264 0.517551 2.770084
1 2.864321 -0.764189 -1.218617
1 3.189712 0.528848 -0.381192
1 1.262232 -2.687350 2.077207
1 2.387099 -1.789095 1.500413
1 1.996433 2.188221 0.711307
1 0.705914 2.517887 1.520888
1 -3.528398 0.790981 -1.047847
1 -4.184071 1.348453 0.584028
1 -1.980149 2.781792 -1.114647
1 -2.635675 3.348076 0.515987
8 3.796111 2.233573 0.168260
1 4.475746 2.256383 0.856506
1 4.082747 2.879753 -0.492028

$[La(H_2O)_7(OH)(Epox)](H_2O)^{2+}$ tricappedtrigonalprism3 (**7La**)

57 0.035157 0.081314 0.176523

8 -1.366596 2.293157 0.749806
8 1.342055 -0.743626 -1.972058
8 -0.399729 1.665827 -1.867022
8 2.418442 1.572368 -0.218130
8 -0.358548 -2.557804 0.085669
8 0.855316 1.454184 1.849723
8 2.062245 -1.464768 0.952910
8 -1.079869 -0.866928 2.355267
8 -2.361172 -0.542084 -0.665746
6 -3.438661 -0.108630 -1.554190
6 -3.757733 -0.745031 -0.277603
1 -0.713743 2.523468 1.443628
1 -2.190990 2.759950 0.927727
1 1.105903 -1.373753 -2.663137
1 2.320268 -0.765979 -1.887414
1 -0.800670 2.535847 -1.742992
1 -0.000372 1.645400 -2.745518
1 2.549354 2.386943 -0.719547
1 2.171267 1.835021 0.704829
1 0.415090 -3.104902 0.279170
1 -1.004771 -3.111345 -0.368946
1 1.148477 1.546000 2.760055
1 2.871036 -1.388556 0.399880
1 2.362246 -1.533186 1.868156
1 -1.144014 -0.402429 3.199399
1 -1.397679 -1.766945 2.499977
1 -3.531007 0.966488 -1.652719
1 -3.507675 -0.682751 -2.470808
1 -4.079117 -0.135775 0.559295
1 -4.064448 -1.784633 -0.261246
8 3.885434 -0.681773 -0.935030
1 3.909722 0.257344 -0.681284
1 4.774910 -0.947566 -1.202697

$[La(H_2O)_7(OH)(Epox)](H_2O)^{2+}$ tricappedtrigonalprism4 (**7La**)

57 0.025292 0.149492 -0.041502
8 0.201237 -2.352760 -0.855810
8 -1.562212 2.134208 0.792520
8 -0.811119 0.231266 -2.127726
8 -0.672466 -0.617862 2.429359
8 -0.063977 2.610736 -1.355796
8 2.007450 -1.130635 1.236567
8 1.192583 1.910473 1.598483
8 2.311567 0.268861 -1.308305
8 -2.399689 -0.948674 0.399842
6 -3.701444 -0.565020 -0.158168
6 -3.192352 -1.918659 -0.356523
1 0.619688 -3.128929 -0.464562
1 -0.002887 -2.570916 -1.773655
1 -2.363017 2.287444 1.307084
1 -1.511380 2.809192 0.095160
1 -1.210451 -0.026630 -2.960741
1 -1.557415 -1.011330 2.426384

1 -0.484086 -0.329607 3.330598
1 0.473799 3.334465 -1.697819
1 -0.407679 2.078377 -2.106626
1 1.935448 -1.504120 2.122485
1 2.928289 -1.257294 0.936001
1 0.682692 2.688950 1.857056
1 2.100948 2.061491 1.885078
1 3.177881 -0.112532 -1.068449
1 2.347108 0.505009 -2.242981
1 -4.461606 -0.383688 0.592965
1 -3.634185 0.146585 -0.972916
1 -3.575626 -2.733234 0.246757
1 -2.766326 -2.184248 -1.316131
8 4.486995 -1.082454 -0.115104
1 5.247996 -0.602280 0.240110
1 4.859014 -1.870944 -0.534300

$[La(H_2O)_7(OH)(Epox)](H_2O)^{2+}$ tricappedtrigonalprism5 (**7La**)

57 0.297466 -0.253785 -0.011747
8 -0.880969 -2.124871 1.460687
8 2.101148 -0.415232 -2.015091
8 1.875919 -2.344509 -0.030033
8 1.054207 -0.543874 2.584271
8 -0.760849 -1.714672 -1.926465
8 2.215961 1.087231 0.111845
8 -0.329760 1.794908 -1.506639
8 1.018891 3.424848 0.139510
8 -0.399062 1.716914 1.652508
8 -2.396608 -0.125634 -0.322471
6 -3.409506 0.889623 -0.609872
6 -3.664781 -0.128390 0.407196
1 -0.629725 -2.149870 2.394150
1 -1.518171 -2.834110 1.311771
1 2.239453 -0.388157 -2.969164
1 2.594417 0.323700 -1.597863
1 1.918437 -3.219994 0.372857
1 2.567639 -2.294841 -0.705597
1 0.930720 0.306218 3.031143
1 1.862592 -0.928717 2.947544
1 -0.422041 -2.329453 -2.588924
1 -1.720455 -1.670471 -2.031503
1 3.005611 1.057306 0.661494
1 -0.507274 1.919081 -2.445894
1 0.062718 2.630066 -1.160986
1 1.392447 4.313730 0.171499
1 1.748745 2.747963 0.109324
1 0.046274 2.542435 1.338112
1 -1.190322 1.989824 2.131629
1 -3.129074 1.892749 -0.312285
1 -3.866665 0.792436 -1.588019
1 -3.578739 0.127400 1.457264
1 -4.307447 -0.969828 0.174120

$[La(H_2O)_7(OH)(Epox)](H_2O)^{2+}$ tricappedtrigonalprism6 (**7La**)

57 0.116047 0.180230 0.037068
8 2.131131 -0.329928 1.609801
8 2.481847 0.586380 -1.245485
8 1.415713 2.507968 0.343807
8 -1.442190 2.311303 -0.406450
8 3.273559 -1.827497 -0.281899
8 -0.316677 0.491321 -2.567798
8 -0.586433 -1.907625 1.561221
8 0.620430 -1.935464 -0.788232
8 -0.837286 1.102217 2.349409
8 -2.471095 -0.253941 -0.310976
6 -3.271927 -1.275026 -0.994281
6 -3.519833 -0.982390 0.414803
1 2.546912 0.083666 2.374293
1 2.775521 -0.959023 1.212529
1 3.064829 -0.184211 -1.061259
1 2.599509 0.801504 -2.178828
1 1.464003 3.265052 0.939559
1 2.289252 2.402871 -0.062849
1 -2.381971 2.145468 -0.561964
1 -1.272550 3.247015 -0.572907
1 3.949923 -2.506553 -0.391847
1 2.392657 -2.187383 -0.552466
1 -0.088850 -0.175520 -3.228016
1 -0.801833 1.184533 -3.032436
1 -0.162715 -2.506647 0.914171
1 -0.457180 -2.281663 2.440646
1 0.409126 -2.561508 -1.486651
1 -0.859544 0.678606 3.216730
1 -1.330578 1.927226 2.440836
1 -3.934361 -0.873465 -1.752187
1 -2.718092 -2.167939 -1.260433
1 -4.365248 -0.362566 0.689828
1 -3.134905 -1.655955 1.170038

$[La(H_2O)_7(OH)(Epox)](H_2O)^{2+}$ tricappedtrigonalprism7 (**7La**)

57 0.018021 -0.332446 0.014285
8 0.053337 0.967877 -2.340689
8 -1.299974 -1.794884 1.192994
8 -1.410502 -1.466932 -1.907570
8 1.289347 -2.498966 -0.959796
8 -0.937630 0.451678 2.419832
8 2.527576 -0.010379 -0.769316
8 1.339180 -1.898154 1.769509
8 1.082965 1.932234 0.836663
8 -2.017620 1.266166 -0.436213
6 -3.468541 1.095038 -0.308387
6 -2.811226 2.229702 0.334992
1 0.780758 1.171466 -2.941211
1 -0.624204 1.645693 -2.466429
1 -1.938735 -2.509696 1.241615
1 -1.491398 -1.148529 -2.815252
1 -2.057105 -2.174253 -1.791884

1 1.028704 -3.095544 -1.672412
1 1.620312 -3.047842 -0.234351
1 -0.714289 0.720769 3.318070
1 -1.378400 -0.426753 2.457228
1 3.012921 -0.768402 -1.117314
1 3.156929 0.719739 -0.617691
1 0.516191 -2.293487 2.112578
1 2.004942 -1.911065 2.467495
1 1.968948 2.282885 0.616505
1 0.697379 2.523090 1.493265
1 -4.006342 1.243030 -1.237524
1 -3.761154 0.241385 0.292146
1 -2.865639 3.209908 -0.124043
1 -2.623331 2.191963 1.401070
8 3.736838 2.413732 0.016470
1 4.435856 2.423954 0.685275
1 3.980939 3.103671 -0.616072

$[La(H_2O)_7(OH)](H_2O)^{2+}$ (**10La**)

57 -0.283030 0.038945 -0.096347
8 -0.479382 0.161637 -2.263783
8 -0.908093 2.556273 -0.539160
8 2.035482 1.310336 -0.258246
8 0.323260 1.414614 2.120285
8 -1.431461 -2.160274 -1.026858
8 1.670919 -1.670850 0.170962
8 -2.920732 0.102395 0.322201
1 -0.452168 0.300211 -3.212788
1 -1.028270 3.376088 -0.043721
1 -1.146570 2.738029 -1.458809
1 2.906703 0.864576 -0.237802
1 2.127123 2.066458 -0.852134
1 -0.012017 1.378834 3.025138
1 1.088865 2.004104 2.130602
1 -1.393619 -2.030285 -1.987154
1 -1.691412 -3.073982 -0.856916
1 2.620810 -1.436900 0.101630
1 1.613957 -2.629927 0.079871
1 -3.505469 0.838759 0.545109
1 -3.445337 -0.498942 -0.224506
8 -1.046910 -1.407981 2.060260
1 -1.980238 -1.502552 2.291666
1 -0.551894 -1.932239 2.702805
8 4.187780 -0.496720 -0.112411
1 4.829593 -0.475120 0.611707
1 4.705773 -0.682396 -0.908890

TS4La

57 -0.696006 -0.212238 0.127696
8 -2.815885 1.074587 1.318616
8 1.089787 0.229060 -1.127171
8 0.927801 2.803458 -1.151802
8 -1.592182 1.867260 -1.219996
8 0.266795 1.950761 1.307368

8 -0.379650 -1.575558 -2.255134
8 0.084352 -0.603394 2.606110
8 -0.313673 -2.798164 0.188909
8 -3.073975 -1.107725 -0.599250
1 -3.263596 1.068246 2.174518
1 -3.035291 1.917077 0.896965
1 1.484728 3.436303 -1.618974
1 1.228577 1.859935 -1.336684
1 -2.182539 1.953771 -1.978225
1 -0.815948 2.457526 -1.383417
1 -0.137483 2.586208 1.910217
1 0.717096 2.478581 0.604545
1 0.418473 -0.991730 -2.296107
1 -0.696871 -1.738746 -3.151392
1 0.634540 0.109364 2.959670
1 0.058670 -1.298063 3.276121
1 -0.228423 -3.579297 0.747752
1 -0.167755 -3.069810 -0.731915
1 -3.885865 -0.756439 -0.211465
1 -3.333820 -1.824718 -1.191233
8 2.781720 -0.097309 -0.289759
1 2.965190 -0.264738 -1.226869
6 4.691064 0.293975 0.260970
6 4.545297 -1.065202 0.360758
1 4.504554 0.942439 1.106328
1 5.139214 0.748688 -0.614372
1 4.842182 -1.725244 -0.445954
1 4.207865 -1.528246 1.278348

Mimoun

$[Ga(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ cis (**5Ga**)

31 -0.199533 -0.097480 0.049995
8 1.341822 1.190265 0.474231
6 -1.583030 -2.000938 -0.561750
8 -0.365103 0.635697 -1.882880
8 -0.235753 -0.787575 2.015773
8 -1.413419 1.203204 0.607966
8 1.322542 -1.337024 -0.414563
1 2.300034 1.107848 0.312752
1 1.058658 2.119067 0.534350
1 0.149389 0.515849 -2.692791
1 -0.713073 1.547934 -1.843096
1 0.313912 -1.421216 2.498578
1 -0.618796 -0.156220 2.646141
8 -0.977361 2.464423 -0.005150
1 1.255081 -2.246103 -0.737548
1 2.280001 -1.046594 -0.373504
1 -1.658524 3.075567 0.320067
6 -2.608233 -1.163238 -0.279750
1 -3.055952 -0.533722 -1.040800
1 -3.041694 -1.103609 0.713410
1 -1.250003 -2.723820 0.177610
1 -1.269510 -2.147246 -1.591898

8 3.702859 -0.186703 -0.172743
1 4.263991 -0.000375 -0.941146
1 4.314886 -0.438709 0.535939

$[Ga(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ trans (**5Ga**)

31 0.216331 0.080449 0.010002
8 1.626698 0.354488 -1.496570
8 -1.258890 -0.070085 1.408433
8 1.589718 0.037920 1.593866
8 -1.287609 -0.077065 -1.393083
8 0.573915 -1.743512 -0.169058
6 0.313080 2.483945 0.512019
1 2.189462 -0.446239 -1.519611
1 2.111104 1.101183 -1.876681
1 -0.996583 -0.410785 2.277657
1 -2.111214 -0.499647 1.142444
1 2.128505 0.702676 2.046176
1 2.126569 -0.771873 1.453734
1 -2.136006 -0.494883 -1.105942
1 -1.020598 -0.484904 -2.231818
8 2.034780 -1.903855 -0.116496
1 2.122603 -2.868148 -0.195098
6 -0.628423 2.546186 -0.454847
1 -1.683578 2.457370 -0.220346
1 -0.379279 2.741248 -1.493173
1 1.353213 2.707725 0.294324
1 0.024135 2.421815 1.556888
8 -3.372830 -1.107361 0.058175
1 -4.248912 -0.691595 0.076994
1 -3.539871 -2.062889 0.059235

$[Ga(H_2O)_4(CH_2CH_2OO(H))](H_2O)^{2+}$ (product 1) (**23Ga**)

31 0.467522 -0.318115 0.010117
8 -3.475411 -0.125392 -0.114505
8 1.425093 -2.178515 0.343159
8 0.189748 -0.379574 2.176316
8 0.630585 -0.916919 -2.077908
8 -0.318893 2.422190 0.299583
8 -1.194088 -1.433613 -0.053395
1 -4.010059 -0.088188 -0.921872
1 -4.113400 -0.141871 0.614408
1 1.935977 -2.610376 -0.358724
1 1.860984 -2.369389 1.188005
1 -0.490434 -0.830199 2.696847
1 0.528055 0.348864 2.718445
8 -0.983266 1.275942 -0.339964
1 -1.200707 -2.394801 0.054398
1 -2.124096 -1.052859 -0.073510
1 -1.914475 1.382951 -0.068405
1 -0.077977 -1.307874 -2.609415
1 1.228762 -0.463645 -2.690706
6 1.769319 1.177777 0.001302
6 0.991962 2.463781 -0.296210
1 1.428440 3.344811 0.181491

1 0.888235 2.658847 -1.365819
1 2.543202 1.000378 -0.747935
1 2.266490 1.222624 0.972328

$[Ga(H_2O)_4(CH_2CH_2O(H)O)](H_2O)^{2+}$ (product 2) (**25Ga**)

31 0.201528 0.395603 0.025540
8 -3.411243 -1.449427 -0.156397
8 -0.091888 2.501048 0.452265
8 0.253228 1.158937 -2.017444
8 -0.373209 0.242180 2.127916
8 1.185496 -2.125722 0.142664
8 -1.758525 0.492741 -0.305443
1 -3.211804 -2.344096 -0.459728
1 -4.373377 -1.359167 -0.160589
1 -0.070197 2.850463 1.355127
1 0.202433 3.202443 -0.146938
1 -0.500821 1.008140 -2.605923
1 1.039121 1.246876 -2.575246
8 -0.029327 -1.531658 -0.417068
1 -2.223420 1.332967 -0.196895
1 -2.415968 -0.290078 -0.283752
1 -1.235341 -0.116568 2.384384
1 0.246017 0.019837 2.838075
6 2.177019 0.119789 0.274894
6 2.462373 -1.285662 -0.170960
1 2.616254 -1.399715 -1.242661
1 3.212071 -1.830565 0.403276
1 2.484467 0.288898 1.307309
1 2.731196 0.819091 -0.353265
1 1.219390 -3.001770 -0.290469

$[Ga(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ isomer 1 (**27Ga**)

31 0.031567 0.236567 -0.034329
8 -3.293411 -1.550527 -0.726715
8 3.538163 -1.313815 -0.624143
8 -0.910573 -0.702548 -1.490978
8 1.633026 0.196907 -1.222454
8 1.051522 -0.464167 1.317329
8 -1.716226 0.028186 1.011353
1 -3.460217 -2.482110 -0.514172
1 -4.108188 -1.230983 -1.144620
1 4.220930 -1.654258 -1.216263
1 3.788679 -1.529844 0.282684
1 -1.809221 -1.128049 -1.382107
1 -0.439554 -1.039538 -2.267369
8 0.214515 -0.937538 2.411719
1 -1.445397 -0.346303 1.880526
1 -2.478393 -0.479448 0.662704
1 2.428056 -0.427040 -0.960916
1 1.979791 0.936157 -1.739593
6 -0.633814 2.482569 -0.649857
6 0.064377 2.592861 0.508434
1 1.126497 2.821820 0.518707
1 -0.437609 2.550198 1.471363

1 -1.714070 2.369295 -0.640707
1 -0.163241 2.645066 -1.615827
1 0.813846 -0.843107 3.169452

$[Ga(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ isomer 2 (**27Ga**)

31 -0.021712 -0.431090 -0.218141
8 3.309837 1.370942 0.321210
8 -1.345179 3.005703 0.049012
8 1.972011 -0.870662 -0.109763
8 0.491323 1.391319 -0.021221
8 -1.774116 -0.213929 -0.763075
8 0.091044 -1.411124 -1.999976
1 3.867728 1.757484 -0.371352
1 3.764133 1.563741 1.155761
1 -2.188209 2.524027 0.037835
1 -1.449239 3.856082 -0.396985
1 2.638239 -0.144131 0.058116
1 2.399291 -1.738147 -0.073957
8 -2.543541 0.443381 0.283490
1 -0.742692 -1.466012 -2.497620
1 0.836331 -1.481405 -2.614567
1 -0.260573 2.161393 -0.031283
1 1.391942 1.707801 0.182890
6 -0.398147 -1.007922 2.183835
6 -0.564114 -2.124413 1.432191
1 0.227097 -2.863378 1.335582
1 -1.537314 -2.387452 1.028084
1 -1.229026 -0.333493 2.371772
1 0.544818 -0.795231 2.678743
1 -3.426925 0.071487 0.125783

$[Ga(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ isomer 3 (**27Ga**)

31 -0.020877 0.086326 0.108316
8 3.457436 -1.322901 -1.138023
8 -3.673155 -1.098614 -0.090053
8 0.950185 -1.181680 -0.989694
8 -1.340768 -0.991675 1.123520
8 0.325280 1.875438 -0.047829
8 -1.468472 0.138034 -1.333387
1 3.984479 -0.767322 -1.729270
1 3.938106 -2.155643 -1.031016
1 -4.040720 -1.927361 -0.434751
1 -4.431678 -0.598174 0.249209
1 1.982232 -1.251114 -1.077885
1 0.532841 -1.444352 -1.824144
8 -0.188630 2.364810 -1.326348
1 -2.391570 -0.159434 -1.207164
1 -1.443107 1.044715 -1.713400
1 -2.281243 -1.126044 0.798052
1 -1.182570 -1.494658 1.934478
6 1.642621 -0.166768 1.811118
6 1.036548 0.864844 2.448669
1 0.291312 0.703494 3.222681
1 1.288698 1.895365 2.220913

1 2.487568 0.018037 1.151932
1 1.488085 -1.194771 2.130713
1 -0.145277 3.325414 -1.192358

TS8Ga

31 0.152196 0.224214 0.171896
8 3.786511 -0.977099 -0.221628
8 -3.173472 -1.808124 -0.444573
8 1.401735 -1.098410 0.957229
8 -1.283018 -0.940511 1.381821
8 -0.954951 0.931919 -1.439338
8 1.712822 0.668596 -1.025482
1 4.128341 -1.699550 -0.770969
1 4.558609 -0.613391 0.239229
1 -3.259748 -2.736739 -0.708769
1 -4.071701 -1.447296 -0.488264
1 2.343749 -1.216340 0.652770
1 1.106865 -1.830120 1.517241
8 -0.894529 -0.567608 -1.311316
1 1.466085 0.977804 -1.912467
1 2.595418 0.238175 -1.023171
1 -2.045150 -1.370078 0.927435
1 -1.504352 -0.844951 2.319016
6 -0.282836 1.975939 1.193049
6 -1.302989 2.285315 0.267367
1 -2.333874 1.996155 0.439416
1 -1.139921 2.975225 -0.554342
1 0.616102 2.588275 1.149800
1 -0.596751 1.684883 2.192516
1 -1.827563 -0.890328 -1.244403

$[Ga(H_2O)_3(CH_2CH_2OO(H))](H_2O)_2^{2+}$ (product 1) (**24Ga**)

31 -0.212868 -0.167212 -0.343928
8 2.539237 2.533894 0.138766
8 -3.847402 0.195220 0.830358
8 -1.216530 0.045447 1.349268
8 -2.055567 0.175035 -1.259409
8 1.957387 -1.423226 1.089859
8 0.263862 1.681534 -0.799759
1 3.298823 2.679039 -0.445377
1 2.575563 3.247489 0.793515
1 -4.449875 -0.549287 0.984919
1 -4.355636 0.989154 1.059006
1 -2.203610 0.068266 1.427662
1 -0.780397 -0.070066 2.206909
8 1.485397 -0.043360 1.050184
1 -0.280721 2.272444 -1.338141
1 1.122806 2.123913 -0.506453
1 2.290399 0.509873 1.019056
1 -2.880571 0.213634 -0.719365
1 -2.274298 -0.163596 -2.140590
6 0.625204 -1.844271 -0.940612
6 1.996665 -1.920420 -0.269408
1 2.330731 -2.949785 -0.113557

1 2.766696 -1.384009 -0.831002
1 0.715889 -1.858394 -2.028364
1 -0.019168 -2.673318 -0.640481

$[Ga(H_2O)_3(CH_2CH_2O(H)O)](H_2O)_2^{2+}$ (product 2) (**26Ga**)

31 -0.087886 -0.186049 -0.180943
8 2.222422 3.123966 0.023642
8 -3.934205 0.190759 0.588339
8 -1.386316 -0.186262 1.327904
8 -1.905036 0.144458 -1.328524
8 2.350677 -1.050828 0.586994
8 0.230720 1.685537 -0.579440
1 2.828030 3.516982 -0.617859
1 2.316564 3.616938 0.848512
1 -4.583362 -0.525375 0.662920
1 -4.419886 1.003035 0.797887
1 -2.367664 -0.055053 1.271570
1 -1.089272 -0.302059 2.241721
8 1.302718 -0.261033 1.235967
1 -0.368797 2.187767 -1.146679
1 1.046542 2.254503 -0.314280
1 -2.788207 0.192958 -0.903483
1 -2.020996 -0.181074 -2.232384
6 0.716968 -1.754569 -1.106900
6 1.785845 -2.276944 -0.185569
1 1.423041 -2.956976 0.583413
1 2.687935 -2.653178 -0.668477
1 1.120100 -1.469284 -2.079454
1 -0.041156 -2.524902 -1.256305
1 2.916881 -1.320455 1.337878

$[In(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ cis (**5In**)

49 -0.160731 -0.082170 0.042554
8 1.461328 1.262378 0.389665
6 -1.623771 -2.110113 -0.588866
8 -0.418178 0.739249 -1.924170
8 -0.198649 -0.733166 2.106138
8 -1.411417 1.302234 0.680823
8 1.408765 -1.380942 -0.447230
1 2.425542 1.152951 0.303850
1 1.221268 2.195261 0.514981
1 -0.145977 0.597302 -2.840228
1 -0.786054 1.641336 -1.818836
1 0.152039 -1.464340 2.634041
1 -0.618860 -0.094145 2.705469
8 -0.999365 2.527399 -0.027220
1 1.374200 -2.293948 -0.764066
1 2.363982 -1.082798 -0.397884
1 -1.668566 3.158345 0.281387
6 -2.630029 -1.265296 -0.283029
1 -3.083733 -0.622063 -1.029866
1 -3.051630 -1.213779 0.716149
1 -1.269651 -2.835987 0.139227
1 -1.307590 -2.240258 -1.621480

8 3.788258 -0.227297 -0.182920
1 4.345358 -0.039651 -0.953881
1 4.402360 -0.498263 0.516702

$[In(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ trans (**5In**)

49 0.181396 0.054561 -0.000103
8 1.689188 0.434747 -1.489156
8 -1.379558 -0.175851 1.431005
8 1.602911 0.180885 1.619678
8 -1.372770 -0.331812 -1.427654
8 0.807032 -1.816432 -0.131621
6 0.087116 2.628104 0.464984
1 2.309315 -0.324501 -1.471944
1 2.031994 1.120354 -2.078375
1 -1.190974 -0.444544 2.342668
1 -2.251905 -0.559775 1.166007
1 2.008154 0.825973 2.214974
1 2.211640 -0.581572 1.500587
1 -2.249700 -0.671671 -1.128636
1 -1.149251 -0.774601 -2.260751
8 2.279766 -1.748447 -0.050837
1 2.517036 -2.688011 -0.105041
6 -0.814333 2.505951 -0.528261
1 -1.867034 2.345609 -0.317923
1 -0.546017 2.650024 -1.570850
1 1.118234 2.904209 0.262196
1 -0.225300 2.598461 1.505499
8 -3.519660 -1.170725 0.068444
1 -4.386335 -0.735843 0.053266
1 -3.710229 -2.120852 0.114148

$[In(H_2O)_4(CH_2CH_2OO(H))](H_2O)^{2+}$ (product 1) (**23In**)

49 0.473284 -0.185752 0.003508
8 -3.503769 -0.862624 -0.102144
8 1.882130 -1.845253 0.318170
8 0.335395 -0.292322 2.234009
8 0.696126 -0.816399 -2.140449
8 -0.941159 2.354975 0.345463
8 -0.996448 -1.690865 0.023995
1 -4.045777 -1.003900 -0.892374
1 -4.112887 -0.957631 0.644894
1 2.424468 -2.232165 -0.385641
1 2.343685 -2.002100 1.155960
1 -0.191673 -0.869860 2.804998
1 0.579109 0.480904 2.765732
8 -1.345787 1.067834 -0.252793
1 -0.857735 -2.643500 0.109995
1 -1.979285 -1.490947 -0.016845
1 -2.309753 1.051411 -0.118824
1 0.144506 -1.422211 -2.656614
1 1.188490 -0.275479 -2.776465
6 1.397190 1.725699 -0.125151
6 0.274169 2.743442 -0.340516
1 0.470982 3.712615 0.127256

1 0.041767 2.905942 -1.395228
1 2.118271 1.770858 -0.944243
1 1.954838 1.940323 0.789521

$[In(H_2O)_4(CH_2CH_2O(H)O)](H_2O)^{2+}$ (product 2) (**25In**)

49 -0.168481 -0.380174 0.007395
8 3.468660 1.649223 -0.096669
8 0.085249 -2.566840 0.227113
8 0.081584 -0.948975 -2.148014
8 0.106557 -0.486965 2.228430
8 -1.200928 2.216405 0.268871
8 1.921145 -0.388200 -0.020767
1 3.178826 2.565729 -0.178657
1 4.434181 1.651286 -0.089312
1 0.004814 -3.044988 1.065426
1 -0.025233 -3.209816 -0.488420
1 0.900016 -0.784731 -2.639381
1 -0.630209 -1.004744 -2.802093
8 0.066478 1.685538 -0.233749
1 2.467573 -1.183683 0.010469
1 2.528531 0.430289 -0.050917
1 0.935893 -0.252625 2.670491
1 -0.600945 -0.375033 2.880049
6 -2.297738 -0.008937 0.005692
6 -2.480937 1.447363 -0.273299
1 -2.519229 1.712397 -1.328327
1 -3.249687 1.964444 0.301280
1 -2.776409 -0.303269 0.940617
1 -2.763027 -0.587014 -0.795641
1 -1.187423 3.138231 -0.054025

$[In(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ isomer 1 (**27In**)

49 -0.015037 0.179284 -0.056382
8 3.474028 -1.572853 0.401115
8 -3.599038 -1.038056 0.388092
8 1.178746 -0.659273 1.441831
8 -1.578677 0.292379 1.350381
8 -1.198925 -0.252434 -1.558357
8 1.698624 -0.227829 -1.266777
1 3.612743 -2.525185 0.279661
1 4.339460 -1.217836 0.656982
1 -4.185162 -1.597915 0.917630
1 -4.159113 -0.621399 -0.283283
1 2.065028 -1.068805 1.244734
1 0.867650 -0.960619 2.307338
8 -0.970067 -1.603540 -0.896503
1 1.509930 -0.457448 -2.191373
1 2.504317 -0.705297 -0.974252
1 -2.437026 -0.163019 1.059989
1 -1.757386 0.847475 2.120781
6 0.918903 2.528364 0.499005
6 0.101915 2.704117 -0.562118
1 -0.937324 2.999284 -0.440832
1 0.476376 2.648741 -1.581621

1 1.981302 2.342601 0.365033
1 0.574267 2.699565 1.515763
1 -1.880708 -1.907099 -0.733408

$[In(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ isomer 2 (**27In**)

49 0.264378 -0.259915 0.208822
8 -3.537556 -0.877974 -0.445473
8 -1.448801 3.457227 -0.207453
8 -1.133840 -1.842053 0.118214
8 -1.347422 0.932366 -0.181888
8 1.653846 0.979766 0.757541
8 0.514098 -0.830563 2.252721
1 -4.248202 -0.885410 0.214142
1 -3.973894 -1.045953 -1.294808
1 -1.380525 4.023595 -0.986413
1 -1.501898 4.032796 0.565929
1 -2.095666 -1.664686 -0.089847
1 -0.991303 -2.796628 0.188445
8 2.364877 1.435831 -0.436177
1 1.261547 -0.380684 2.683291
1 0.019215 -1.327749 2.919304
1 -1.343002 1.962411 -0.184802
1 -2.253983 0.608769 -0.343945
6 1.088038 -0.754022 -2.185878
6 1.899131 -1.478195 -1.381945
1 1.749363 -2.546007 -1.239699
1 2.787871 -1.025680 -0.947942
1 1.325942 0.283819 -2.410410
1 0.253971 -1.211352 -2.711147
1 2.991414 2.065102 -0.047318

$[In(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ isomer 3 (**27In**)

49 0.038976 0.153175 0.049893
8 -3.444447 -1.192579 -1.422053
8 3.828651 -0.644484 -0.685488
8 -0.997575 -0.621114 -1.540417
8 1.692264 0.878611 -1.007977
8 -0.903535 -0.194881 1.717637
8 1.367357 -1.413897 0.480846
1 -3.806680 -1.921320 -0.900866
1 -4.098677 -0.966373 -2.096407
1 4.228864 -1.125301 -1.426212
1 4.572996 -0.344002 -0.141463
1 -2.001543 -0.878017 -1.503690
1 -0.614405 -1.001237 -2.342829
8 -0.674041 -1.598142 2.081117
1 2.312489 -1.557057 0.296198
1 1.048088 -1.923930 1.255316
1 2.578281 0.406663 -0.972962
1 1.776049 1.677364 -1.547773
6 -1.245548 2.347092 -0.101877
6 -0.467674 2.632602 0.966190
1 0.445165 3.214396 0.866429
1 -0.763332 2.340071 1.969887

1 -2.216322 1.874499 0.033087
1 -1.015706 2.729680 -1.093659
1 -1.025165 -1.617277 2.984984

$[In(H_2O)_3(CH_2CH_2OO(H))](H_2O)_2^{2+}$ (product 1) (**24In**)

49 -0.179677 -0.182033 -0.321862
8 2.487985 2.733411 0.151455
8 -3.904163 0.207242 0.889421
8 -1.255269 0.016968 1.465195
8 -2.133032 0.103030 -1.199454
8 2.040777 -1.314466 1.198107
8 0.224993 1.803435 -0.787039
1 3.235371 2.905534 -0.440395
1 2.501032 3.453955 0.798777
1 -4.506991 -0.534158 1.056318
1 -4.415001 1.004559 1.098660
1 -2.238055 0.074393 1.535133
1 -0.855871 -0.050031 2.345093
8 1.579059 0.066446 1.036895
1 -0.309955 2.408577 -1.318432
1 1.070062 2.263751 -0.491013
1 2.379194 0.620910 1.089569
1 -2.945453 0.177388 -0.642414
1 -2.397052 -0.153164 -2.095535
6 0.854207 -1.939633 -0.890793
6 2.175583 -1.910359 -0.123584
1 2.534945 -2.908032 0.145458
1 2.968305 -1.390652 -0.668054
1 1.028370 -1.970479 -1.967515
1 0.253721 -2.811531 -0.624792

$[In(H_2O)_3(CH_2CH_2OO(H))](H_2O)_2^{2+}$ (product 2) (**26In**)

49 -0.098122 -0.177721 -0.191132
8 2.179047 3.290845 0.023864
8 -4.011699 0.138888 0.591203
8 -1.441871 -0.154138 1.433228
8 -1.986267 0.027750 -1.269958
8 2.444936 -0.939649 0.691003
8 0.191629 1.822919 -0.594359
1 2.785890 3.690154 -0.612323
1 2.283817 3.767393 0.856905
1 -4.647006 -0.588273 0.678503
1 -4.521671 0.946581 0.756043
1 -2.421548 -0.052630 1.392745
1 -1.151703 -0.265345 2.349993
8 1.322711 -0.257164 1.335744
1 -0.406211 2.373036 -1.116929
1 0.997310 2.392273 -0.323485
1 -2.859281 0.096040 -0.817283
1 -2.139161 -0.204699 -2.196946
6 0.963412 -1.806128 -1.109510
6 2.025343 -2.214103 -0.133465
1 1.698408 -2.930163 0.618560
1 2.991756 -2.484578 -0.559679

1 1.384430 -1.526815 -2.075829
1 0.278692 -2.642455 -1.262511
1 3.013842 -1.176424 1.449743

$[Sc(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ cis (**5Sc**)

21 -0.161302 -0.054568 0.130735
8 1.542106 1.232596 0.556534
6 -1.531041 -2.281664 -0.652004
8 -0.539492 0.791750 -1.842834
8 -0.246226 -0.856891 2.193745
8 -1.399109 1.267931 0.632799
8 1.535889 -1.315029 -0.622720
1 2.491413 1.051289 0.376269
1 1.451266 2.132161 0.901404
1 -0.202799 0.696877 -2.743697
1 -1.125371 1.574412 -1.804438
1 0.191353 -1.603491 2.627839
1 -0.754675 -0.390805 2.875878
8 -1.785497 2.408293 -0.121515
1 1.535291 -2.179331 -1.056306
1 2.472466 -1.005343 -0.582015
1 -2.557017 2.746184 0.364544
6 -2.579924 -1.524904 -0.293712
1 -3.090321 -0.885226 -1.006222
1 -3.002181 -1.568949 0.705133
1 -1.103095 -3.009541 0.032831
1 -1.198778 -2.318148 -1.686512
8 3.891274 0.046997 -0.234454
1 4.405280 0.395008 -0.978933
1 4.548751 -0.254949 0.410632

$[Sc(H_2O)_4(OOH)(C_2H_4)](H_2O)^{2+}$ trans (**5Sc**)

21 -0.253806 -0.016439 0.069189
8 -1.459512 0.712885 1.769288
8 1.287200 -0.450692 -1.425576
8 -1.738135 0.183295 -1.515031
8 1.444825 -0.382109 1.392816
8 -1.154281 -1.651942 0.293763
6 -0.174717 2.803681 -0.706009
1 -2.110258 0.097242 2.142562
1 -1.592811 1.568022 2.202518
1 1.124862 -0.667611 -2.354459
1 2.198177 -0.748942 -1.195600
1 -2.065903 0.836579 -2.147446
1 -2.379169 -0.559769 -1.463554
1 2.324064 -0.699430 1.075869
1 1.410123 -0.496335 2.353258
8 -2.504056 -1.895629 -0.104269
1 -2.560353 -2.866743 -0.086316
6 0.809741 2.705414 0.196490
1 1.827341 2.468826 -0.098577
1 0.660238 2.962709 1.241127
1 -1.167705 3.149541 -0.433632
1 0.021531 2.660506 -1.765116

8 3.573263 -1.209933 -0.110882
1 4.405557 -0.715885 -0.165705
1 3.829645 -2.145055 -0.101660

TS7Sc

21 0.394055 -0.216288 0.027834
8 1.339729 -1.638630 1.483935
8 0.391770 1.659182 -1.003001
8 2.469999 -0.208285 -0.835362
8 -0.996749 1.186024 -1.008370
6 0.710895 1.431256 1.504308
6 0.616378 2.457838 0.468082
8 0.285572 -2.051249 -1.381701
1 1.649541 -1.364424 2.359786
1 1.465229 -2.596775 1.422430
1 2.773714 0.429854 -1.497986
1 3.257480 -0.649630 -0.486123
1 -1.303819 1.387489 -1.910472
1 1.694680 1.382306 1.973029
1 -0.082603 1.473712 2.249925
1 -0.250980 3.111267 0.450280
1 1.527346 2.972544 0.167166
1 -0.483436 -2.630253 -1.482864
1 0.921667 -2.312487 -2.063070
8 -3.830990 -0.130517 0.047447
1 -4.525825 -0.691799 -0.321385
1 -4.282997 0.584680 0.514287
8 -1.485175 -1.021078 0.724168
1 -2.403312 -0.672316 0.483817
1 -1.588736 -1.580269 1.505405

$[Sc(H_2O)_4(CH_2CH_2OO(H))](H_2O)^{2+}$ (product 1) (**23Sc**)

21 0.667705 -0.254625 0.022633
8 -3.326527 -1.276399 -0.036323
8 2.729965 -1.033535 0.272358
8 0.750290 -0.197883 2.250862
8 1.046866 -0.647027 -2.132575
8 -1.393496 2.013885 0.327001
8 -0.697034 -2.057158 -0.077463
1 -3.903490 -1.353523 -0.811010
1 -3.898745 -1.451838 0.725712
1 3.320336 -1.348996 -0.428243
1 3.264980 -0.965939 1.077628
1 0.637020 -0.904824 2.903200
1 0.629451 0.638743 2.727013
8 -1.312181 0.577336 -0.003854
1 -0.483376 -2.999567 -0.036668
1 -1.682603 -1.977380 -0.080590
1 -2.239055 0.254082 0.044368
1 0.682214 -1.357604 -2.680359
1 1.395387 0.024045 -2.738926
6 0.968231 1.896856 -0.228491
6 -0.342724 2.623666 -0.452809
1 -0.370775 3.648522 -0.065142

1 -0.642350 2.640487 -1.504401
1 1.684357 2.122680 -1.028455
1 1.448746 2.221364 0.708344

$[Sc(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ isomer 1 (**27Sc**)

21 0.027138 0.153123 0.033602
8 3.833570 -1.137726 0.052782
8 -3.418803 -1.499494 0.013303
8 1.375966 -1.087148 1.274120
8 -1.547073 -0.212312 1.505771
8 -1.135135 0.194505 -1.480415
8 1.838963 0.291482 -1.145822
1 4.163198 -1.943931 -0.373394
1 4.611385 -0.724432 0.457941
1 -3.811599 -2.346121 0.275113
1 -4.130588 -1.009106 -0.425961
1 2.312444 -1.265484 1.018939
1 1.159435 -1.658483 2.023945
8 -0.949063 -1.239625 -1.206597
1 1.840620 0.508016 -2.090265
1 2.707392 -0.114608 -0.912941
1 -2.373813 -0.634215 1.156138
1 -1.692021 0.022326 2.432704
6 0.285852 2.708849 0.722924
6 -0.719822 2.889156 -0.150182
1 -1.758518 2.889791 0.165564
1 -0.536777 3.097399 -1.200512
1 1.323559 2.819513 0.416928
1 0.096299 2.618167 1.791083
1 -1.864498 -1.539919 -0.982512

$[Sc(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ isomer 2 monodentate (**27Sc**)

21 0.030682 -0.063936 0.134748
8 -1.632382 0.638497 -1.010734
8 -1.583701 -1.483240 0.726628
8 0.379893 2.341360 -1.579450
8 1.419268 -1.635305 -0.055512
8 0.908772 1.264419 -0.829974
6 0.107652 0.690999 2.614158
6 0.795658 1.738577 2.121923
1 -2.554809 0.313417 -1.095341
1 -1.462643 1.388785 -1.610519
1 -2.485453 -1.446053 0.321619
1 -1.610624 -2.148362 1.428594
1 1.135388 2.625809 -2.122190
1 1.243910 -2.582584 0.035748
1 2.394130 -1.546904 -0.379167
1 0.623880 -0.175773 3.024204
1 -0.962792 0.757665 2.795945
1 0.302993 2.659333 1.823969
1 1.878945 1.729720 2.048018
8 3.825295 -1.431451 -0.831181
1 4.598131 -1.603482 -0.277690
1 4.116588 -1.478346 -1.750905

8 -3.869829 -0.903567 -0.659328
1 -4.661069 -0.570007 -0.209579
1 -4.199289 -1.483718 -1.362509

$[Sc(H_2O)_3(OOH)(C_2H_4)](H_2O)_2^{2+}$ isomer 2 bidentate (**27Sc**)

21 -0.029771 0.089595 -0.073983
8 1.456901 -0.358575 1.427518
8 1.698237 -0.613147 -1.321951
8 -1.104161 0.262532 1.498627
8 -1.129377 -1.512354 -1.013423
8 -1.965221 0.804218 0.446824
6 0.299321 2.472718 -1.190356
6 0.349573 2.890593 0.086353
1 2.369881 -0.705448 1.299057
1 1.269957 -0.286252 2.375413
1 2.549810 -0.914998 -0.924112
1 1.817256 -0.602846 -2.282178
1 -0.828930 -2.256983 -1.552385
1 -2.079393 -1.658895 -0.765955
1 -2.737596 0.187212 0.430021
1 -0.652638 2.395222 -1.715317
1 1.202351 2.371184 -1.785642
1 1.296634 3.088297 0.580252
1 -0.551526 3.094540 0.656652
8 -3.636151 -1.354848 -0.013983
1 -4.425044 -1.259938 -0.569490
1 -3.912540 -1.898937 0.739357
8 3.775878 -1.302804 0.335840
1 4.596982 -0.787957 0.361756
1 4.047762 -2.225751 0.454627

TS8Sc

21 -0.068012 0.061125 0.080712
8 -1.709222 0.255778 -1.331219
8 -1.704078 -0.908831 1.206271
8 0.758417 1.701080 -0.972061
8 1.028081 -1.717480 0.461806
8 1.828220 0.706049 -0.835121
6 0.233404 1.701608 1.550396
6 0.772302 2.594842 0.547104
1 -2.611738 -0.130026 -1.228267
1 -1.685397 0.789789 -2.138425
1 -2.601482 -1.069733 0.831505
1 -1.765104 -0.996126 2.168215
1 0.689556 -2.504944 0.909138
1 1.997513 -1.893945 0.211868
1 2.276342 0.718008 -1.699615
1 0.932513 1.403256 2.331731
1 -0.737027 1.998408 1.949376
1 0.150688 3.402232 0.167021
1 1.830913 2.832902 0.556227
8 3.478808 -2.093218 -0.244302
1 4.224540 -1.939783 0.351423
1 3.750964 -2.802243 -0.842451

8 -3.938171 -1.009134 -0.397365
1 -4.734677 -0.504704 -0.171119
1 -4.260025 -1.839358 -0.780656

$[Sc(H_2O)_3(CH_2CH_2OO(H))](H_2O)_2^{2+}$ (product 1) (**24Sc**)

21 -0.102583 -0.003733 0.100750
8 3.499093 -2.051369 -0.338152
8 -3.981976 -0.892912 -0.416749
8 -1.740509 0.423582 -1.270887
8 -1.734658 -1.022192 1.150987
8 0.773610 1.846079 -0.821215
8 1.029721 -1.785065 0.349743
1 4.228267 -1.936976 0.286137
1 3.797042 -2.703040 -0.987079
1 -4.759504 -0.392583 -0.124673
1 -4.334679 -1.671992 -0.873389
1 -2.647930 0.044100 -1.198535
1 -1.727240 1.064885 -1.995938
8 1.756750 0.748669 -0.848905
1 0.705726 -2.616734 0.721494
1 2.006714 -1.919797 0.101920
1 2.246817 0.892926 -1.678109
1 -2.642707 -1.114531 0.775891
1 -1.782040 -1.210179 2.099513
6 0.355870 1.529612 1.574258
6 0.891950 2.507567 0.571594
1 0.276959 3.391095 0.388750
1 1.940177 2.786013 0.659103
1 1.089377 1.218469 2.320358
1 -0.545907 1.889334 2.075106

$[Y(H2O)6(OOH)](H2O)(C2H4)^{2+}$ (**4Y**•C_2H_4)

39 0.345225 -0.376173 0.035546
8 -0.856702 -2.523065 0.068408
8 2.336429 0.480801 -1.011193
8 -1.669495 0.288932 1.180602
8 0.706808 1.879660 0.822020
8 -0.989744 0.260324 -1.768621
6 -4.289893 1.793685 0.145571
6 -4.532408 0.529094 -0.208982
8 -0.119884 -0.923969 -1.992128
1 -1.177218 -2.641610 -0.841035
1 -1.407264 -3.059396 0.653394
1 2.494906 0.230695 -1.931615
1 2.800968 1.326904 -0.839945
1 -2.497708 0.564307 0.710995
1 -1.946497 0.066727 2.078963
1 0.022931 2.404291 1.256503
1 1.462382 2.468703 0.614311
1 -0.832300 0.803460 -2.555370
1 -3.824937 2.496992 -0.538370
1 -4.614399 2.189857 1.102689
1 -5.066316 -0.151241 0.447362
1 -4.269925 0.152931 -1.192622

8 1.933157 -2.255646 -0.055356
1 2.856596 -2.224210 -0.339103
1 1.597757 -3.136078 -0.275204
8 1.109978 -0.914015 2.293640
1 1.135142 -0.397693 3.110212
1 1.627302 -1.715985 2.452379
8 3.074760 3.011182 -0.118994
1 3.838856 3.154893 0.457963
1 3.067293 3.766896 -0.724376

$[Y(H_2O)_6(OOH)(C_2H_4)](H_2O)^{2+}$ isomer 2 or 3 (**5Y**)

39 0.187912 0.001066 0.216979
8 2.587394 0.224886 -0.033273
8 1.204483 -0.549388 2.363919
8 -1.220056 -1.692867 1.442366
8 0.436419 1.251580 -1.510042
8 -1.429200 -0.531815 -1.487105
8 0.641465 2.222472 1.094668
8 -1.878187 0.969245 1.044408
6 0.717161 -2.939573 -0.751018
6 1.468008 -2.331834 -1.674938
8 1.542820 2.193224 -1.449927
1 3.382961 -0.317826 0.013616
1 2.738918 0.940966 -0.684864
1 0.820141 -1.135299 3.029419
1 2.071908 -0.275340 2.690282
1 -1.970314 -1.372850 1.961919
1 -1.311263 -2.652561 1.375677
1 -1.168864 -0.088552 -2.310117
1 -2.392929 -0.400431 -1.391173
1 1.036338 2.580315 1.899598
1 0.963063 2.760696 0.343772
1 -1.829437 1.866002 1.402072
1 -2.727792 0.891047 0.557770
1 1.167158 -3.434071 0.105129
1 -0.349806 -3.064477 -0.905970
1 1.038535 -1.920288 -2.582254
1 2.548234 -2.288779 -1.592162
1 1.505132 2.619403 -2.319997
8 -3.991634 0.401168 -0.691132
1 -4.755229 -0.145250 -0.455855
1 -4.354366 1.116124 -1.234356

$[Y(H_2O)_6(CH_2CH_2OO(H))](H_2O)^{2+}$ (product 1) isomer 2 or 3 (**23Y**)

39 0.003538 0.294708 0.045315
8 -0.994850 -0.709772 2.023702
8 -0.021136 2.676287 -0.519979
8 0.899697 1.520130 1.997644
8 0.138763 -0.235359 -2.304311
8 2.320643 0.771229 -0.789992
8 1.446232 -1.523089 0.775883
8 -2.691555 -1.517629 0.122139
6 -2.324972 0.889590 -0.347387
6 -3.255617 -0.294988 -0.479817

8 -1.380703 -1.710050 -0.525585
1 -1.102892 -0.388718 2.926777
1 -1.840303 -1.120659 1.743105
1 0.586104 3.426954 -0.501736
1 -0.869402 3.006671 -0.848731
1 1.580159 1.224639 2.616509
1 0.599873 2.383753 2.311270
1 -0.612466 -0.614337 -2.780049
1 0.807599 0.010223 -2.955120
1 2.708989 1.575221 -1.155228
1 3.051985 0.126648 -0.687088
1 1.148755 -2.188095 1.409846
1 2.367149 -1.727423 0.515029
1 -2.438616 1.510130 -1.246234
1 -2.631423 1.518479 0.501163
1 -4.187695 -0.234856 0.092889
1 -3.504338 -0.541954 -1.513738
1 -1.357908 -2.673906 -0.631346
8 4.024636 -1.402955 -0.269937
1 4.795338 -1.318176 0.309828
1 4.310823 -1.986141 -0.987728

$[Y(H_2O)_5(OOH)(C_2H_4)](H_2O)_2^{2+}$ pentagbipiram1 (**27Y**)

39 0.046511 -0.051985 0.259893
8 1.875593 -1.597149 0.133782
8 -0.316270 -1.882938 1.833741
8 -2.323806 0.199879 0.509642
8 1.593434 0.717319 -1.423182
8 -1.013433 -1.346725 -1.464737
8 1.283087 0.983931 1.958289
6 -1.035910 2.658010 -1.359258
6 -0.463100 3.146908 -0.255191
8 -0.171723 0.827041 2.194910
1 2.728252 -1.484599 -0.335513
1 2.009658 -2.230228 0.850723
1 -0.642331 -2.791024 1.869965
1 -0.408287 -1.490916 2.716850
1 -2.687315 0.649630 1.284008
1 -3.055858 -0.229889 0.024246
1 1.512343 1.512275 -1.963222
1 2.494766 0.353186 -1.565846
1 -0.578473 -1.836081 -2.174449
1 -1.982756 -1.469270 -1.571308
1 1.455400 1.901369 2.218796
1 -2.045830 2.263631 -1.347043
1 -0.560558 2.727174 -2.333638
1 0.511838 3.624124 -0.284062
1 -0.979887 3.163648 0.698619
8 3.975102 -0.699778 -1.446441
1 4.771402 -0.331055 -1.037046
1 4.285938 -1.186204 -2.223672
8 -3.782553 -1.320408 -1.322394
1 -4.289438 -2.100224 -1.053324

1 -4.314187 -0.897006 -2.012083

$[Y(H_2O)_5(OOH)(C_2H_4)](H_2O)_2^{2+}$ pentagbipiram2 (**27Y**)

39 0.348194 -0.151656 -0.053673
8 0.028669 2.105891 0.630571
8 -0.817793 -2.189643 -0.450078
8 1.950644 -2.037011 -0.057545
8 2.495180 0.984838 0.029503
8 0.841761 0.164593 -2.040640
8 1.786610 1.163527 -2.468857
8 -1.990555 0.301400 -0.029052
1 -0.797956 2.634586 0.611604
1 0.780939 2.711515 0.611116
1 -1.771571 -2.299793 -0.659648
1 -0.357690 -3.000201 -0.701419
1 2.554874 -2.091676 -0.811616
1 2.300135 -2.632947 0.618232
1 2.703557 1.218251 -0.904421
1 3.304701 1.034939 0.551101
1 1.912795 0.946881 -3.405169
1 -2.688603 -0.316251 -0.325824
1 -2.388098 1.191541 0.057278
6 -0.029090 -0.894021 2.898430
6 1.139744 -0.256633 3.024546
1 -0.972791 -0.355791 2.918645
1 -0.089980 -1.977776 2.868932
1 2.077960 -0.797553 3.101953
1 1.187661 0.821380 3.142425
8 -3.504778 -1.885820 -0.922357
1 -3.842388 -1.912949 -1.829341
1 -4.181183 -2.315576 -0.379421
8 -2.554126 3.020085 0.356517
1 -3.080180 3.348126 1.099865
1 -2.780577 3.588943 -0.393393

$[Y(H_2O)_5(OOH)(C_2H_4)](H_2O)_2^{2+}$ pentagbipiram3 (**27Y**)

39 -0.065358 0.066061 -0.079143
8 2.178472 0.440849 0.514715
8 -2.231313 0.634427 0.736582
8 -0.063724 2.048284 0.700530
8 -1.690999 -1.124062 -1.422363
8 0.426160 1.432480 -1.951093
8 1.240400 -1.738312 -1.036482
8 1.074982 2.867371 0.328451
1 2.334882 1.386233 0.700605
1 3.015727 -0.002856 0.286000
1 -2.269071 1.539189 1.082873
1 -3.129355 0.346442 0.482734
1 -1.578767 -1.631401 -2.235886
1 -2.661456 -1.031414 -1.277931
1 0.523712 1.407309 -2.910507
1 0.667475 2.324407 -1.635373
1 2.224987 -1.739327 -0.995990
1 0.974080 -2.609041 -1.356671

1 0.898577 3.694324 0.803250
6 -0.327092 -1.893297 2.138264
6 0.025403 -0.817689 2.853406
1 0.401606 -2.641875 1.842528
1 -1.371030 -2.119285 1.937442
1 -0.712744 -0.115466 3.226953
1 1.056899 -0.632378 3.133199
8 -4.299565 -0.627792 -0.647754
1 -4.894202 -0.104491 -1.204730
1 -4.854497 -1.320444 -0.260733
8 3.955774 -1.414446 -0.610015
1 4.448769 -2.037383 -0.056624
1 4.562010 -1.173398 -1.325163

$[Y(H_2O)_5(OOH)(C_2H_4)](H_2O)_2^{2+}$ pentagbipiram4 (**27Y**)

39 -0.265922 0.012147 0.054545
8 2.088200 0.370963 -0.128285
8 -0.000702 2.367656 -0.292707
8 0.731304 -2.038018 0.606795
8 -0.222664 -0.602585 -2.227390
8 -0.209055 0.166996 2.453007
8 -1.841981 -1.392483 -0.155036
8 -1.462779 -2.617716 -0.844153
1 2.759788 -0.332775 -0.011787
1 2.541755 1.223974 -0.269514
1 0.868718 2.817691 -0.399006
1 -0.693942 3.027383 -0.420717
1 1.670009 -2.309359 0.591808
1 0.164010 -2.774112 0.306350
1 0.231012 -0.407450 -3.056059
1 -0.759575 -1.410405 -2.345052
1 -0.145990 -0.644112 2.977759
1 -0.376968 0.888359 3.074097
1 -2.288102 -3.126552 -0.817022
6 -3.048794 1.175195 0.940268
6 -3.124855 1.455476 -0.365909
1 -2.944722 1.960607 1.683198
1 -3.197994 0.162018 1.301211
1 -3.320842 0.678952 -1.097383
1 -3.088371 2.477415 -0.733519
8 3.514515 -1.993352 0.374225
1 3.971019 -2.477441 -0.328736
1 4.076467 -2.092143 1.156126
8 2.639760 3.111858 -0.531941
1 2.987321 3.444279 -1.372340
1 3.066493 3.649346 0.151054

$[Y(H_2O)_5(OOH)(C_2H_4)](H_2O)_2^{2+}$ cappedtrigonalprismatic4 (**27Y**)

39 -0.113695 0.091373 0.095954
8 -1.756654 0.649196 -1.545927
8 -2.049165 -1.255244 0.549015
8 2.192004 0.590729 0.217013
8 -0.200902 0.991480 2.285981
8 0.796835 -0.924939 -1.849460

8 -0.155805 2.197104 -0.196264
8 0.783181 2.888589 0.675849
1 -1.695906 1.578868 -1.815439
1 -2.696586 0.380175 -1.584251
1 -2.167615 -1.976736 1.179270
1 -2.922548 -1.100399 0.119664
1 2.906173 0.286891 -0.374871
1 2.305361 1.544932 0.385098
1 -0.300687 0.752647 3.215051
1 0.027082 1.941714 2.229131
1 1.758662 -0.937593 -2.056610
1 0.314311 -1.127071 -2.661417
1 0.663006 3.814294 0.413548
6 1.070310 -2.688746 1.060311
6 0.952378 -2.044700 2.225515
1 1.973196 -2.611919 0.463513
1 0.320699 -3.390071 0.707317
1 0.097493 -2.201188 2.877484
1 1.747696 -1.413350 2.608034
8 -4.222557 -0.534177 -0.987360
1 -4.944621 -0.002563 -0.621397
1 -4.645926 -1.164180 -1.588669
8 3.545687 -0.620671 -1.954961
1 3.923206 -0.041437 -2.633009
1 4.173976 -1.352448 -1.870692

$[Y(H_2O)_5(OOH)(C_2H_4)](H_2O)_2^{2+}$ cappedtrigonalprismatic5 (**27Y**)

39 0.022311 -0.167748 0.099815
8 2.057043 -0.094510 -1.002635
8 -1.624073 1.240245 1.274050
8 -0.882765 1.158044 -1.645043
8 1.301563 1.614527 1.074716
8 0.609131 -1.314001 2.108203
8 0.245707 -2.087081 -0.732388
8 1.542998 -2.614974 -1.090369
1 2.284119 -0.996019 -1.327899
1 2.852342 0.463228 -0.923427
1 -2.110219 1.056979 2.088487
1 -2.135322 1.919864 0.784776
1 -0.669564 1.088989 -2.585241
1 -1.569786 1.850281 -1.536107
1 0.984607 2.300105 1.675111
1 2.230028 1.827046 0.828462
1 0.932437 -1.062693 2.983661
1 0.725677 -2.272100 2.021941
1 1.311930 -3.346297 -1.683172
6 -2.531370 -2.059260 0.660835
6 -2.779481 -1.516612 -0.535786
1 -1.893346 -2.930800 0.754668
1 -3.027509 -1.709993 1.561337
1 -3.489358 -0.703963 -0.653493
1 -2.349474 -1.934468 -1.439720
8 -2.767889 2.933513 -0.652771

1 -2.600567 3.887383 -0.654779
1 -3.702613 2.840917 -0.889286
8 3.831001 1.852329 -0.028212
1 4.628184 1.586022 0.452001
1 4.091686 2.628191 -0.544790

$[Y(H_2O)_5(OOH)(C_2H_4)](H_2O)_2^{2+}$ cappedtrigonalprismatic7 (**27Y**)

39 0.295129 -0.291207 -0.078986
8 0.621343 1.991582 0.322967
8 -1.230721 -2.026229 -0.714370
8 1.534503 -2.353447 0.162282
8 2.403353 -0.028960 -0.335846
8 0.565874 0.234719 -2.367109
8 2.787913 1.158289 -1.076569
8 -1.881817 0.703066 -0.038884
1 0.002241 2.745089 0.373198
1 1.505094 2.291465 0.042291
1 -2.208530 -1.935599 -0.765059
1 -0.992908 -2.895729 -1.061120
1 2.453931 -2.143008 -0.078332
1 1.525891 -3.213091 0.602246
1 1.460168 0.603398 -2.506513
1 0.080277 0.269668 -3.199674
1 3.756299 1.108417 -1.059908
1 -2.732775 0.252477 -0.203115
1 -2.046630 1.660929 0.087798
6 -0.309514 -0.748531 2.786809
6 0.933671 -0.273085 2.933527
1 -0.505186 -1.816067 2.727180
1 -1.176192 -0.096915 2.846959
1 1.126178 0.784179 3.082741
1 1.797856 -0.928592 2.961872
8 -3.864366 -1.210790 -0.661370
1 -4.388464 -1.148190 -1.473042
1 -4.472441 -1.556982 0.007922
8 -1.740296 3.471576 0.391279
1 -2.042960 3.877854 1.216083
1 -1.963112 4.109009 -0.302123

$[Y(H_2O)_5(OOH)(C_2H_4)](H_2O)_2^{2+}$ cappedtrigonalprismatic9 (**27Y**)

39 0.192285 -0.068264 0.132207
8 0.736656 -0.442079 -1.830368
8 0.229510 -0.134885 2.571977
8 -0.066142 2.314869 0.125932
8 1.731943 -1.925457 0.243153
8 -1.039077 -2.065272 0.647016
8 1.860462 -1.220743 -2.267943
8 -2.101850 0.393717 -0.225804
1 0.583637 0.479996 3.228530
1 -0.223389 -0.833782 3.064126
1 -0.900208 2.777614 -0.115099
1 0.642605 2.968354 0.089329
1 2.359699 -2.344011 0.844406
1 2.038652 -2.070956 -0.682130

1 -1.988183 -2.231058 0.460223
1 -0.566046 -2.904142 0.566501
1 1.640098 -1.418842 -3.191105
1 -2.807676 -0.281811 -0.285667
1 -2.487978 1.265398 -0.445968
6 3.031208 1.240321 -0.312635
6 2.922846 1.203388 1.020448
1 2.855097 2.149605 -0.879150
1 3.363257 0.387293 -0.894090
1 3.201376 0.320105 1.586872
1 2.679955 2.089629 1.600100
8 -2.581121 3.107829 -0.665072
1 -3.168214 3.629092 -0.098677
1 -2.705534 3.455534 -1.560215
8 -3.687875 -1.912680 -0.128937
1 -4.424947 -2.007647 0.491304
1 -3.975703 -2.352726 -0.941893

$[Y(H_2O)_5(OOH)(C_2H_4)](H_2O)_2^{2+}$ cappedtrigonalprismatic10 (**27Y**)

39 0.046629 -0.051322 0.263659
8 1.877836 -1.597227 0.137374
8 -0.313836 -1.863492 1.854565
8 -2.324645 0.202787 0.490698
8 1.591727 0.722601 -1.416047
8 -0.999948 -1.378602 -1.444982
8 1.274356 0.974087 1.973740
6 -1.034330 2.665672 -1.379339
6 -0.467607 3.155927 -0.272771
8 -0.187875 0.853372 2.184881
1 2.726136 -1.485596 -0.340053
1 2.022894 -2.219334 0.861760
1 -0.625583 -2.776302 1.897105
1 -0.416440 -1.465342 2.733706
1 -2.696214 0.660006 1.256842
1 -3.051676 -0.233575 0.003417
1 1.507301 1.519777 -1.952367
1 2.491059 0.356903 -1.566880
1 -0.558398 -1.885084 -2.138394
1 -1.968315 -1.499127 -1.561317
1 1.463265 1.890384 2.226759
1 -2.041374 2.263856 -1.370753
1 -0.556999 2.740502 -2.352371
1 0.503992 3.640178 -0.298329
1 -0.985880 3.166377 0.680239
8 3.967893 -0.703110 -1.458582
1 4.767940 -0.337456 -1.053737
1 4.272338 -1.188487 -2.239002
8 -3.770907 -1.339917 -1.330612
1 -4.282144 -2.114239 -1.053999
1 -4.295601 -0.925458 -2.030961

$[Y(H_2O)_5(OOH)(C_2H_4)](H_2O)_2^{2+}$ cappedtrigonalprismatic11 (**27Y**)

39 -0.000342 0.077476 -0.123846
8 1.617834 -1.326510 0.897255

8 -1.977772 0.265107 -1.487968
8 1.946293 0.536545 -1.434737
8 0.186648 0.939813 1.796494
8 -1.612016 -1.103234 1.115831
8 0.233252 -0.069966 2.845359
8 0.021284 -2.043445 -1.338056
1 1.572205 -1.187090 1.863374
1 2.550862 -1.428866 0.631053
1 -2.229585 0.880312 -2.188161
1 -2.790367 -0.228874 -1.225467
1 2.158374 1.244066 -2.056212
1 2.780346 0.040288 -1.259946
1 -1.509110 -0.997738 2.077692
1 -2.514872 -1.394184 0.896076
1 0.342145 0.472788 3.641298
1 -0.264715 -2.284030 -2.228526
1 0.331115 -2.851080 -0.906217
6 0.405017 3.150739 -0.386293
6 -0.915388 3.084466 -0.176915
1 1.108940 3.035027 0.432149
1 0.806395 3.434510 -1.354978
1 -1.625556 3.300983 -0.968684
1 -1.317303 2.901293 0.814482
8 4.049748 -1.003593 -0.530204
1 4.791306 -0.555410 -0.097587
1 4.452706 -1.707862 -1.058279
8 -4.016415 -1.232369 -0.365347
1 -4.791052 -0.773860 -0.008338
1 -4.367104 -2.031860 -0.783493

TS7Y

39 -0.238620 -0.202116 0.031385
8 -2.153572 -1.825500 0.177735
8 1.536565 0.451868 -1.437688
8 -0.639087 -0.855705 2.357033
8 1.926411 -0.922259 1.048104
8 -2.352936 0.996700 0.120750
6 0.351935 1.938672 1.194838
6 -0.459039 2.782137 0.370560
8 -1.434307 1.779041 -0.703443
1 -3.069882 -1.539915 0.063687
1 -2.141013 -2.785325 0.073708
1 1.419815 0.571141 -2.388006
1 2.474511 0.613487 -1.209976
1 -0.565875 -0.226662 3.087043
1 -1.286155 -1.523415 2.621419
1 1.967580 -1.092099 1.998014
1 2.772552 -0.497906 0.792160
1 -3.004351 1.633867 0.454960
1 1.420826 2.031337 1.007322
1 0.125656 1.986653 2.258646
1 -1.279469 3.339839 0.814295
1 -0.003016 3.319043 -0.458764

8 -1.035063 -0.255367 -2.330021
1 -1.277945 -0.886672 -3.018602
1 -1.537626 0.561074 -2.486646
8 0.502415 -2.507715 -0.590105
1 1.358764 -2.724988 -0.194509
1 0.357883 -3.129246 -1.314571
8 4.028307 0.469233 -0.186299
1 4.781632 -0.010179 -0.560354
1 4.405046 1.275272 0.195236

TS8Y

39 -0.006927 0.094020 0.052072
8 1.920416 -0.681529 1.268069
8 -0.174027 0.607649 2.527774
8 -2.328794 -0.187232 0.603926
8 1.713960 -0.660420 -1.471172
8 -0.631521 -2.154433 -0.423499
8 0.804035 2.297390 0.418550
6 -0.720030 1.190023 -2.054226
6 -1.058100 2.440535 -1.442383
8 -0.651438 2.390808 0.276163
1 2.788759 -1.003721 0.950945
1 1.977841 -0.519615 2.218174
1 -0.704416 0.197623 3.223635
1 -0.117265 1.550081 2.743823
1 -2.887367 0.522807 0.944778
1 -2.904959 -0.950606 0.388878
1 1.677210 -0.423922 -2.406210
1 2.622151 -0.968782 -1.268776
1 -0.058606 -2.775742 -0.889872
1 -1.527902 -2.550929 -0.369313
1 1.152104 3.176570 0.200623
1 -1.578470 0.600634 -2.379182
1 0.041747 1.257497 -2.828486
1 -0.487587 3.329452 -1.696927
1 -2.100419 2.672319 -1.230984
8 4.097758 -1.469850 -0.276936
1 4.891888 -0.918719 -0.329120
1 4.417188 -2.382951 -0.309593
8 -3.335702 -2.666941 -0.128208
1 -3.682598 -3.279395 0.536635
1 -3.897855 -2.786252 -0.907534

$[Y(H_2O)_5(CH_2CH_2OO(H))](H_2O)_2^{2+}$ (product 1) pentagbipiram3 (**24Y**)

39 0.115291 -0.105065 0.109675
8 -0.433960 1.806960 1.549302
8 -0.526285 -1.601970 1.888221
8 2.093804 -1.150365 0.942511
8 -0.634578 1.675167 -1.376514
8 2.001092 0.840213 -0.984604
8 -2.339566 -0.354617 0.138557
6 -0.563591 -1.736765 -1.496747
6 -1.984561 -2.199851 -1.283565
1 -0.735166 2.677787 1.212702

1 -0.404240 1.871042 2.512455
1 -0.393516 -1.817788 2.819225
1 -1.339361 -2.052083 1.574745
1 2.076048 -1.979681 1.436523
1 3.015920 -1.000415 0.640226
1 -1.119742 1.458334 -2.183677
1 -0.905346 2.575723 -1.100478
1 1.901865 1.481065 -1.699694
1 2.944772 0.579520 -0.924212
1 -3.195269 -0.080994 0.502180
1 0.140731 -2.570953 -1.368390
1 -0.429851 -1.390635 -2.527990
1 -2.694746 -1.800725 -2.008819
1 -2.122996 -3.284028 -1.217079
8 -1.226476 4.014025 0.034601
1 -2.127015 4.366306 0.084573
1 -0.653781 4.791548 -0.036036
8 4.417025 -0.329401 -0.314730
1 5.115456 0.152337 0.151684
1 4.875304 -0.920613 -0.929727
8 -2.495617 -1.817329 0.055946

$[Y(H_2O)_5(CH_2CH_2OO(H))](H_2O)_2^{2+}$ (product 1) cappedtrigonalprismatic9 (**24Y**)

39 -0.018990 0.046459 0.055466
8 1.946716 -0.599854 1.301690
8 -0.253705 0.709482 2.468915
8 -2.351153 -0.208478 0.583244
8 1.695020 -0.798350 -1.431965
8 -0.641570 -2.197196 -0.411378
8 0.745416 2.324232 0.396022
6 -0.576263 1.226329 -1.975584
6 -0.913041 2.552535 -1.380139
8 -0.684477 2.521629 0.136969
1 2.811772 -0.934089 0.986835
1 1.996986 -0.472250 2.257084
1 -0.835716 0.352353 3.152501
1 -0.093924 1.636787 2.696038
1 -2.929861 0.516426 0.851827
1 -2.917254 -0.976946 0.357609
1 1.662479 -0.527098 -2.358107
1 2.606821 -1.094020 -1.229685
1 -0.070151 -2.792639 -0.912423
1 -1.534952 -2.600221 -0.359919
1 1.171973 3.171452 0.184589
1 -1.455264 0.759499 -2.430320
1 0.191202 1.313091 -2.747688
1 -0.341017 3.412260 -1.734068
1 -1.973394 2.819668 -1.366398
8 4.102704 -1.503319 -0.211368
1 4.896756 -0.961271 -0.323939
1 4.420069 -2.416823 -0.171052
8 -3.349005 -2.694973 -0.141591
1 -3.713143 -3.296187 0.524293

1 -3.896526 -2.820482 -0.930325

[La(H2O)7(OOH)](H2O)(C2H4)$^{2+}$ (**4La•**C_2H_4)

57 -0.613045 -0.053499 -0.043436
6 4.708148 -1.185930 -0.648674
6 4.702765 -1.081797 0.681303
8 -1.694531 -0.552571 2.013181
8 -0.592256 0.340147 2.454684
8 -2.951151 1.120925 0.359369
8 0.241875 -2.214990 1.261443
8 -2.536200 -1.699429 -0.841169
8 0.345182 -1.983578 -1.584813
8 1.910749 0.507273 -0.124440
8 -0.255427 2.515906 -0.273905
1 5.087353 -0.390786 -1.282672
1 4.403846 -2.099116 -1.150249
1 4.393507 -1.904686 1.317859
1 5.075865 -0.197165 1.187382
1 -0.980055 0.838191 3.187650
1 -3.700742 1.636498 0.038499
1 -3.158651 0.771980 1.244322
1 1.036756 -2.574926 1.673285
1 -0.429087 -2.118036 1.967096
1 -3.428941 -1.687053 -0.470912
1 -2.401965 -2.589655 -1.191344
1 0.618697 -2.814869 -1.174548
1 0.647966 -2.003734 -2.501571
1 2.687260 -0.088662 -0.095910
1 2.266069 1.413995 -0.051308
1 -0.950294 3.156648 -0.078899
1 0.602205 2.987598 -0.208356
8 -1.319642 0.569135 -2.514476
1 -1.100611 1.362212 -3.020677
1 -2.006741 0.105147 -3.010912
8 2.385301 3.315482 -0.019673
1 2.855267 3.766056 -0.735459
1 2.689189 3.739777 0.795183

[La(H_2O)$_7$(OOH)(C_2H_4)](H_2O)$^{2+}$ trigonalprism2 (**5La**)

57 -0.014744 -0.218493 0.105947
8 -0.268460 0.687184 -2.260632
8 -1.933803 -1.186612 1.679708
8 -2.160404 -0.777061 -0.812174
8 -0.257024 -2.626247 -0.890401
8 -0.049885 0.677276 2.613174
8 2.219973 -0.952132 -1.056553
8 1.441836 -1.662451 1.763824
8 1.753111 1.730308 0.219258
6 -2.363743 2.309893 0.430174
6 -1.306264 3.089391 0.190999
1 0.204774 1.129216 -2.973117
1 -1.207707 0.546083 -2.533437
1 -2.632346 -1.161685 0.991846
1 -2.129610 -1.916537 2.280219

1 -1.172374 -2.556291 -1.218036
1 -0.017046 -3.559197 -0.838791
1 0.456389 1.356632 3.076296
1 -0.881645 0.564722 3.093922
1 2.237850 -1.577667 -1.791480
1 3.066663 -0.463481 -1.060258
1 1.385297 -1.590816 2.725174
1 2.097166 -2.343771 1.568913
1 2.691205 1.633860 -0.047020
1 1.580673 2.675455 0.308007
1 -2.919625 1.838612 -0.372997
1 -2.748502 2.175829 1.436427
1 -0.974945 3.296734 -0.821702
1 -0.806055 3.625495 0.992806
8 -2.731764 0.016795 -1.884815
1 -3.412549 -0.568328 -2.248268
8 4.280221 0.941170 -0.715839
1 5.011069 0.784479 -0.101051
1 4.681371 1.383197 -1.477850

$[La(H_2O)_7(OOH)(C_2H_4)](H_2O)^{2+}$ trigonalprism3 (**5La**)

57 -0.105960 0.002929 0.044116
8 -2.446583 -0.858770 0.774402
8 1.987707 1.452335 0.699496
8 -0.615525 1.192561 2.359951
8 0.600069 -1.363163 2.216854
8 0.621113 1.379738 -2.093628
8 -0.203693 -2.379884 -0.065567
8 2.072330 -1.123644 -0.715385
8 -1.270929 -0.764608 -2.162349
6 -1.660976 3.221882 -0.360505
6 -2.697609 2.387210 -0.266684
1 -2.537171 -1.787625 0.482674
1 -3.250331 -0.608165 1.242426
1 2.045618 2.095721 1.416118
1 2.904689 1.233074 0.430753
1 -0.550832 0.580702 3.107056
1 -1.068284 1.982433 2.679974
1 1.350139 -1.504478 2.807319
1 0.326161 -2.233998 1.867666
1 0.583521 0.965696 -2.966070
1 1.154877 2.178611 -2.185353
1 3.014181 -0.876149 -0.711017
1 1.975220 -2.073830 -0.870944
1 -1.468066 -1.715765 -2.022141
1 -1.897023 -0.435110 -2.817858
1 -1.297215 3.783927 0.494354
1 -1.195816 3.441450 -1.314990
1 -3.223601 2.233451 0.669940
1 -3.119891 1.900881 -1.140173
8 -1.449769 -2.916686 -0.607407
1 -1.282735 -3.870922 -0.615954
8 4.419904 0.384627 -0.246815

1 5.086496 0.076751 0.383368
1 4.924296 0.791790 -0.965019

$[La(H_2O)_7(CH_2CH_2OO(H))](H_2O)^{2+}$ (product 1) isomer 2 (**23La**)

57 -0.006393 0.315249 -0.025861
8 1.444061 1.323327 -2.034428
1 1.991248 0.643626 -2.452807
1 1.625842 2.159576 -2.479430
8 -1.641250 2.238412 -0.878319
1 -1.554309 3.084736 -1.333869
1 -2.555293 1.948369 -1.005882
8 0.859212 2.728837 0.995001
1 1.794422 2.856312 1.202679
1 0.459252 3.607448 1.018890
8 -1.117748 -0.763429 -2.137265
1 -1.223912 -0.568965 -3.075880
1 -1.923071 -1.225609 -1.826209
8 -0.525723 0.670385 2.553067
1 -0.915181 -0.013639 3.112639
1 -0.501596 1.483981 3.072560
8 1.751214 -1.273810 -1.350093
1 1.336045 -1.987841 -1.851415
1 2.566654 -1.639592 -0.953330
8 2.231081 0.050071 1.324330
1 2.973107 -0.537965 1.071420
1 2.224829 0.087540 2.288780
8 4.025825 -1.809129 0.229141
1 4.132842 -2.663739 0.670535
1 4.910423 -1.569229 -0.081196
8 -2.903292 -1.444487 -0.205125
6 -0.708272 -2.055929 0.822638
6 -2.179988 -2.347632 0.730925
1 -0.366547 -2.192970 1.855663
1 -0.138196 -2.774026 0.221932
1 -2.449008 -3.301795 0.262973
1 -2.709842 -2.282616 1.685249
8 -2.692144 -0.062945 0.241033
1 -3.433611 0.080717 0.850673

$[La(H_2O)_6(OOH)(C_2H_4)](H_2O)_2^{2+}$ firstintermediate1 (**27La**)

57 -0.224359 -0.013029 0.173760
8 -1.679327 -1.764287 -0.330939
8 -2.049304 -0.731939 1.945722
8 0.534208 0.275055 2.654337
8 -0.256092 -0.411992 -2.355831
8 0.193905 2.481948 -0.460887
8 1.067086 -2.178350 0.089510
8 2.326744 0.471816 0.025331
6 -3.131522 2.201399 0.078315
6 -3.141188 1.342996 -0.944434
8 -1.225888 -2.698306 -1.350192
1 -2.730725 -0.431909 2.560072
1 -2.379240 -1.536458 1.499548
1 1.345184 0.624976 3.044114

1 0.038625 -0.149336 3.367822
1 -0.669915 -1.290289 -2.494372
1 0.047043 -0.074846 -3.205901
1 -0.472044 3.146675 -0.674700
1 1.072838 2.906591 -0.557989
1 2.018520 -2.386032 0.041436
1 0.548269 -2.901418 -0.304341
1 3.009170 -0.228335 0.000166
1 2.755462 1.325005 -0.173330
1 -3.433755 1.908723 1.078747
1 -2.908953 3.255706 -0.058053
1 -2.917362 1.664241 -1.956916
1 -3.446956 0.308548 -0.823622
1 -1.996857 -3.274462 -1.462292
8 2.883951 3.191170 -0.604722
1 3.266394 3.800539 0.042449
1 3.281382 3.437613 -1.451897
8 3.859448 -1.916534 -0.004731
1 4.400402 -2.191968 0.748540
1 4.359365 -2.185924 -0.787903

$[La(H_2O)_6(OOH)(C_2H_4)](H_2O)_2^{2+}$ firstintermediate2 (**27La**)

57 0.215828 -0.105327 -0.157362
8 1.587209 -2.106777 0.761890
8 0.800817 -1.463618 -2.387784
8 0.143091 1.657978 -2.136241
8 0.610754 0.221024 2.071674
8 -0.108008 2.340103 0.705095
8 -1.148197 -2.306384 -0.156292
8 -2.304975 0.382970 -0.209131
6 3.130133 1.506347 -0.747379
6 3.590683 0.457996 -0.060304
8 1.079329 -0.828946 2.947879
1 2.264360 -2.741740 0.502702
1 1.684980 -1.916729 1.727198
1 1.471224 -1.347574 -3.073853
1 0.367348 -2.307007 -2.576174
1 -0.099593 1.567388 -3.066594
1 0.325362 2.595511 -1.988456
1 0.214748 2.296103 1.621147
1 -0.967186 2.803887 0.731505
1 -2.123146 -2.409283 -0.145895
1 -0.761655 -3.062676 0.304739
1 -3.029201 -0.270950 -0.202603
1 -2.680311 1.255779 0.022610
1 3.225755 1.565214 -1.826661
1 2.727114 2.379585 -0.242602
1 3.566813 0.434061 1.024057
1 4.073612 -0.377098 -0.557719
1 1.437888 -0.337907 3.701096
8 -2.868740 3.028055 0.625734
1 -3.241565 3.706871 0.046128
1 -3.302434 3.160071 1.480651

8 -3.904879 -1.967692 -0.149987
1 -4.459699 -2.244475 -0.892782
1 -4.412732 -2.185152 0.644537

$[La(H_2O)_6(OOH)(C_2H_4)](H_2O)_2^{2+}$ firstintermediate3 (**27La**)

57 0.201775 0.005866 0.207294
8 1.935228 -0.551540 2.132776
8 1.808198 -1.634780 -0.174976
8 0.439083 -0.383723 -2.318672
8 -0.758109 0.076350 2.631373
8 -0.293364 2.540618 -0.160626
8 -0.945666 -2.228946 -0.025031
8 -2.341335 0.353100 -0.163680
6 2.798041 2.127936 -1.199418
6 3.353967 1.508564 -0.156007
8 1.499339 -2.594113 -1.224841
1 2.366550 -1.332221 1.735432
1 2.564887 -0.146178 2.742658
1 0.116236 -0.111427 -3.184865
1 0.924009 -1.230727 -2.417325
1 -0.233308 -0.314976 3.343227
1 -1.624102 0.289287 3.000477
1 0.346305 3.249722 -0.301048
1 -1.188585 2.931707 -0.250567
1 -1.874630 -2.487956 -0.166656
1 -0.350967 -2.916217 -0.373170
1 -2.981831 -0.376303 -0.284515
1 -2.808533 1.200546 -0.285683
1 2.594027 1.608622 -2.129959
1 2.612271 3.198384 -1.189909
1 3.628560 2.052708 0.742446
1 3.625739 0.459092 -0.204027
1 2.312882 -3.118197 -1.273677
8 -3.008032 3.107252 -0.436914
1 -3.334510 3.458792 -1.277399
1 -3.492639 3.591945 0.246213
8 -3.729576 -2.103880 -0.407803
1 -4.128411 -2.379384 -1.245008
1 -4.333286 -2.423315 0.277333

$[La(H_2O)_6(OOH)(C_2H_4)](H_2O)_2^{2+}$ firstintermediate4 (**27La**)

57 -0.013926 -0.033541 -0.029533
8 -1.987112 0.882847 -1.550297
8 -2.217481 -1.252187 0.432048
8 1.183750 0.203514 2.254247
8 0.265979 -1.051987 -2.403153
8 1.544394 1.937821 -0.780296
8 0.182066 -2.098318 0.978514
8 2.345936 -0.984137 -0.516147
6 -1.825073 1.890545 2.059780
6 -1.069895 2.827673 1.481320
8 1.454289 -2.387551 1.623948
1 -2.901271 0.530056 -1.493753
1 -2.002053 1.580452 -2.216916

1 -2.073689 -2.077936 0.919488
1 -3.124499 -1.227624 0.077152
1 1.549054 0.825112 2.893281
1 1.433891 -0.702656 2.528196
1 -0.309227 -1.180411 -3.166969
1 1.044117 -1.613112 -2.525777
1 1.389067 2.880198 -0.917405
1 2.496602 1.781385 -0.967320
1 2.507027 -1.712991 0.113637
1 3.182485 -0.518993 -0.694711
1 -2.822787 1.664720 1.699005
1 -1.503974 1.365730 2.953543
1 -0.106450 3.116246 1.890609
1 -1.432401 3.405313 0.636372
1 1.317927 -3.289200 1.951389
8 4.170418 1.085556 -1.204469
1 4.880396 1.378846 -0.616162
1 4.556255 1.094987 -2.091826
8 -4.431644 -0.426121 -1.094042
1 -5.184056 0.023822 -0.684500
1 -4.817578 -0.996908 -1.773393

TS8La

57 0.272538 0.018611 0.207912
6 1.031192 -1.443995 -1.901923
6 2.187031 -0.684346 -2.272143
1 0.233256 -1.463399 -2.642491
1 1.244825 -2.438594 -1.509872
1 3.176970 -1.067445 -2.029410
1 2.184063 -0.141770 -3.212899
8 2.355335 0.708726 -1.225741
8 1.267924 1.625461 -1.554572
1 1.630280 2.214064 -2.233170
8 2.112167 1.485571 1.393680
1 2.411751 1.858465 2.231450
1 2.827713 1.599753 0.746245
8 1.936583 -1.779816 1.274578
1 2.224957 -1.786282 2.196836
1 2.597196 -2.286031 0.783763
8 -0.442786 -0.382325 2.732440
1 -0.561392 0.175728 3.511270
1 -0.969457 -1.181935 2.871099
8 -0.984273 -2.278761 0.733883
1 -0.446408 -3.074806 0.831461
1 -1.789039 -2.542571 0.241715
8 -2.155975 0.089157 -0.647902
1 -2.679654 -0.695895 -0.897837
1 -2.727605 0.876235 -0.733430
8 -0.843034 2.363987 0.643357
1 -0.329157 3.161049 0.820384
1 -1.728018 2.652221 0.343304
8 -3.250796 -2.506433 -0.912769
1 -3.185234 -2.989137 -1.748773

1 -4.119512 -2.734280 -0.553160
8 -3.388878 2.627448 -0.507303
1 -4.176751 2.774058 0.034433
1 -3.512938 3.175640 -1.294712

$[La(H_2O)_6(CH_2CH_2OO(H))](H_2O)_2^{2+}$ (product 1) (**24La**)

57 0.243294 -0.019984 0.250441
6 1.097942 -1.182212 -1.915225
6 2.309965 -0.372682 -2.232069
1 0.360415 -1.152053 -2.721344
1 1.351490 -2.232342 -1.741578
1 3.270179 -0.868741 -2.065714
1 2.335423 0.114210 -3.208468
8 2.476263 0.773974 -1.229266
8 1.355223 1.692174 -1.406556
1 1.648627 2.313193 -2.091485
8 2.133466 1.303091 1.541364
1 2.375121 1.587859 2.431114
1 2.897931 1.474253 0.970126
8 1.874988 -1.945277 1.115950
1 2.194398 -2.099114 2.014638
1 2.479069 -2.416050 0.527309
8 -0.548237 -0.716881 2.698254
1 -0.680467 -0.277313 3.547567
1 -1.054797 -1.540904 2.722307
8 -1.054376 -2.347594 0.460668
1 -0.519303 -3.151033 0.438751
1 -1.859398 -2.534072 -0.064602
8 -2.168756 0.191379 -0.620925
1 -2.704229 -0.552747 -0.957060
1 -2.717056 0.998779 -0.654111
8 -0.771882 2.375369 0.737614
1 -0.241185 3.145781 0.972606
1 -1.650773 2.703997 0.463194
8 -3.315151 -2.326635 -1.206231
1 -3.249087 -2.703316 -2.094978
1 -4.189822 -2.583549 -0.882577
8 -3.331374 2.752096 -0.352512
1 -4.103844 2.895478 0.211761
1 -3.459185 3.332580 -1.115734

TS7La

57 0.203828 -0.183411 0.028805
6 1.229953 1.327475 -1.956298
6 1.496737 2.502775 -1.192499
8 0.934147 2.286952 0.480953
8 -0.523606 2.343986 0.438516
8 0.720675 0.526074 2.534398
8 2.882211 -0.264620 0.298962
8 1.035331 -2.434289 1.240115
8 1.389444 -2.039626 -1.531422
8 -1.932125 0.274031 -1.536382
8 -2.002409 -0.268392 1.482437
1 0.522252 1.455310 -2.773504

1 2.112231 0.774555 -2.276255
1 2.515201 2.723463 -0.878435
1 0.928024 3.405840 -1.388601
1 -0.733664 3.219528 0.794835
1 0.996638 0.208990 3.402547
1 1.053351 1.434543 2.432434
1 3.339236 -0.765919 0.985994
1 3.516863 0.386684 -0.025364
1 0.909753 -2.886564 2.083545
1 1.468513 -3.058411 0.641478
1 2.227135 -1.901689 -1.992438
1 0.844544 -2.603186 -2.096568
1 -1.838497 0.847659 -2.307308
1 -2.827233 0.430438 -1.173467
1 -1.972525 0.051201 2.392474
1 -2.909545 -0.113529 1.156595
8 -1.282715 -2.323723 -0.858981
1 -1.980903 -2.084018 -1.482739
1 -1.556476 -3.142884 -0.427943
8 -4.320581 0.405298 -0.021468
1 -5.048299 -0.209004 -0.192431
1 -4.747896 1.254414 0.159062

cis-[Ga(H2O)4(OOH)(C2H4)](H2O)$^{2+}$ (**5Ga**)

31 0.293220 -0.120668 -0.144940
8 1.215335 -1.309241 -1.604018
8 -0.325816 1.193697 1.029128
8 2.168924 0.075057 0.724560
8 0.703301 2.244202 1.026021
6 0.022206 -2.253432 1.018506
6 -0.498259 -1.454084 1.978382
8 0.883106 1.356006 -1.519220
1 1.376579 -2.264584 -1.615672
1 1.753249 -0.892649 -2.295851
1 2.205141 0.909340 1.232569
1 3.059506 -0.170787 0.437518
1 0.311629 2.897373 1.628165
1 1.055597 -2.581500 1.084965
1 -0.629474 -2.770878 0.320384
1 -1.557517 -1.217896 2.015431
1 0.116567 -1.038776 2.769191
1 0.277377 1.611519 -2.231915
1 1.047340 2.163373 -0.991498
8 -3.618957 0.425828 -0.156841
1 -3.771438 1.327346 0.155100
1 -4.484528 0.043848 -0.354854
8 -1.415313 -0.364424 -1.126944
1 -2.317940 -0.022464 -0.762633
1 -1.560218 -0.976461 -1.860584

TS9Ga

31 0.068087 -0.004301 0.141789
8 -1.216746 0.092635 -1.513539
8 -1.684705 -0.286295 1.106777

8 1.697224 0.157631 -0.849855
8 0.849905 -0.603976 2.067068
6 0.522789 2.080445 0.454773
6 1.823177 2.102647 -0.076052
1 -2.189630 0.213926 -1.469086
1 -0.896634 0.294783 -2.403705
1 -2.575178 -0.081329 0.721327
1 -1.731191 -0.396945 2.066758
1 1.402749 -0.069821 2.655850
1 1.134086 -1.526124 2.162222
1 0.439995 2.168299 1.537842
1 -0.239488 2.625265 -0.097242
1 2.021174 2.484240 -1.070006
1 2.695879 1.933941 0.544124
8 0.269821 -2.046723 -0.116177
1 -0.416089 -2.679344 -0.370672
1 1.084232 -2.206813 -0.642904
8 -3.785929 0.265047 -0.480039
1 -4.277475 1.099292 -0.430926
1 -4.452344 -0.413833 -0.667786
8 2.492105 -1.022396 -1.113871
1 2.840014 -0.858136 -2.006481

[Ga(H2O)4{CH2CH2O(OH)}](H2O)$^{2+}$ (**28Ga**)

31 -0.193503 0.405067 -0.161796
8 -0.735724 -1.553630 0.352636
8 -2.135451 0.653848 -0.101459
8 2.116611 -1.395881 0.140608
8 -0.402230 2.658147 -0.155655
6 1.262500 0.273529 -1.488608
6 2.138815 -0.957331 -1.236690
1 -1.616220 -1.971737 0.281105
1 -0.037921 -2.213345 0.486229
1 -2.812051 -0.085002 -0.105857
1 -2.532260 1.530593 -0.208404
1 -0.224596 3.216172 -0.927843
1 -0.138211 3.172876 0.621892
1 1.835970 1.196780 -1.385534
1 0.852920 0.252637 -2.501114
1 1.764664 -1.845018 -1.753329
1 3.171942 -0.788739 -1.547120
8 0.482418 0.697302 1.695647
1 0.006697 0.465622 2.507479
1 1.419569 0.357758 1.751013
8 -3.522254 -1.585430 -0.024308
1 -3.945816 -1.949601 -0.817063
1 -4.134751 -1.770643 0.704392
8 2.751558 -0.373404 0.962597
1 3.541337 -0.830240 1.301114

TS10Ga

31 -0.109302 0.162950 0.011821
8 -1.323765 -1.542324 -0.180561
8 1.813461 -0.785143 0.140462

8 0.574332 0.187126 -1.740356
8 2.803683 -0.725068 -1.195105
6 0.811677 -0.195235 1.887712
6 2.254002 -0.461903 1.510568
8 0.542833 2.318495 -0.003106
1 -2.303665 -1.532568 -0.130034
1 -1.017134 -2.437376 -0.377154
1 1.932530 -0.353059 -1.716202
1 0.045070 0.261345 -2.541959
1 2.984341 -1.656933 -1.427059
1 0.322952 -1.027789 2.383870
1 0.689713 0.761703 2.396935
1 2.897139 0.416062 1.502864
1 2.729685 -1.328779 1.961587
1 0.781213 2.957551 0.683678
1 0.966944 2.601563 -0.826577
8 -3.935314 -0.646673 0.056872
1 -4.458768 -0.811680 0.856109
1 -4.564767 -0.690921 -0.679204
8 -1.884642 1.076856 0.055230
1 -2.768822 0.626662 0.075180
1 -1.966845 2.039438 0.014347

8Ga

31 0.118356 -0.153781 -0.126813
8 1.745883 0.790831 -0.971154
8 -0.591633 1.693396 -0.077875
8 -0.559972 -1.143059 -1.446454
8 -2.874449 -2.194573 -0.087931
6 -1.372006 2.525561 0.882718
6 -1.994510 2.123369 -0.375264
8 -1.204710 -0.866857 1.165448
1 2.685769 0.558293 -0.807560
1 1.681068 1.646981 -1.416418
1 -2.497235 -2.377744 -0.960725
1 -0.129211 -1.146220 -2.308161
1 -3.476425 -2.909534 0.155095
1 -0.945237 3.515627 0.986214
1 -1.641195 2.011620 1.797151
1 -2.706456 1.306625 -0.381694
1 -2.030266 2.815153 -1.207653
1 -1.350621 -0.719335 2.107390
1 -1.946591 -1.481092 0.740016
8 3.970939 -0.340732 0.192019
1 4.605524 0.184473 0.703914
1 4.496477 -1.025425 -0.250381
8 1.510273 -0.831568 1.117123
1 2.486056 -0.759734 0.929890
1 1.327756 -1.605552 1.670006

cis-[In(H2O)4(OOH)(C2H4)](H2O)$^{2+}$ (**5In**)

49 -0.376617 -0.075565 -0.050206
8 -2.022080 -0.227595 -1.442323
8 0.891450 0.031395 1.453086

8 -1.880305 -0.366324 1.509549
8 1.931156 -0.994962 1.344055
6 -0.884151 2.397236 -0.195034
6 0.161351 2.601729 0.637131
8 -0.468479 -2.238178 -0.293972
1 -2.554380 0.465138 -1.861642
1 -2.304173 -1.082412 -1.804322
1 -1.515568 -0.354825 2.409837
1 -2.846985 -0.345877 1.570089
1 2.165384 -1.123479 2.276532
1 -1.901369 2.405212 0.189569
1 -0.751941 2.506040 -1.269799
1 1.170901 2.742007 0.264251
1 0.038264 2.650690 1.714066
1 0.290909 -2.693869 -0.690187
1 -0.816172 -2.826391 0.393806
8 3.265688 0.287347 -0.753017
1 3.303837 -0.155707 0.112710
1 4.143991 0.295352 -1.153671
8 0.974557 -0.088896 -1.616334
1 1.986943 0.061519 -1.379516
1 0.845476 -0.056818 -2.572554

TS9In

49 0.039175 0.007360 0.079418
8 -1.432332 0.384123 -1.489218
8 -1.672024 -0.065340 1.351539
8 1.808298 0.121316 -0.919208
8 1.245636 -1.087660 1.555689
6 0.726690 2.135380 0.516420
6 1.999089 2.000437 -0.059167
1 -2.399820 0.408797 -1.312062
1 -1.255615 0.809289 -2.341050
1 -2.585426 -0.012612 0.973649
1 -1.724392 0.080756 2.306282
1 1.235423 -1.316889 2.494870
1 2.138181 -1.263225 1.194958
1 0.690652 2.170401 1.605584
1 0.025120 2.802288 0.020467
1 2.222465 2.407561 -1.037738
1 2.860481 1.720738 0.536346
8 -0.408444 -2.011624 -0.528619
1 0.033446 -2.779473 -0.137479
1 -0.674901 -2.251961 -1.427618
8 -3.878120 0.228561 -0.213099
1 -4.440315 1.011565 -0.105846
1 -4.491446 -0.504186 -0.378125
8 2.686036 -1.006659 -0.703714
1 3.299530 -0.960342 -1.454192

$[In(H2O)4\{CH2CH2O(OH)\}](H2O)^{2+}$ (**28In**)

49 0.087218 -0.057543 0.009284
8 1.888471 -0.941606 -1.075043
8 1.681977 0.703956 1.207094

8 -2.385517 -0.239939 -0.444245
8 -0.927256 1.721231 0.756025
6 -0.942578 -1.857578 0.515275
6 -2.403241 -1.446631 0.419213
1 2.814203 -0.788911 -0.785441
1 1.856775 -1.812969 -1.495935
1 2.638280 0.497854 1.040440
1 1.596960 1.045423 2.108350
1 -0.645435 2.560190 1.144873
1 -1.907428 1.726248 0.661468
1 -0.679478 -2.202191 1.516615
1 -0.682080 -2.648229 -0.189902
1 -3.050868 -2.181472 -0.058575
1 -2.823533 -1.145433 1.378030
8 0.280905 1.121659 -1.741970
1 -0.306257 1.840148 -2.019475
1 0.866254 0.891281 -2.478476
8 4.119004 -0.085061 0.356175
1 4.642292 -0.720490 0.868710
1 4.759796 0.553212 0.006966
8 -3.314067 0.754078 0.048759
1 -4.026398 0.755644 -0.613870

In Second TS Alternative (**TS10In**)

49 0.077816 0.156404 -0.090655
8 1.328808 -1.243717 0.980593
8 -1.803588 -0.665784 0.177110
8 -0.620457 1.128022 1.538294
8 -2.768138 0.067419 1.467114
6 -0.956959 -1.366628 -1.607245
6 -2.307338 -1.435855 -1.012142
8 -0.541103 2.004038 -1.145733
1 2.310012 -1.276063 0.925561
1 1.025345 -1.926110 1.595443
1 -1.734992 0.682012 1.712372
1 -0.230384 1.602832 2.279331
1 -2.946926 -0.667464 2.078637
1 -0.352787 -2.266501 -1.546850
1 -0.873015 -0.780887 -2.521554
1 -3.090417 -0.860981 -1.499121
1 -2.647469 -2.411293 -0.676400
1 -0.762966 2.185481 -2.071036
1 -1.001107 2.663530 -0.602103
8 3.945253 -0.688968 0.304810
1 4.456993 -1.277709 -0.271456
1 4.579371 -0.349220 0.955228
8 1.969154 0.861860 -0.655732
1 2.831192 0.428473 -0.423483
1 2.130493 1.702024 -1.107813

7In

49 -0.220146 -0.456727 0.003943
8 1.289818 0.098959 -1.430802
8 -0.942894 1.502354 0.042691

8 -0.231748 -2.374932 -0.038056
8 -1.609004 -0.770199 -1.613700
6 -0.703618 2.795198 0.721599
6 -0.875572 2.763284 -0.730322
8 -1.561460 -0.797959 1.654210
1 2.238827 0.164514 -1.174342
1 1.239453 -0.174048 -2.358197
1 -1.689294 -1.735545 -1.716218
1 0.474937 -3.022914 -0.033565
1 -2.368023 -0.338315 -2.028223
1 0.290947 2.891753 1.139388
1 -1.532199 3.092717 1.352976
1 -1.830854 3.036753 -1.162099
1 -0.006010 2.836605 -1.372155
1 -2.300677 -0.348155 2.085640
1 -1.667097 -1.760351 1.753910
8 3.654258 0.257256 -0.029551
1 4.192670 1.063380 -0.025214
1 4.291608 -0.473293 -0.045917
8 1.322783 0.066745 1.410757
1 2.267151 0.133980 1.137112
1 1.286830 -0.196128 2.341626

TS9Sc

21 -0.022910 -0.100836 0.037496
8 -1.675821 -0.334217 -1.379058
8 -1.731974 0.105125 1.405615
8 1.931572 0.198439 -0.671761
8 1.105353 -0.462077 1.876499
6 0.389347 2.108508 -0.340561
6 1.812028 1.986756 -0.413131
1 -2.619776 -0.152420 -1.160916
1 -1.605397 -0.468690 -2.335077
1 -2.661891 0.141983 1.071986
1 -1.749270 0.364535 2.337310
1 0.920208 -0.770118 2.774255
1 2.061771 -0.581335 1.704430
1 0.008068 2.516987 0.598917
1 -0.106008 2.520205 -1.216454
1 2.334667 2.248023 -1.326209
1 2.410826 2.089218 0.487162
8 0.515867 -2.135277 -0.705004
1 1.461209 -2.335129 -0.802920
1 0.017365 -2.938739 -0.909225
8 -4.029145 0.161243 -0.073638
1 -4.517414 0.990967 -0.189320
1 -4.706505 -0.528026 0.005559
8 2.920779 -0.666967 -0.046885
1 3.731955 -0.481646 -0.550910

$[Sc(H2O)4\{CH2CH2O(OH)\}](H2O)^{2+}$ (**28Sc**)

21 -0.094108 -0.141779 0.164543
8 -1.944528 -1.290334 -0.104436
8 -1.610222 1.426729 0.349333

8 2.139950 -0.156575 -0.340236
8 0.868163 1.101716 1.701756
6 0.481242 0.079411 -1.938805
6 1.947624 0.364947 -1.748918
1 -2.835080 -0.875264 -0.197282
1 -2.006458 -2.197603 -0.434577
1 -2.563672 1.304085 0.127120
1 -1.454556 2.369941 0.497176
1 0.571239 1.512401 2.525222
1 1.846087 1.155599 1.657983
1 -0.051626 0.915858 -2.398454
1 0.287637 -0.825705 -2.520448
1 2.651757 -0.179219 -2.377792
1 2.203247 1.423495 -1.718563
8 0.563850 -2.111921 0.935416
1 1.469052 -2.424038 0.785831
1 0.134188 -2.746451 1.527540
8 -4.074423 0.419423 -0.262952
1 -4.508263 0.599869 -1.110999
1 -4.785912 0.410138 0.395542
8 3.122444 0.589552 0.415272
1 3.923574 0.039376 0.359420

TS10Sc

21 0.097854 0.309449 0.011316
8 1.407351 -1.007829 1.133606
8 -1.695768 -0.724041 0.011663
8 -0.917597 1.041003 1.674064
8 -2.932902 -0.223924 1.145871
6 -0.676027 -1.244342 -1.676797
6 -2.076095 -1.424224 -1.229480
8 -0.621962 2.124874 -1.046442
1 2.381553 -1.084960 0.995545
1 1.144242 -1.639089 1.818689
1 -1.880269 0.575720 1.678778
1 -0.748113 1.546100 2.480159
1 -3.127420 -1.058994 1.602893
1 -0.024793 -2.111830 -1.623102
1 -0.527799 -0.582465 -2.531130
1 -2.843322 -0.854922 -1.749601
1 -2.407569 -2.432486 -0.991195
1 -0.642676 2.365720 -1.984570
1 -1.226404 2.732443 -0.591760
8 3.977028 -0.700204 0.260286
1 4.416755 -1.378951 -0.274821
1 4.666191 -0.344441 0.842551
8 2.048491 0.938652 -0.759791
1 2.890651 0.463843 -0.554275
1 2.269643 1.729023 -1.272190

7Sc

21 -0.018251 -0.705558 0.015288
8 1.281198 0.312335 -1.463064
8 -1.413261 1.032905 0.084996

8 0.714775 -2.381108 -0.003418
8 -1.341059 -1.362828 -1.642389
6 -1.479325 2.474328 0.374778
6 -2.521916 1.848716 -0.436000
8 -1.178495 -1.306150 1.805427
1 2.140826 0.718958 -1.213185
1 1.319090 0.097121 -2.404553
1 -1.265610 -2.287545 -1.920971
1 1.158199 -3.234462 -0.015401
1 -2.083563 -0.974349 -2.124031
1 -0.704207 3.053455 -0.112728
1 -1.673656 2.697438 1.417116
1 -3.480671 1.612303 0.010667
1 -2.503043 1.980441 -1.512085
1 -1.908988 -0.871535 2.265938
1 -1.093541 -2.202873 2.160868
8 3.462204 1.329765 -0.107165
1 3.703069 2.267652 -0.136567
1 4.303102 0.848227 -0.109925
8 1.336218 0.393158 1.369800
1 2.187345 0.781626 1.064430
1 1.399729 0.247365 2.323206

[Y(H2O)6(OOH)(C2H4)](H2O)$^{2+}$ (**5Y**)

39 0.222322 -0.108285 0.173219
8 -1.442652 -0.270548 -1.526164
8 0.291752 1.282979 2.206181
8 2.591705 0.051137 0.635372
8 0.928425 -2.192630 -0.745306
8 -1.955483 -0.532475 1.175808
8 1.129576 0.364578 -1.731707
6 -1.258395 2.860564 -0.183967
6 -0.012158 3.063597 -0.622918
1 -2.385133 -0.521690 -1.556161
1 -1.075675 -0.226244 -2.420633
1 0.167276 2.237620 2.286660
1 0.580262 0.957247 3.069422
1 3.031672 -0.007128 -0.240585
1 3.144806 0.593954 1.210047
1 1.521784 -2.028350 -1.504548
1 0.915723 -3.138635 -0.559929
1 -2.241300 -0.253656 2.054555
1 -2.766526 -0.761848 0.667967
1 -1.602040 3.237029 0.775174
1 -2.009256 2.395647 -0.813331
1 0.303826 2.757907 -1.613669
1 0.720599 3.607209 -0.033268
8 2.389294 -0.330932 -1.968452
1 2.681750 0.051057 -2.810244
8 0.707299 -1.545917 2.134197
1 1.612312 -1.869049 2.248604
1 0.130280 -2.145391 2.625943
8 -3.978830 -1.049889 -0.651411

1 -4.752503 -0.472642 -0.725045
1 -4.313795 -1.945321 -0.803348

TS9Y

39 -0.004716 0.304315 0.014873
8 1.244784 -1.520628 -0.875205
8 0.170945 2.208743 1.607936
8 -2.219524 1.223972 0.123078
8 -0.864907 0.160129 -2.296215
8 2.331210 0.588862 0.588109
8 -1.491725 -1.554131 -0.146086
6 -0.533696 -0.897400 2.135668
6 -1.572107 -1.737420 1.617783
1 2.184702 -1.766615 -0.753369
1 0.751578 -2.301188 -1.160530
1 -0.033038 2.151710 2.551256
1 0.287807 3.144961 1.398497
1 -2.932742 0.621108 -0.154374
1 -2.619049 2.004081 0.525109
1 -1.686946 -0.357957 -2.347816
1 -0.437723 0.116733 -3.160331
1 2.608553 1.141253 1.329548
1 3.046645 -0.061650 0.418935
1 -0.897286 -0.120451 2.809746
1 0.327867 -1.423312 2.542960
1 -1.432351 -2.813527 1.607887
1 -2.609296 -1.444839 1.757579
8 -2.738484 -1.232180 -0.828052
1 -3.180594 -2.092707 -0.909745
8 0.723185 2.341423 -1.235972
1 0.202782 2.758302 -1.936405
1 1.620127 2.694377 -1.306839
8 3.932824 -1.550717 -0.180551
1 4.277837 -2.176371 0.472847
1 4.633430 -1.457058 -0.842049

$[Y(H_2O)_6\{CH_2CH_2O(OH)\}](H_2O)^{2+}$ (**28Y**)

39 -0.049950 0.296774 0.023096
8 -1.328569 -1.465317 1.001349
8 -0.231443 2.194172 -1.574729
8 2.102244 1.435219 0.031699
8 0.929185 -0.169112 2.233330
8 -2.378665 0.546792 -0.591457
8 1.672184 -1.435559 -0.074170
6 0.535937 -0.864897 -2.038065
6 1.825115 -1.487219 -1.587121
1 -2.221858 -1.780299 0.750380
1 -0.945902 -2.100655 1.618884
1 -0.027121 2.079655 -2.512728
1 -0.438077 3.127737 -1.435083
1 2.897752 0.954233 0.309021
1 2.393604 2.192318 -0.491116
1 1.786292 -0.630375 2.219543
1 0.745941 0.100300 3.141316

1 -2.629306 1.082510 -1.354288
1 -3.072905 -0.136668 -0.473296
1 0.715765 -0.197111 -2.886060
1 -0.189623 -1.616455 -2.357786
1 1.994280 -2.539126 -1.821689
1 2.715068 -0.902024 -1.820041
8 2.919143 -1.266552 0.666157
1 3.302980 -2.160400 0.678724
8 -0.828570 2.317317 1.311810
1 -0.320640 2.904274 1.888084
1 -1.759149 2.546838 1.439595
8 -3.901306 -1.703475 0.003306
1 -4.126992 -2.340570 -0.689821
1 -4.672006 -1.673545 0.588359

TS10Y

39 0.023572 0.195964 -0.025109
8 -0.011707 1.498238 -2.062241
8 1.642426 -0.715087 1.503099
8 -1.682126 1.935566 0.074074
8 2.017371 -0.340122 -1.346763
8 -2.086627 -0.709842 -0.294395
6 -0.608793 -2.046418 -1.123865
6 -2.004059 -2.171055 -0.666839
8 -1.018882 -0.134920 2.166043
1 0.537979 1.406147 -2.851468
1 -0.812588 1.979595 -2.312615
1 2.586843 -0.877297 1.288014
1 1.426850 -1.221450 2.296406
1 -1.708919 2.836784 0.417386
1 -2.551880 1.512301 0.253776
1 2.908966 -0.447140 -0.958555
1 1.939204 -1.015306 -2.033692
1 0.094067 -2.683232 -0.582541
1 -0.476186 -2.069737 -2.203005
1 -2.773329 -2.356392 -1.414846
1 -2.173393 -2.760892 0.233615
1 -1.979886 -0.287521 2.061419
1 -0.872268 0.152004 3.075947
8 -3.283306 -0.128729 0.637232
1 -4.083912 -0.462671 0.201017
8 4.173276 -0.961959 0.373811
1 4.906413 -0.372950 0.603034
1 4.576855 -1.835941 0.267720
8 1.459981 2.165584 0.479596
1 1.622202 2.873850 -0.158363
1 1.907516 2.422234 1.296605

$[Y(H_2O)_5(OH)(CH_2CH_2O)](H_2O)_2^{2+}$ (**8Y**)

39 0.109505 -0.438300 0.150275
8 0.004591 -0.259835 2.587772
8 1.500539 0.818052 -1.428776
8 -1.358070 -1.804184 0.691523
8 2.357952 -0.179640 1.036155

8 -1.037996 1.571674 0.372580
6 -2.318098 2.143039 0.823265
6 -1.642147 2.697968 -0.348550
8 -1.000108 -0.355247 -1.979973
1 0.275152 0.376862 3.261621
1 -0.705982 -0.799569 2.960896
1 2.418021 1.142047 -1.329597
1 1.154702 1.149582 -2.266468
1 -1.676126 -2.633911 1.054885
1 -3.050275 -1.230822 -0.239216
1 3.112167 0.303820 0.636511
1 2.654544 -0.547413 1.877938
1 -2.243511 2.656438 1.774329
1 -3.158023 1.475058 0.675811
1 -2.001980 2.441114 -1.337763
1 -1.075334 3.616570 -0.254393
1 -1.983443 -0.438991 -1.822462
1 -0.795840 -0.847254 -2.784343
8 -3.359672 -0.592215 -0.908243
1 -4.245942 -0.847141 -1.191818
8 4.086994 1.349785 -0.508677
1 4.872215 0.987662 -0.943801
1 4.345254 2.233560 -0.209779
8 1.164837 -2.434405 -0.716566
1 0.663508 -3.260920 -0.721140
1 2.059118 -2.640913 -1.016584

[La(H2O)7(OOH)](H2O)(C2H4)$^{2+}$ (**4La•**C_2H_4)

57 -0.149604 0.324914 0.035039
8 -0.652488 -1.856379 -0.599683
6 4.989245 -1.069280 0.589359
6 4.944870 -1.156796 -0.742239
8 0.346791 -0.390813 -2.431236
8 2.421686 0.776870 -0.180317
8 -0.913451 2.385099 1.535166
8 1.080030 -0.151442 2.281474
8 -1.581520 -0.856149 1.877448
8 -2.514299 0.942888 -0.685176
1 4.534381 -1.826085 1.221393
1 5.548915 -0.285379 1.090050
1 5.466705 -0.446655 -1.376250
1 4.448199 -1.982518 -1.241890
1 0.993845 -0.364199 -3.146123
1 -0.068883 -1.274261 -2.430068
1 2.787966 1.590387 -0.550426
1 3.178961 0.148136 -0.129348
1 -1.813568 2.735008 1.485288
1 -0.524490 2.750456 2.341171
1 1.985366 -0.038906 2.596827
1 0.596307 -0.665123 2.943452
1 -1.795580 -1.741804 1.504602
1 -2.325842 -0.591593 2.431776
1 -2.821865 1.572946 -1.347202

1 -3.185124 0.197270 -0.657034
8 -1.658610 -2.707359 0.000904
1 -1.284763 -3.593474 -0.120992
8 0.142193 2.550981 -1.424544
1 0.191704 2.591472 -2.389014
1 0.067888 3.465090 -1.119634
8 -4.004899 -1.194590 -0.481196
1 -4.907730 -1.395839 -0.753403
1 -3.473149 -2.001399 -0.575831

TS9La

57 -0.473284 -0.023998 0.016582
8 1.759868 -1.256145 0.547066
6 0.294154 -2.340247 -1.226570
6 1.656309 -2.402830 -0.839616
8 -0.148708 -1.068761 2.372255
8 -2.577890 -1.657960 0.039189
8 -1.359587 2.598130 -0.336854
8 -2.017049 0.152507 -2.131434
8 1.068266 0.951939 -1.836633
8 0.975222 1.902267 1.115375
1 0.110428 -1.968842 -2.235342
1 -0.304613 -3.215372 -0.982995
1 2.016822 -3.267967 -0.293700
1 2.416076 -1.939734 -1.461840
1 -0.541628 -1.347632 3.207484
1 0.717865 -1.501996 2.271681
1 -3.431589 -1.527085 0.472480
1 -2.483107 -2.608582 -0.108614
1 -0.687300 3.212458 -0.008820
1 -1.840312 3.062194 -1.034357
1 -2.692254 -0.530788 -2.240046
1 -1.992626 0.648379 -2.959378
1 1.147189 0.722359 -2.770042
1 1.930229 1.342260 -1.562026
1 1.079495 2.021901 2.068223
1 1.861570 2.065274 0.717301
8 3.035123 -0.607719 0.833343
1 3.556554 -1.316656 1.239502
8 -2.405561 0.935738 1.582671
1 -2.832579 0.768111 2.431856
1 -2.617992 1.845840 1.328504
8 3.213162 1.801759 -0.427917
1 3.958586 2.388255 -0.611430
1 3.560846 0.959935 -0.073014

[La(H2O)7{CH2CH2O(OH)}](H2O)$^{2+}$ (**28La**)

57 -0.536761 -0.051247 0.006143
8 1.941952 -1.167597 0.408070
6 0.466333 -2.250363 -1.041776
6 1.930502 -2.120528 -0.761093
8 -0.038208 -1.040908 2.372636
8 -2.442957 -1.899874 -0.129987
8 -1.532853 2.613816 -0.134797

8 -2.030642 0.189893 -2.153108
8 0.985499 1.057581 -1.787184
8 0.896306 1.859018 1.181095
1 0.273678 -2.191710 -2.117961
1 0.078984 -3.207462 -0.680116
1 2.454146 -3.018390 -0.424169
1 2.503233 -1.635082 -1.552094
1 -0.478168 -1.228951 3.210421
1 0.800593 -1.524900 2.366164
1 -3.352946 -1.977019 0.183971
1 -2.140933 -2.792596 -0.346417
1 -0.851825 3.194835 0.233109
1 -2.052654 3.156087 -0.742259
1 -2.618621 -0.538880 -2.392792
1 -2.068117 0.823920 -2.880062
1 1.064976 0.840173 -2.723543
1 1.833219 1.474066 -1.513519
1 1.008504 1.935518 2.137234
1 1.768146 2.080407 0.780659
8 3.259482 -0.590394 0.664775
1 3.745980 -1.307700 1.102514
8 -2.573296 0.667653 1.559228
1 -3.173810 0.356039 2.247462
1 -2.773998 1.602711 1.403516
8 3.134301 1.972255 -0.378092
1 3.799861 2.650340 -0.554087
1 3.597437 1.163476 -0.092082

TS10La

57 0.047704 0.143982 0.072603
8 -2.163301 -0.965374 -0.467964
6 -0.992851 -2.318428 0.816926
6 -2.412092 -2.091351 0.514242
8 0.461739 -1.211287 -2.140019
8 2.095928 -1.371406 0.839748
8 2.332076 0.949741 -0.964685
8 0.796268 0.485083 2.564601
8 -2.070354 1.150480 1.305204
8 -1.305199 1.486325 -1.730320
1 -0.744169 -2.213184 1.875086
1 -0.551997 -3.199365 0.357262
1 -2.950118 -2.867413 -0.029667
1 -3.021361 -1.692465 1.325202
1 1.054368 -1.093539 -2.892159
1 -0.159100 -1.912929 -2.376334
1 3.010946 -1.318028 0.497765
1 1.923465 -2.300401 1.040865
1 2.500989 1.870779 -1.198233
1 3.194460 0.487473 -0.954182
1 1.538711 -0.057678 2.863324
1 0.369391 0.837187 3.355921
1 -2.286589 1.876046 1.901882
1 -2.898883 0.886495 0.862073

1 -2.224210 1.133967 -1.695742
1 -1.150134 1.797214 -2.630003
8 -3.385554 0.023861 -0.832670
1 -4.008881 -0.562233 -1.290146
8 0.380088 2.861606 0.271528
1 0.851631 3.455081 0.869950
1 -0.284293 3.398613 -0.181108
8 4.527240 -0.729270 -0.445041
1 5.272283 -0.396270 0.075259
1 4.922566 -1.315721 -1.105469

[La(H2O)6(OH)(CH2CH2O)](H2O)2^{2+} (**8La**)
57 -0.094636 -0.279185 -0.023441
8 1.256619 1.935182 0.004256
6 2.136938 2.675015 0.917329
6 2.639289 2.268132 -0.391623
8 -0.788734 1.367156 -1.987462
8 -1.900240 1.437810 1.072632
8 -2.482620 -0.936778 -0.821247
8 -1.016728 -0.984052 2.375571
8 1.918169 -0.751077 1.487657
8 1.222863 -1.197544 -1.633961
1 2.432726 2.111191 1.794345
1 1.826359 3.700880 1.077746
1 2.688545 2.999130 -1.190141
1 3.291066 1.405131 -0.471487
1 -1.113309 1.142610 -2.868586
1 -0.363570 2.231359 -2.059736
1 -2.813212 1.451663 0.717925
1 -1.738043 2.318717 1.432630
1 -2.724122 -1.836493 -1.073628
1 -3.300550 -0.405605 -0.761071
1 -1.676052 -0.406833 2.782636
1 -0.919073 -1.750140 2.954531
1 2.072018 -0.980736 2.410165
1 2.751500 -0.939164 0.966603
1 2.994762 -1.269649 -1.060003
1 1.350795 -1.197955 -2.587314
8 3.673087 -1.026844 -0.392716
1 4.479914 -1.525322 -0.564104
8 -0.287261 -2.903906 -0.201787
1 -0.465493 -3.756866 0.211141
1 0.385305 -3.025895 -0.894475
8 -4.407883 1.008617 -0.173179
1 -5.176268 0.778555 0.368414
1 -4.744572 1.621569 -0.841840

[Ga(H_2O)$_3$(OOH)$_2$](H_2O)$^+$ (**20Ga**)
31 -0.321640 0.081313 -0.000123
8 0.013335 1.674286 -0.870578
8 0.864472 0.557436 1.615218
8 -1.573447 -0.545499 1.199331
8 0.964001 -1.309867 -0.541964
1 1.131174 1.488518 1.460231

1 0.455370 0.473828 2.487998
1 1.946329 -1.327497 -0.329320
1 0.794407 -1.797883 -1.357456
8 3.508326 -1.429647 -0.074222
1 4.196122 -0.894714 -0.486372
1 3.942929 -2.062192 0.508990
8 -1.466412 -0.482659 -1.644541
1 -1.628031 0.185794 -2.325213
1 -2.321580 -0.769046 -1.256278
8 1.005403 2.461915 -0.139960
1 0.709198 3.360150 -0.346544
8 -2.825114 -0.878931 0.522799
1 -3.179597 -1.553942 1.119097

TS6Ga

31 -0.556131 -0.229783 -0.019002
8 -2.196415 0.569549 -0.460233
8 2.562107 2.640927 -0.298937
8 -0.973013 -1.315789 -1.780136
8 -0.441281 0.940240 1.709335
8 0.678968 -1.536354 0.527511
8 -2.447728 1.765708 0.345632
8 -0.979096 -2.054773 0.838586
1 2.526232 3.388214 0.309455
1 3.318600 2.792705 -0.878024
1 -1.845692 -1.132618 -2.157391
1 -0.934155 -2.262124 -1.574799
1 -1.278337 1.456286 1.696415
1 -0.304387 0.542679 2.577382
1 -3.415348 1.772787 0.359523
1 -0.863508 -2.312841 1.761613
8 0.489391 1.163229 -1.064693
1 1.254762 1.707188 -0.739314
1 -0.106847 1.739494 -1.562193
6 2.755382 -1.446462 -0.443134
6 2.899220 -0.797054 0.727972
1 2.837238 -2.523777 -0.504142
1 2.607741 -0.914982 -1.376345
1 2.877815 0.285211 0.784836
1 3.094872 -1.335756 1.646488

$[Ga(H_2O)_3(OOH)(OH)(Epox)](H_2O)^+$ (**22Ga**)

31 -0.324342 -0.468440 0.259078
8 -2.042149 -0.907875 -0.404507
8 -2.624107 0.272655 -1.052412
8 -0.157253 -0.573614 2.056540
8 -0.035505 0.739525 -1.333728
1 -3.414334 -0.115531 -1.454238
1 0.650785 -0.960462 2.405145
1 0.222323 1.673334 -1.087666
1 -0.928585 0.788520 -1.734048
8 0.575539 3.053573 -0.272380
1 -0.098032 3.074972 0.426136
1 0.717227 3.954786 -0.583149

8 0.024068 -2.418432 -0.488503
1 -0.822121 -2.766013 -0.811089
1 0.468548 -3.104485 0.026800
8 -1.345031 1.549684 1.106896
1 -2.273249 1.507108 0.831587
1 -1.293791 1.217905 2.018950
8 1.880215 -0.582241 0.160466
6 2.830310 -0.464528 -0.943244
6 2.921547 0.445024 0.201440
1 3.506664 -1.308179 -1.013108
1 2.388916 -0.115029 -1.868264
1 2.550955 1.459903 0.111349
1 3.661935 0.265638 0.972025

$[In(H_2O)_3(OOH)_2](H_2O)^+$ (**20In**)

49 0.297206 -0.192604 -0.027173
8 2.007524 0.145934 0.872543
8 -0.068648 -1.689200 1.457058
8 1.103947 0.717040 -1.786801
8 -0.969064 -1.123116 -1.199167
8 -1.827891 -2.018981 -0.415396
8 -0.821159 1.387121 0.737512
1 0.485985 -2.069183 2.147941
1 -0.752650 -2.313892 1.145208
1 1.999158 1.063264 -1.599299
1 0.976558 0.529034 -2.723631
1 -2.142103 -2.613621 -1.110446
1 -1.769515 1.640580 0.530010
1 -0.467441 1.987230 1.406076
8 -3.276716 2.101654 0.281077
1 -3.560124 2.790068 -0.331217
1 -4.048837 1.558569 0.476508
8 2.738662 1.201392 0.159921
1 3.622615 1.090779 0.536333

TS6In

49 -0.515368 -0.237064 -0.114023
8 -2.213536 0.771134 -0.355040
8 2.732053 2.710915 -0.377511
8 -0.297003 0.031102 -2.277981
8 -1.164078 -0.459234 1.940508
8 0.895763 -1.643482 -0.081115
8 -2.326974 1.648140 0.829014
8 -0.607691 -2.231136 -0.765750
1 3.391722 3.050523 0.238544
1 2.894189 3.146967 -1.222077
1 -1.001350 0.511755 -2.734351
1 -0.143233 -0.801399 -2.748738
1 -1.879492 0.164290 2.157250
1 -0.940191 -1.014277 2.694692
1 -3.178611 2.071446 0.653966
1 -0.698811 -3.042494 -0.252388
8 0.434098 1.599587 0.376221
1 1.279786 2.026156 0.085961

1 -0.231269 2.277817 0.573275
6 3.076692 -0.969841 0.096556
6 2.677666 -1.056309 1.378243
1 3.430839 -1.837462 -0.443885
1 3.116868 -0.018058 -0.421002
1 2.375748 -0.179059 1.940474
1 2.689639 -1.999395 1.909818

$[In(H_2O)_3(OOH)(OH)(Epox)](H_2O)^+$ (**22In**)

49 0.238399 -0.179702 -0.070312
8 1.718731 0.853518 -0.965855
8 -0.967304 -1.242640 1.287538
8 -3.013568 -1.797872 -0.104393
8 1.369057 0.265744 1.780682
8 -0.857246 1.616242 0.487441
8 2.974009 0.406620 -0.322763
8 -1.052077 -0.693514 -1.463663
1 -0.709405 -1.676147 2.107132
1 -1.837841 -1.613224 0.923364
1 -3.533919 -2.579211 -0.315494
1 -2.493091 -1.524669 -0.898579
1 2.257544 0.525639 1.462410
1 1.051469 0.962371 2.368903
1 3.624072 0.937723 -0.802642
1 -0.841428 -0.586269 -2.394292
8 1.624329 -1.888760 -0.175378
1 1.450732 -2.684227 -0.692903
1 2.496154 -1.530659 -0.429102
6 -1.136514 2.775074 -0.367589
6 -2.243389 1.971834 0.151967
1 -0.880167 3.715036 0.105217
1 -0.823281 2.650151 -1.397319
1 -2.727739 1.253964 -0.498520
1 -2.802684 2.318751 1.011984

$[Sc(H_2O)_3(OOH)_2](H_2O)^+$ (**20Sc**)

21 -0.290373 -0.320823 -0.025156
8 -1.860832 0.483151 -0.931142
8 -1.362355 -2.193597 -0.506272
8 -1.266639 0.315016 1.828997
8 1.311292 -1.383101 -0.481019
8 1.573803 -0.978147 0.913977
8 0.743728 1.569503 -0.370102
1 -2.284000 -2.246699 -0.790495
1 -0.916190 -3.027478 -0.703880
1 -1.930699 0.993910 1.601169
1 -1.126081 0.291532 2.781935
1 2.362697 -0.406260 0.817885
1 1.715090 1.646285 -0.449523
1 0.291448 2.355849 -0.700876
8 3.391310 0.857536 -0.227954
1 4.170309 1.323995 0.101048
1 3.689313 0.331938 -0.983094
8 -2.147382 1.758279 -0.275346

1 -2.937443 2.045078 -0.754995

TS6Sc

21 0.270961 -0.394422 0.261349
8 0.326445 -1.489026 -1.419514
8 -3.668626 1.831772 0.233747
8 2.382767 -1.103827 0.422372
8 -0.459278 -2.302755 1.155714
8 0.932959 1.443808 0.651467
8 -0.915309 -2.244790 -1.569103
8 0.359840 0.572611 2.097489
1 -4.445783 1.666923 0.778957
1 -3.817881 2.672951 -0.211905
1 2.725508 -1.880827 -0.035414
1 3.080595 -0.716312 0.964231
1 -0.809689 -2.890065 0.464439
1 -0.773453 -2.589768 2.019651
1 -0.763652 -2.699242 -2.409467
1 -0.063993 1.320897 2.532485
8 -1.751572 0.057495 -0.370358
1 -2.453223 0.714836 -0.148663
1 -2.063661 -0.551543 -1.058432
6 2.201986 2.507336 -0.775908
6 1.045581 2.371985 -1.460100
1 2.373335 3.343965 -0.112136
1 3.032390 1.829878 -0.933969
1 0.905530 1.575717 -2.184796
1 0.240586 3.087217 -1.351784

$[Sc(H_2O)_3(OOH)(OH)(Epox)](H_2O)^+$ (**22Sc**)

21 0.095961 -0.303136 0.479586
8 0.516942 -1.118263 -1.382750
8 -3.863339 1.869216 0.060185
8 2.144545 -1.237058 0.727649
8 -0.812432 -2.340005 0.648524
8 1.171619 1.528858 -0.114069
8 -0.680010 -1.745395 -1.950467
8 -0.145550 0.102383 2.296025
1 -4.610265 1.628234 0.618657
1 -3.963960 2.804094 -0.149326
1 2.267505 -1.880004 0.013351
1 2.516588 -1.599548 1.540526
1 -1.010158 -2.670132 -0.247882
1 -1.464337 -2.675272 1.272797
1 -0.352948 -2.056304 -2.805261
1 -0.274162 0.265510 3.230668
8 -1.708699 0.377222 -0.500694
1 -2.493751 0.926949 -0.266754
1 -1.846640 -0.060899 -1.355429
6 2.504679 2.087479 0.053177
6 1.946060 1.900777 -1.289716
1 2.502055 3.071335 0.507143
1 3.234374 1.378970 0.427164
1 2.258355 1.056700 -1.893356

1 1.533127 2.751011 -1.819586

$[Y(H_2O)_5(OOH)_2](H_2O)^+$ (**20Y**)

39 -0.202820 0.149955 -0.059675
8 0.968954 1.665742 -1.522356
8 1.407428 -1.401535 -0.978503
8 -0.453483 1.986672 -1.251411
8 -1.118979 -1.708641 -0.856757
8 -2.605079 0.615009 -0.084474
8 1.809074 0.394058 1.280108
1 0.990782 1.616019 -2.488376
1 0.966994 -2.247209 -1.149989
1 2.353999 -1.532809 -0.808844
1 -2.901992 1.222654 -0.773022
1 -3.038572 -0.245512 -0.243243
1 1.936801 1.240219 1.725377
1 2.679468 0.022615 1.046497
8 -0.324416 2.185429 1.417561
1 -0.959624 2.469262 2.084833
1 -0.432722 2.765781 0.638145
8 -0.984318 -1.094689 1.863808
1 -1.612429 -1.769726 1.542426
1 -0.995332 -1.080651 2.825265
8 -2.394000 -2.042335 -0.219959
1 -2.677642 -2.812681 -0.730275
8 4.000854 -1.009258 0.149039
1 4.667823 -0.544858 -0.373380
1 4.484156 -1.674940 0.655439

TS6Y

39 -0.007797 -0.248947 0.119475
8 0.686091 -2.309807 -0.633220
8 0.708041 -1.800176 1.957154
8 -2.085401 1.260925 0.857390
8 -1.174274 0.039833 -1.994112
8 1.878139 -1.017250 -0.694002
8 0.311399 1.860591 -0.621223
8 -0.040193 2.896816 0.361390
8 0.670960 1.012986 2.077047
1 0.858936 -2.620802 -1.528816
1 0.276809 -2.239354 2.698111
1 1.121175 -2.487074 1.405854
1 -1.636110 2.123172 0.707464
1 -2.372052 1.269582 1.779182
1 -0.954273 0.949003 -2.250263
1 -2.142564 -0.044715 -2.032532
1 0.215139 3.705798 -0.101899
1 1.346718 0.767300 2.717770
1 0.754865 1.957191 1.846008
8 -1.999055 -1.638267 0.416209
1 -1.875721 -2.568269 0.190878
1 -2.830608 -1.338157 -0.002995
6 3.629347 0.383639 -0.288188
6 3.195834 0.587981 -1.547290

1 3.315080 1.031620 0.521978
1 4.345410 -0.391603 -0.049312
1 2.511744 1.395728 -1.777468
1 3.556421 -0.016287 -2.369310
8 -3.802197 -0.084192 -0.952961
1 -4.730323 -0.066174 -1.213712
1 -3.635727 0.680594 -0.376974

$[Y(H_2O)_5(OOH)(OH)(Epox)](H_2O)^+$ (**22Y**)

39 -0.015487 -0.315434 -0.266963
8 -0.579330 0.235561 -2.319866
8 -0.233340 -2.256043 -1.856791
8 -0.834849 -1.959324 1.317722
8 -0.921215 1.549811 1.017070
8 1.633888 1.386782 -0.790690
8 1.000955 0.054380 1.774030
8 1.450798 -1.193782 2.406132
8 1.995709 -1.624645 -0.206549
1 -0.272894 0.848376 -2.990591
1 -0.846564 -2.992647 -1.947553
1 -0.457485 -1.576379 -2.536229
1 -0.206307 -2.006995 2.065179
1 -1.459384 -2.688666 1.361892
1 -0.496669 1.352347 1.872588
1 -1.867250 1.728323 1.160598
1 1.853459 -0.872524 3.223533
1 2.135453 -2.439618 -0.700749
1 2.292744 -1.740263 0.714159
8 -2.461207 -0.397996 -0.675368
1 -2.311109 -0.029593 -1.571653
1 -3.107967 0.164229 -0.221158
6 2.711852 1.986090 -0.023367
6 1.707029 2.832043 -0.675118
1 2.641879 1.791891 1.040318
1 3.685058 1.864201 -0.485069
1 0.911750 3.267574 -0.081046
1 1.946354 3.330361 -1.607848
8 -3.776246 1.652097 0.965644
1 -4.210497 2.404718 0.544137
1 -4.341186 1.413078 1.711301

$[La(H_2O)_6(OOH)_2](H_2O)^+$ (**20La**)

57 -0.232365 -0.053202 0.047760
8 0.445504 1.932749 1.552321
8 1.635968 1.113678 -0.977292
8 1.055069 -1.786186 -1.403509
8 -1.794120 1.096012 -1.240296
8 -3.201362 0.721953 -1.084523
1 -0.102197 2.561494 2.033559
1 1.097299 2.431016 1.001527
1 0.761395 -2.267347 -2.183881
1 2.029502 -1.656460 -1.459468
1 -3.631749 1.331862 -1.699215
8 2.140625 -0.804988 1.490299

1 2.848984 -0.896774 0.814730
1 2.472170 -0.166976 2.133783
8 -2.381536 0.524619 1.471322
1 -2.835490 0.309992 2.291700
1 -3.049294 0.780689 0.803534
8 -0.227971 -1.942801 1.887700
1 0.706963 -2.066167 2.121763
1 -0.746953 -2.647540 2.287481
8 -2.025759 -1.700362 -1.003397
1 -2.358734 -2.602644 -1.003847
1 -2.740405 -1.106286 -1.308512
8 2.099189 2.379229 -0.417264
1 2.009141 2.975981 -1.173439
8 3.443323 -0.714790 -0.906261
1 2.945678 0.149734 -1.052343
1 4.327085 -0.650985 -1.282500

TS6La

57 -0.067824 -0.386627 0.206815
8 -2.139999 -1.596080 -0.145391
8 -2.374903 0.152385 -0.457243
8 -0.867334 -0.498315 -2.514176
8 0.072461 -2.324271 1.969549
8 0.385635 -2.693327 -1.439448
8 -0.411320 1.222226 1.909541
8 2.206933 -0.731233 -1.101214
8 1.952870 -0.364119 2.088503
8 1.071869 1.925122 -0.397952
8 0.759565 2.002920 2.333394
1 -3.005447 -1.705151 0.261269
1 -0.771241 -0.011327 -3.338556
1 -1.727445 -0.231758 -2.102472
1 -0.598764 -2.910126 2.335423
1 0.708207 -2.106898 2.665619
1 -0.260275 -2.386724 -2.099554
1 0.132938 -3.592172 -1.201652
1 2.177502 -1.550596 -1.614625
1 2.771777 -0.081725 -1.551531
1 1.777582 0.511450 2.497573
1 2.904602 -0.446381 1.968571
1 1.895041 2.106328 -0.876980
1 1.076110 2.428146 0.436497
1 0.384583 2.539398 3.044691
6 -3.057204 2.078490 0.016972
6 -2.495953 2.333685 -1.186642
1 -4.105361 1.824311 0.101486
1 -2.503902 2.223267 0.936832
1 -3.069968 2.255358 -2.102368
1 -1.466930 2.665304 -1.268183
8 3.477916 1.672695 -2.022012
1 4.365406 1.900978 -1.717721
1 3.430971 1.989003 -2.933145

$[La(H_2O)_6(OOH)(OH)(Epox)](H_2O)^+$ (**22La**)

57 -0.362796 -0.110579 0.062363
8 -2.499299 0.968361 0.059836
8 0.198795 2.260873 -0.914899
8 -2.080176 0.087769 -2.324678
8 -2.483154 -1.187240 1.486647
8 -1.702373 -2.214673 -1.038141
8 0.309763 0.851900 2.120651
8 0.896892 -1.548467 -1.752333
8 0.637616 -2.027160 1.622866
8 2.292421 0.221514 0.174154
8 1.488909 0.248547 2.754531
1 -2.907339 1.803222 0.300872
1 -2.110768 0.567251 -3.158109
1 -2.540371 0.623233 -1.621835
1 -2.901663 -0.355574 1.140778
1 -2.617633 -1.200835 2.440120
1 -2.177122 -1.728373 -1.738682
1 -2.370846 -2.559574 -0.431463
1 0.398943 -2.324050 -2.038655
1 1.846515 -1.756096 -1.794837
1 1.004296 -1.508258 2.368279
1 0.221272 -2.814767 1.987160
1 2.960193 -0.379896 -0.190868
1 2.469259 0.337317 1.126332
1 1.526063 0.725921 3.593652
6 0.238665 3.475903 -0.111037
6 1.368768 3.118349 -0.971121
1 -0.463739 4.234512 -0.436960
1 0.304935 3.288119 0.955779
1 1.490651 3.617966 -1.925800
1 2.256112 2.678734 -0.532156
8 3.715917 -1.731404 -1.430414
1 4.122504 -2.520488 -1.050751
1 4.321019 -1.431032 -2.120339

$[Ga(H_2O)_4O_2](H_2O)^+$ (**12Ga**)

31 -0.335036 0.022603 -0.065991
8 -1.953693 0.876373 0.932788
8 0.953463 -1.096725 -1.300032
8 0.480157 -0.874770 1.554312
8 -1.638272 -1.533940 -0.355437
8 2.731911 0.012635 0.480530
1 -1.966742 1.743373 0.484671
1 -1.903071 1.050609 1.884197
1 0.971166 -0.529248 -2.091542
1 1.853089 -1.027097 -0.913453
1 1.450009 -0.652577 1.506772
1 0.362587 -1.794803 1.827281
1 -1.461970 -2.166052 -1.068055
1 -2.590282 -1.360065 -0.310122
1 2.289483 0.850720 0.176324
1 3.655053 0.199136 0.688839
8 -0.296243 1.410549 -1.286051

8 0.688525 1.579044 -0.043509

TS5Ga

31 0.474863 -0.410689 -0.098039
8 -1.301492 -0.818029 -0.609709
8 0.343496 -1.512395 -1.494150
8 0.621626 1.009772 1.325210
8 2.552234 -0.825721 0.241262
8 0.935463 1.191904 -1.437041
8 0.104096 -1.700733 1.577501
1 0.271511 0.777022 2.195644
1 0.394415 1.944482 1.092367
1 2.816779 -1.384266 -0.506505
1 3.253119 -0.178646 0.397045
1 0.686918 0.706620 -2.245138
1 0.504153 2.059341 -1.430891
1 -0.699797 -2.102019 1.198954
1 0.730478 -2.416272 1.754167
6 -3.073794 0.013704 -0.629004
6 -3.114401 -0.160792 0.720620
1 -3.497423 -0.720000 -1.300226
1 -2.849765 0.980040 -1.062752
1 -2.819986 0.625983 1.406104
1 -3.467424 -1.087343 1.155705
8 0.121437 3.450434 0.287078
1 -0.726524 3.909685 0.348933
1 0.797076 4.137410 0.364901

$[Ga(H_2O)(OH)2(C2H4O)](H2O)_3^+$ (**15Ga**)

31 -0.138665 -0.127493 -0.345065
8 0.267321 1.833418 -0.198845
8 1.237022 -0.744015 0.863700
8 -1.639381 -0.379652 0.586129
8 0.540299 -0.612609 -1.937989
6 1.576122 2.495307 -0.072038
6 0.594886 2.606921 1.009813
1 1.930761 -1.310306 0.411442
1 0.848788 -1.145535 1.698182
1 -2.488941 -0.308278 0.107939
1 -0.005323 -0.527177 -2.725691
1 1.693953 3.304375 -0.781685
1 2.407861 1.809589 0.036555
1 0.716684 2.002383 1.900715
1 -0.012216 3.498730 1.100147
8 2.784611 -1.850383 -0.858722
1 3.334330 -2.621785 -1.028000
1 2.228099 -1.680104 -1.638200
8 -0.335285 -1.350958 2.792051
1 -1.153985 -1.167997 2.293071
1 -0.518724 -2.006702 3.471687
8 -3.939595 -0.164390 -0.957116
1 -4.471042 -0.932032 -1.196847
1 -4.557613 0.572460 -0.892622

$[In(H_2O)_4O_2](H_2O)^+$ (**12In**)

49 -0.338099 0.014040 0.072445
8 -0.952001 -1.562707 -0.964495
8 -1.562746 -1.427490 0.500673
8 1.191082 1.237500 -0.714707
8 -0.789324 1.498136 1.570986
8 1.248004 -0.949664 1.161829
8 -1.589620 0.796860 -1.516580
1 1.008674 1.710767 -1.539084
1 2.114743 0.885062 -0.733714
1 -1.514836 1.302821 2.182831
1 -0.365310 2.322285 1.845682
1 0.892779 -1.833806 1.359879
1 2.160032 -1.034282 0.834547
1 -1.726863 -0.203308 -1.676412
1 -2.443037 1.247522 -1.502957
8 3.497549 -0.162204 -0.429336
1 3.795898 -0.736844 -1.148675
1 4.301225 0.208357 -0.038827

TS5In

49 -0.091660 -0.443508 -0.013125
8 1.755219 0.121216 0.461588
8 0.980700 -1.509903 1.201166
8 -1.415802 0.807560 -0.999038
8 -1.377837 -2.204209 -0.351122
8 -0.933337 -0.073167 1.963095
8 0.794456 -0.821836 -1.988230
1 -1.267385 1.038700 -1.924817
1 -2.053842 1.465804 -0.591198
1 -0.992932 -2.890708 0.219891
1 -2.330970 -2.351340 -0.407489
1 -0.114806 -0.655859 2.183828
1 -0.958952 0.699075 2.540026
1 1.725368 -0.685742 -1.726243
1 0.742733 -1.657138 -2.472626
6 2.894637 1.631884 0.580572
6 2.431273 2.109533 -0.613296
1 3.821291 1.077074 0.632926
1 2.539701 2.042368 1.516556
1 1.603272 2.808017 -0.658689
1 2.898778 1.833794 -1.551128
8 -3.070041 2.521655 0.054660
1 -2.940507 3.475841 0.108400
1 -4.002719 2.352956 0.233076

$[In(H_2O)_3(OH)2(C2H4O)](H2O)^+$ (**16In**)

49 0.114645 -0.461085 -0.128855
8 -1.518723 -1.926700 -0.516732
8 1.475699 1.101577 0.596327
8 0.771421 -1.959140 0.961010
8 -1.229417 1.100874 -0.661610
8 -0.840708 -0.208320 1.850685
8 0.694108 -0.162065 -1.965423
6 2.936483 1.093354 0.511640

6 2.170513 2.070987 -0.260837
1 -1.225549 -2.739851 -0.075806
1 -1.858213 -2.159045 -1.389612
1 1.580634 -2.459570 0.849400
1 -1.135075 1.269193 -1.609768
1 -2.120456 1.385142 -0.341776
1 -0.825141 0.589615 2.391753
1 -0.341271 -0.909296 2.312237
1 1.108078 -0.807790 -2.539631
1 3.348008 0.227938 0.004960
1 3.413603 1.384995 1.439232
1 2.080062 3.087801 0.101297
1 2.011203 1.890315 -1.317231
8 -3.602634 1.895152 0.269086
1 -3.942744 2.796798 0.252767
1 -4.350690 1.319857 0.464528

$[Sc(H_2O)_5(OO)]^+$ (**11Sc**)

21 -0.093113 0.024358 0.038040
8 0.542742 0.298110 2.197946
8 -0.233874 -0.829803 -2.075654
8 1.261966 1.830699 -0.569579
8 2.144938 -0.732797 -0.259209
8 -1.757014 1.584169 -0.277885
1 0.098045 -0.409107 2.689516
1 0.701201 1.030940 2.803741
1 -0.642420 -1.686400 -1.866705
1 -0.618886 -0.512364 -2.901274
1 1.173340 2.749599 -0.846428
1 2.192365 1.585018 -0.665536
1 2.256115 -1.323989 -1.015817
1 2.507403 -1.206526 0.501382
1 -2.586024 1.134877 -0.057252
1 -1.938054 2.528870 -0.330142
8 -0.458298 -1.784965 0.510934
8 -1.648925 -0.915717 0.584656

$[Sc(H_2O)_4O_2](H_2O)^+$ (**12Sc**)

21 -0.462056 -0.011285 0.004850
8 -1.686152 1.880020 -0.542584
8 -0.609816 -0.963649 1.615582
8 -1.717160 -0.008316 1.410345
8 1.284944 -1.426185 -0.464043
8 1.198274 1.488097 -0.107969
8 -1.721864 -1.274198 -1.368487
1 -2.343420 2.019318 0.154462
1 -2.012025 2.311691 -1.341073
1 2.209065 -1.120970 -0.411631
1 1.225675 -2.232160 0.066474
1 1.092290 2.438127 0.018714
1 2.144552 1.256808 -0.018301
1 -1.492216 -1.947623 -2.020277
1 -2.540633 -1.555381 -0.935248
8 3.628407 0.148877 -0.015715

1 4.331610 0.283635 -0.665151
1 4.075208 0.026376 0.833151

TS5Sc

21 0.048284 0.640436 -0.110181
8 1.666643 -0.405784 -0.640127
8 1.079681 1.215099 -1.460156
8 -1.329049 -0.388379 1.526366
8 -0.770738 2.788173 -0.049691
8 -1.575041 -0.258920 -1.363577
8 1.391774 1.203040 1.651595
1 -1.164351 -0.448347 2.474236
1 -2.113216 -0.928490 1.319107
1 -0.305597 3.266702 -0.751012
1 -1.540508 3.306100 0.210977
1 -1.428367 -0.290217 -2.316801
1 -2.313353 -0.845043 -1.121227
1 2.225218 0.869079 1.279942
1 1.567109 2.082593 2.006720
6 2.131626 -2.271116 -0.659584
6 2.283741 -2.117811 0.687343
1 2.973960 -2.183309 -1.331162
1 1.238507 -2.721432 -1.073773
1 1.476465 -2.334621 1.377100
1 3.228201 -1.800746 1.111074
8 -3.411358 -1.762246 0.161032
1 -3.430254 -2.727897 0.125793
1 -4.335259 -1.487830 0.232739

$[Sc(H_2O)_4(=O)(C2H4O)](H2O)^+$ (**18Sc**)

21 -0.033069 0.377118 -0.019454
8 -0.692264 0.647667 -1.589961
8 2.100538 0.882622 -0.630993
8 1.170550 -1.470647 0.679044
8 -1.038578 1.260942 1.842449
1 2.897670 0.350456 -0.460143
1 2.102406 1.134791 -1.563008
1 2.129854 -1.620579 0.604937
1 0.751320 -2.266692 1.024072
1 -1.520362 0.967815 2.622627
1 -1.230082 2.196472 1.676950
8 -1.556256 -1.310408 0.339703
6 -2.086380 -2.015739 -0.836980
6 -2.957867 -1.149509 -0.048094
1 -2.134671 -3.089860 -0.701083
1 -1.694499 -1.628212 -1.770577
1 -3.193304 -0.167477 -0.441709
1 -3.649720 -1.581378 0.665652
8 -0.403674 2.818772 -0.184252
1 -0.698364 2.443060 -1.051193
1 0.149001 3.588995 -0.355303
8 3.930435 -1.151106 0.175831
1 4.562112 -0.993036 0.889781
1 4.402566 -1.685087 -0.476602

$[Sc(H_2O)_3(OH)_2(C2H4O)](H2O)^+$ (**16Sc**)
21 -0.146326 -0.666328 -0.011641
8 1.419891 -2.273844 0.434509
8 -1.437531 1.132626 -0.353700
8 -0.795545 -1.589430 -1.518560
8 1.097860 0.743825 1.306773
8 1.436842 0.206936 -1.416107
8 -1.013416 -1.121973 1.623589
6 -2.868853 1.149334 -0.618970
6 -2.335668 1.794132 0.583495
1 1.620295 -2.911523 -0.261621
1 1.223539 -2.778651 1.233749
1 -1.288319 -2.151834 -2.115367
1 0.971578 0.685824 2.260175
1 1.908765 1.241666 1.107704
1 2.147799 0.848517 -1.247490
1 1.320841 0.085847 -2.364771
1 -1.619775 -1.634296 2.158914
1 -3.346902 0.180348 -0.535496
1 -3.137169 1.749809 -1.480090
1 -2.214439 2.870830 0.605408
1 -2.418738 1.285800 1.537051
8 3.252180 1.939239 -0.102517
1 4.171408 1.667050 0.016085
1 3.278865 2.893662 -0.248844
$[Y(H_2O)_7O_2]^+$ (**11Y**)
39 0.081725 0.069453 0.031906
8 0.927692 2.409301 0.230546
8 -1.391226 1.067715 -1.697636
8 1.559411 0.158179 -1.941995
8 -0.560439 -0.850706 2.300787
8 -2.193753 -1.135248 -0.445001
8 2.274603 -0.201494 1.134382
8 0.613856 -1.985422 0.162460
8 0.085728 -1.768023 -1.210083
1 1.654141 2.874373 -0.198960
1 0.406886 3.062256 0.713532
1 -2.088326 0.396426 -1.796360
1 -1.082927 1.306104 -2.580341
1 1.289955 -0.796350 -2.045814
1 2.486636 0.255919 -2.181514
1 -0.111483 -0.804586 3.153244
1 -0.384648 -1.743119 1.939270
1 -1.515904 -1.755061 -0.867321
1 -2.856561 -1.652182 0.024782
1 3.074817 0.159371 1.529335
1 2.399307 -1.144240 0.924520
8 -1.585668 1.558979 1.166464
1 -2.023644 1.169869 1.934749
1 -2.277142 1.936318 0.607138
$[Y(H_2O)_6O_2](H_2O)^+$ (**12Y**)
39 0.350139 0.053041 0.030727

8 1.799113 1.552021 1.346364
8 -1.251698 1.922677 0.066497
8 1.466851 -1.589070 1.487834
8 1.274943 -1.086605 -1.448053
8 0.347808 -2.018590 -0.747881
8 1.587101 1.555995 -1.520107
1 2.493685 2.028912 0.873837
1 2.026362 1.562560 2.283914
1 -2.185608 1.625548 0.117090
1 -1.201718 2.804541 0.450213
1 1.286868 -2.223850 0.742768
1 2.352426 -1.751519 1.829529
1 1.385136 2.366415 -2.001904
1 1.900223 0.904502 -2.168996
8 -1.261056 -0.595589 1.722598
1 -2.210925 -0.461059 1.539943
1 -1.148872 -1.406776 2.232247
8 -1.584027 -0.678261 -1.517229
1 -1.615898 -0.469701 -2.458506
1 -0.972172 -1.501366 -1.411241
8 -3.414402 0.245741 0.243176
1 -3.103842 -0.266578 -0.532924
1 -4.378149 0.253210 0.240075

TS5Y

39 0.297623 0.352436 0.116259
8 0.224079 -0.925508 -1.505815
8 -1.413038 -0.912087 -0.563743
8 -0.272175 1.448914 -2.256570
8 2.625207 -0.307114 0.160199
8 0.246785 -1.933203 1.255493
8 -1.226012 2.319317 0.051715
1 0.186483 1.872689 -2.989576
1 -0.198531 0.449030 -2.374656
1 3.332068 -0.252239 0.811768
1 2.671762 -1.208771 -0.266352
1 0.920601 -2.523358 0.870979
1 -0.553648 -2.084711 0.707587
1 -1.340669 2.337280 -0.918979
1 -2.073607 2.524851 0.460805
8 1.975104 -2.642088 -0.841492
1 1.215606 -2.154699 -1.312641
1 2.332059 -3.324981 -1.418037
8 1.598878 2.454686 0.309448
1 2.516769 2.613108 0.059965
1 1.140153 3.303969 0.297877
8 0.056486 0.346199 2.564366
1 0.063472 -0.588654 2.827773
1 0.009342 0.897672 3.352245
6 -3.216689 -0.889682 0.803546
6 -3.286787 -0.908236 -0.561941
1 -3.170719 -1.806939 1.377093
1 -3.224990 0.039082 1.361750

1 -3.439067 -1.836200 -1.095507
1 -3.496038 -0.007561 -1.124638
[Y(H_2O)$_4$(OH)2(C2H4O)](H2O)$_2^+$ (**17Y**)
39 0.234660 0.420818 -0.130439
8 -1.813000 1.416218 0.688226
8 1.135420 1.425825 1.935850
8 -0.789877 -1.087884 1.473252
8 2.074940 1.337657 -0.706381
8 1.641302 -1.559878 0.305763
8 -0.630179 -0.586091 -1.786696
8 -3.047481 -1.649765 -1.229536
1 -2.604251 0.879535 0.918875
1 -2.088892 2.298853 0.420445
1 1.912694 1.963696 1.737577
1 0.819398 1.643356 2.819447
1 -0.429100 -1.980137 1.525384
1 -1.765471 -1.135604 1.580461
1 -0.403968 -0.769233 -2.701146
1 2.972744 1.382642 -1.034173
1 -3.593073 -1.830383 -1.999966
1 -2.172867 -1.295115 -1.542039
8 -0.109376 2.655903 -1.201748
1 -0.528720 2.837068 -2.050274
1 0.862676 2.683259 -1.332333
6 3.060233 -1.663401 0.618604
6 2.537183 -2.234255 -0.623366
1 3.270807 -2.311430 1.461415
1 3.586431 -0.716836 0.585880
1 2.689850 -1.704106 -1.556380
1 2.361225 -3.301046 -0.695920
8 -3.444750 -0.668187 1.156843
1 -3.508079 -1.082477 0.250567
1 -4.253634 -0.858385 1.643277
[La(H_2O)$_7O_2$](H_2O)$^+$ (**12La**)
57 -0.166419 -0.011947 0.068463
8 -2.111363 0.643987 -1.161061
8 -2.205537 0.929248 0.290062
8 2.370158 0.562250 0.307144
1 3.258761 0.185501 0.126188
1 2.488591 1.442204 0.688369
8 -0.229810 2.289742 -1.498905
1 0.049954 2.686322 -2.329669
1 -1.162219 1.911200 -1.608895
8 0.510731 2.442843 1.069848
1 0.096562 2.894800 1.813715
1 0.197680 2.894281 0.260208
8 0.383021 -1.545600 -1.997124
1 0.856954 -1.575804 -2.834058
1 -0.489195 -1.976122 -2.108018
8 0.292440 -2.267366 1.361593
1 0.661142 -3.126101 1.127108
1 -0.357682 -2.403657 2.063903

8 -2.054914 -1.851754 -1.062109
1 -2.432960 -0.925645 -1.235287
1 -2.769713 -2.458489 -0.846010
8 -1.524909 -0.403902 2.411554
1 -1.600558 -0.152194 3.338622
1 -2.287400 -0.015747 1.927027
8 4.839418 -0.493498 -0.198612
1 5.417410 -0.236045 -0.925343
1 5.404662 -0.911126 0.460614

$[La(H_2O)_5O_2](H_2O)_3^+$ (**13La**)

57 0.263049 0.075063 -0.554721
8 0.660555 0.205230 1.693768
8 1.972082 0.217617 0.959419
8 -2.063842 1.258101 -0.852303
1 -2.937761 0.895988 -0.613861
1 -2.109482 2.221703 -0.833348
8 0.651778 2.866922 1.931842
1 1.346494 3.300959 2.437373
1 0.728122 1.892976 2.103966
8 0.465902 2.657809 -0.642367
1 0.914194 3.310366 -1.190438
1 0.616709 2.916830 0.326296
8 -1.551684 -1.554212 0.227513
1 -2.510676 -1.406488 0.244507
1 -1.275387 -1.980047 1.076536
8 1.633744 -2.206424 0.046686
1 1.247985 -2.842320 0.667458
1 2.127723 -1.552150 0.608107
8 1.586315 -1.214910 -2.427787
1 1.934892 -1.235572 -3.325596
1 1.958869 -1.965946 -1.931251
8 -0.101940 -2.234730 2.360484
1 0.284282 -1.315564 2.384485
1 -0.178777 -2.561681 3.262333
8 -4.201968 -0.377452 -0.016031
1 -4.853892 -0.727869 -0.636889
1 -4.694632 -0.173425 0.789618

TS5La

57 -0.164591 0.054868 -0.496064
8 0.427062 0.198902 1.605118
8 1.970730 -0.097926 0.594894
8 -2.329346 1.518649 -0.864303
8 1.314652 2.692342 1.685560
8 0.448658 2.576601 -0.743746
8 -2.177983 -1.207835 0.504783
8 0.767543 -2.447143 0.166178
8 0.373555 -1.739105 -2.370396
1 -3.233504 1.286458 -0.580686
1 -2.262644 2.478587 -0.924298
1 1.067100 3.241904 2.434602
1 1.064765 1.746082 1.892872
1 0.875957 3.160045 -1.379074

1 0.808766 2.809804 0.174020
1 -3.104835 -0.929452 0.554228
1 -1.905309 -1.599504 1.370221
1 0.320420 -2.797068 0.956387
1 1.517566 -1.912003 0.517096
1 0.435743 -1.991547 -3.297216
1 0.638721 -2.497740 -1.819126
8 -0.638394 -1.962855 2.550977
1 -0.119897 -1.103182 2.427459
1 -0.663411 -2.187253 3.486040
8 -4.660431 0.281714 0.141173
1 -5.337890 -0.066879 -0.452584
1 -5.138922 0.631126 0.903962
6 3.714218 -0.517483 -0.809395
6 3.805139 0.274913 0.298806
1 3.475832 -0.102363 -1.782132
1 3.904789 -1.582347 -0.759845
1 4.191985 -0.116803 1.229649
1 3.761920 1.353326 0.225680

$[La(H_2O)_5(=O)(C2H4O)](H2O)_3^+$ (**19La**)

57 -0.058687 -0.007895 -0.365945
8 0.200127 0.237432 1.696652
8 2.501823 -0.541740 -0.640740
8 -1.838581 1.790622 -1.106765
8 1.810847 2.179120 1.933585
8 0.983456 2.418189 -0.496272
8 -2.432942 -0.847883 0.403207
8 0.051093 -2.635639 0.443851
8 -0.614241 -2.017187 -2.124232
1 -2.784507 1.754323 -0.870638
1 -1.544565 2.705414 -1.024099
1 1.751957 2.761836 2.696217
1 1.154226 1.394932 2.057647
1 1.466568 3.006332 -1.084589
1 1.347523 2.545498 0.440545
1 -3.256938 -0.341624 0.365424
1 -2.298763 -1.164656 1.327968
1 -0.360822 -2.543509 1.346247
1 0.881824 -3.106195 0.573417
1 -1.013474 -2.260754 -2.965336
1 -0.703796 -2.770705 -1.519840
8 -1.115125 -1.631778 2.591562
1 -0.502338 -0.764898 2.418722
1 -1.203525 -1.824234 3.529126
8 -4.454670 1.203334 -0.206486
1 -5.172445 1.008035 -0.822071
1 -4.859104 1.698054 0.517435
6 3.798429 -0.083249 -1.104265
6 3.572900 -0.303522 0.325474
1 3.803809 0.929959 -1.491590
1 4.339671 -0.820531 -1.686622
1 3.946155 -1.211684 0.784780

1 3.391411 0.539291 0.983987

$[La(H_2O)_5(OH)2(C2H4O)](H2O)_2^+$ (**17La**)

57 0.130813 -0.099779 0.162151
8 0.494449 -1.535403 -1.706722
8 -2.345047 -0.882241 -0.298335
6 -3.712520 -0.480156 -0.024075
6 -3.362867 -1.118141 -1.297830
8 1.845058 1.782119 -0.394953
8 -0.829436 1.879604 -1.314298
8 2.650135 -1.135262 -0.255756
8 0.064029 -2.730525 0.602106
8 1.669935 -0.597104 2.238102
8 -1.115637 1.050396 1.756092
1 0.296507 -1.795734 -2.607912
1 -3.858766 0.592943 0.020974
1 -4.191489 -1.070018 0.749471
1 -3.592111 -2.165798 -1.459326
1 -3.267887 -0.509477 -2.190784
1 2.808354 1.737439 -0.533317
1 1.503813 2.593003 -0.788343
1 -1.570237 2.347415 -0.828194
1 -1.020307 1.912928 -2.257042
1 3.413949 -0.615522 -0.545805
1 2.222640 -1.527250 -1.053347
1 0.141827 -2.838073 -0.372322
1 -0.568565 -3.372928 0.937741
1 1.557631 -0.647547 3.192595
1 2.321310 -1.259883 1.968110
1 -1.214007 1.150410 2.705558
8 -2.639935 2.664364 0.372013
1 -2.139170 2.137211 1.068368
1 -2.832807 3.536998 0.727917
8 4.551838 1.081497 -0.786612
1 5.216745 1.253059 -0.107929
1 5.005467 1.198450 -1.630701

Cyclohexene

6 -0.665002 1.305173 0.056885
6 0.664755 1.305207 -0.057174
6 1.496908 0.048241 -0.109971
6 0.698490 -1.192463 0.316831
6 -0.698455 -1.192227 -0.317451
6 -1.496804 0.047969 0.110825
1 -1.194969 2.252716 0.112612
1 1.194609 2.252757 -0.114037
1 1.887500 -0.086025 -1.128669
1 2.380273 0.166343 0.528145
1 1.243575 -2.102769 0.049092
1 0.595714 -1.196043 1.408716
1 -0.595835 -1.194562 -1.409358
1 -1.243407 -2.102874 -0.050596
1 -2.381284 0.165888 -0.525741
1 -1.885525 -0.086841 1.130171

TS [Ga(H2O)4(OOH)](H2O)$^{2+}$ + Cyclohexene

31	-1.133730	-0.364929	0.025794
8	-4.218776	2.077687	-0.487841
8	-1.169567	-2.352993	-0.313580
8	-1.688403	-0.976716	1.954693
8	-0.445421	-0.223668	-1.905726
8	0.298272	0.516765	0.742538
8	-2.957340	-0.079954	-0.538345
1	-4.685708	2.448313	-1.248871
1	-4.580113	2.495137	0.305371
1	-0.741179	-2.751643	-1.087498
1	-1.136156	-2.978050	0.428513
1	-2.575973	-0.993593	2.343646
1	-1.091366	-0.560109	2.599644
8	-0.952093	1.559974	0.920502
1	-3.535249	-0.800543	-0.826158
1	-3.485136	0.822346	-0.498184
1	-0.544249	2.367383	0.570461
1	-0.912513	0.107261	-2.687193
1	0.500889	0.024608	-1.968357
6	2.571810	-0.735432	0.953543
6	3.370187	0.444344	1.423083
6	2.357554	-1.023078	-0.346623
6	3.675977	1.447499	0.302519
6	2.925206	-0.192907	-1.474880
6	4.058263	0.730341	-0.996326
1	3.273129	-0.851577	-2.276357
1	2.150584	0.450082	-1.946738
1	4.951758	0.119402	-0.831341
1	4.311296	1.448172	-1.779272
1	2.797076	2.078948	0.125851
1	4.479395	2.117357	0.614682
1	2.856622	0.931116	2.258035
1	4.303564	0.053643	1.851270
1	1.880026	-1.967978	-0.605236
1	2.241548	-1.440836	1.712299

TS [In(H2O)4(OOH)](H2O)$^{2+}$ + Cyclohexene

49	1.098298	-0.295337	-0.021828
8	-0.383902	-1.479486	-0.414705
8	0.896597	-2.032420	-1.304884
1	0.446887	-2.381102	-2.086900
8	3.136856	-0.522019	-0.554052
1	3.920164	0.033434	-0.433217
1	3.369826	-1.266615	-1.131683
8	1.484060	-1.518222	1.713937
1	2.290458	-1.802402	2.169210
1	0.835293	-2.239651	1.776428
8	0.813891	1.214988	-1.482415
1	0.326899	1.051342	-2.303403
1	0.842909	2.180801	-1.307153
8	1.513088	1.342614	1.207360
1	1.513529	1.314495	2.175274

1 1.392093 2.281327 0.902314
8 1.097989 3.622622 -0.149248
1 1.816793 4.247057 -0.334011
1 0.319287 4.172424 0.029899
6 -2.447617 -1.116250 0.900231
6 -3.507395 -1.338272 -0.136324
6 -1.962639 0.104657 1.221897
6 -3.753633 -0.101540 -1.009596
6 -2.472939 1.384635 0.597838
6 -3.796165 1.172338 -0.157810
1 -2.603362 2.134627 1.385889
1 -1.722400 1.807097 -0.091379
1 -4.607483 1.091752 0.572739
1 -4.019971 2.046304 -0.773946
1 -2.955973 -0.019573 -1.759126
1 -4.686447 -0.218479 -1.564435
1 -3.250798 -2.210518 -0.744151
1 -4.427707 -1.618879 0.394246
1 -1.297207 0.189725 2.082475
1 -2.145681 -1.979681 1.485142

TS $[Sc(H2O)5(\underline{O}OH)]^{2+}$ + Cyclohexene

21 1.482506 -0.033848 -0.050336
8 2.846881 0.851957 -1.666423
8 1.050770 -0.718104 2.019420
8 2.995458 -1.691699 -0.179047
8 0.614851 1.994756 -0.180972
8 -0.354656 -0.672704 -0.325949
8 3.099676 1.081508 1.163135
1 3.430760 0.289397 -2.195525
1 2.643659 1.625256 -2.211533
1 0.175699 -1.132185 2.081609
1 1.557547 -0.974805 2.801520
1 3.776346 -1.944891 0.331754
1 2.714379 -2.465381 -0.692313
8 0.726753 -1.282222 -1.500470
1 3.120978 1.366870 2.087060
1 3.896206 1.436548 0.743419
1 0.198032 -1.110961 -2.293216
1 0.934181 2.870200 0.076812
1 -0.346090 2.055241 -0.323741
6 -2.309158 -0.731000 1.112912
6 -3.243336 -1.440770 0.186499
6 -2.074630 0.604399 1.076266
6 -3.713992 -0.562858 -0.981353
6 -2.785862 1.524126 0.115254
6 -4.024972 0.862389 -0.512853
1 -3.061929 2.444544 0.639607
1 -2.115845 1.842417 -0.706483
1 -4.822939 0.838823 0.236309
1 -4.391899 1.472875 -1.340084
1 -2.936899 -0.533445 -1.753166
1 -4.595111 -1.010087 -1.444930

1 -2.773487 -2.363011 -0.170723
1 -4.101630 -1.773667 0.787688
1 -1.461417 1.054727 1.853910
1 -1.899328 -1.323313 1.931184

TS [Y(H2O)6(OOH)](H2O)$^{2+}$ + Cyclohexene

39 -1.014591 0.230270 -0.001434
8 0.097164 0.462946 -1.932096
8 -0.247189 -2.046365 0.013329
8 -2.711119 1.761511 0.957673
8 -2.721003 -0.229256 -1.611673
8 -2.769793 -1.084060 1.196125
8 1.119889 0.223901 -0.563561
1 0.578474 -0.090462 -2.558755
1 -0.554192 -2.958568 0.075949
1 0.690639 -2.043087 -0.236165
1 -2.866592 2.643350 0.593886
1 -3.477910 1.532624 1.497191
1 -2.588067 -0.106705 -2.560185
1 -3.598275 -0.639278 -1.471091
1 -2.670291 -1.589875 2.012164
1 -3.596275 -1.383415 0.763742
8 -0.656723 2.597319 -0.618712
1 -0.340091 3.378532 -0.148086
1 -0.102881 2.504228 -1.412792
8 -0.281836 0.544720 2.278068
1 0.628877 0.369332 2.553212
1 -0.701939 1.049629 2.986539
8 -4.917178 -1.589736 -0.552288
1 -5.100711 -2.484465 -0.873496
1 -5.787275 -1.182931 -0.431659
6 2.928384 0.636285 0.897783
6 3.923658 1.193102 -0.075201
6 2.750296 -0.689260 1.105312
6 4.476699 0.133531 -1.038461
6 3.536807 -1.747596 0.376977
6 4.791171 -1.172864 -0.301566
1 3.808698 -2.539949 1.081715
1 2.903757 -2.235283 -0.381581
1 5.551914 -0.987126 0.463925
1 5.212559 -1.911734 -0.986375
1 3.740948 -0.057242 -1.826716
1 5.372739 0.516654 -1.530906
1 3.472674 2.025034 -0.624844
1 4.739772 1.638785 0.510536
1 2.090827 -1.034508 1.901678
1 2.421908 1.358875 1.534033

TS [La(H2O)7(OOH)](H2O)$^{2+}$ + Cyclohexene

57 -1.108344 -0.386719 0.038996
8 0.420127 -2.130643 0.598495
8 1.334718 -0.734140 0.024439
1 1.122659 -2.496166 1.146771
8 0.186691 0.553986 2.117991

1 0.319327 1.278578 2.739378
1 1.060134 0.262749 1.786554
8 -2.092968 -2.804998 -0.279099
1 -1.390097 -3.450724 -0.113650
1 -2.887329 -3.289103 -0.533239
8 -2.330948 -0.944406 2.340176
1 -1.767246 -0.869092 3.122443
1 -2.973722 -1.638609 2.535418
8 -0.036627 -1.021878 -2.264438
1 -0.147474 -1.549784 -3.063457
1 0.836174 -1.220391 -1.869352
8 -2.722511 1.589406 0.808456
1 -3.209801 1.550760 1.640896
1 -2.676238 2.526708 0.533025
8 -3.366226 -0.312211 -1.396898
1 -3.664176 -0.754642 -2.201552
1 -4.014661 0.378254 -1.208396
8 -0.701167 1.803254 -1.323180
1 -1.070724 2.697406 -1.190381
1 -0.218546 1.799739 -2.158751
8 -2.146133 4.056358 -0.433183
1 -2.798904 4.491577 -0.999519
1 -1.698924 4.775505 0.034725
6 2.932445 0.452720 -1.177733
6 4.077392 -0.510345 -1.286465
6 2.727333 1.251196 -0.101596
6 4.803225 -0.730978 0.048055
6 3.649250 1.267836 1.089057
6 4.998875 0.594440 0.791764
1 3.798888 2.305167 1.407221
1 3.175372 0.766319 1.946916
1 5.606415 1.270449 0.180741
1 5.548034 0.437714 1.722575
1 4.219311 -1.417331 0.670503
1 5.766290 -1.212771 -0.132527
1 3.726540 -1.461347 -1.701272
1 4.773514 -0.108878 -2.036426
1 1.928727 1.987129 -0.137204
1 2.321280 0.596750 -2.064757