Electronic Supplementary Information

Density functional theory study of aluminium(III) hydrolysis in aqueous solution

*Wenjing Yang, Zhaosheng Qian, Qiang Miao,Yingjie Wang and Shuping Bi**

School of Chemistry and Chemical Engineering, State Key Laboratory of Coordination Chemistry of China & Key Laboratory of MOE for Life Science, Nanjing University, Nanjing 210093, China

1. The calculated Gibbs free energies and the solvation energies of the gas phase structures using the supermolecule density functional calculations

Table S1 The Gibbs free energies and the solvation energies of the most stable structures

Charge	Complex	Gibbs free energies / a.u.	Solvation energies / kcal·mol^{-1}
+3	$Al(H_2O)_6^{3+}$•12H_2O	-1617.446535	-287.00
+2	$Al(OH)(H_2O)_5^{2+}$•12H_2O	-1617.254043	-134.18
+1	*trans*-$Al(OH)_2(H_2O)_4^{+}$•12H_2O	-1616.957174	-43.38
0	*trans*-$Al(OH)_3(H_2O)_2$•13H_2O	-1616.558109	-11.63
-1	$Al(OH)_4^{-}$ •14H_2O	-1616.084592	-35.14
0	H_2O	-76.430410	-6.94
+1	H_3O^{+}	-76.692613	-107.41

2. The calculated Gibbs free energies and the solvation energies of the solution phase structures using the supermolecule density functional calculations

Table S2 The Gibbs free energies and the solvation energies of the solution phase structures

Charge	Complex	$G_{(aq)}$ / a.u.
+3	$Al(H_2O)_6^{3+}$•12H_2O	-1617.956263
+2	$Al(OH)(H_2O)_5^{2+}$•12H_2O	-1617.516179
+1	*trans*-$Al(OH)_2(H_2O)_4^{+}$•12H_2O	-1617.073484
0	*trans*-$Al(OH)_3(H_2O)_2$•13H_2O	-1616.627671
-1	$Al(OH)_4^{-}$ •14H_2O	-1616.193071
0	H_2O	-76.443627
+1	H_3O^{+}	-76.874444

3. The calculation of ΔG^0 using solution phase geometries

ΔG^0 can be computed directly from the Gibbs free energy of the solution phase geometries without thermodynamica cycles. Two approaches shown as follows have been used in the calculation:

Approach I $Al(H_2O)_6^{3+} \rightarrow Al(OH)_m(H_2O)_n^{(3-m)+} + mH^+$

ΔG^0 can be obtained by the following equation:

$$\Delta G^0=\Delta G_{(aq)}=G_{(aq)}(Al(OH)_m(H_2O)_n^{(3-m)+})+mG_{(gas)}(H^+)+m\Delta G_{sol}(H^+)-G_{(aq)}(Al(H_2O)_6^{3+})$$

in which $G_{(gas)}(H^+)$ is -6.28 kcal/mol and $\Delta G_{sol}(H^+)$ is -264.61 kcal/mol.

Approach II $Al(H_2O)_6^{3+} + mH_2O \rightarrow Al(OH)_m(H_2O)_n^{(3-m)+} + mH_3O^+$

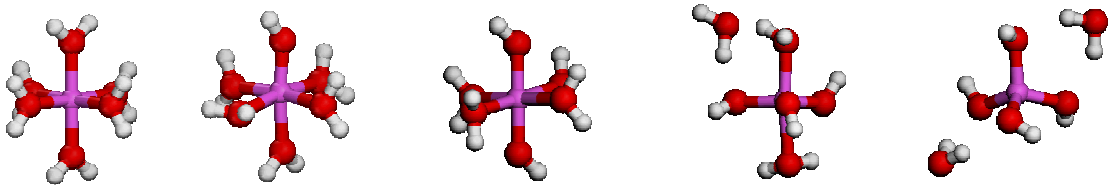
ΔG^0 can be obtained by the following equations:

$$\Delta G^0=\Delta G_{(aq)}-mRT\ln[H_2O]$$

$$\Delta G_{(aq)}=G_{(aq)}(Al(OH)_m(H_2O)_n^{(3-m)+})+mG_{(aq)}(H_3O^+)-G_{(aq)}(Al(H_2O)_6^{3+})-mG_{(aq)}(H_2O)$$

The parameters m, R and T are the number of water molecules acting as reactant, the gas constant and temperature in Kelvin, respectively.

4. The optimized structures of the gas phase structures without using the supermolecule medel.



$Al(H_2O)_6^{3+}$ $Al(OH)(H_2O)_5^{2+}$ *trans*-$Al(OH)_2(H_2O)_4^+$ *trans*-$Al(OH)_3(H_2O)_2$ $Al(OH)_4^-$

Fig. S1 The optimized structures of the hydrolysis products with one hydration shell

5. The calculated Gibbs free energies and the solvation energies of the gas phase structures without using the supermolecule density functional calculations

Table S3 The Gibbs free energies and the solvation energies of the structures with one hydration shell

Charge	Complex	Gibbs free energies / a.u.	Solvation energies / kcal·mol^{-1}
+3	$Al(H_2O)_6^{3+}$	-699.996952	-470.13
+2	$Al(OH)(H_2O)_5^{2+}$	-699.946462	-210.66
+1	*trans*-$Al(OH)_2(H_2O)_4^+$	-699.745995	-69.44
0	*trans*-$Al(OH)_3(H_2O)_2$	-699.395537	-17.30
-1	$Al(OH)_4^-$	-698.903103	-55.17

6. Cartesian coordinates of the most stable gas phase structures optimized using the supermolecule density functional calculations at B3LYP/6-31+G(d,p)

$Al(H_2O)_6^{3+}•12H_2O$

Al	1.50000000	0.00000000	0.00000000
O	0.41020477	1.55638888	0.00000000
O	0.41020477	-0.77819444	1.34787231
O	0.41020477	-0.77819444	-1.34787231
O	2.58979523	-1.55638888	0.00000000
O	2.58979523	0.77819444	-1.34787231
O	2.58979523	0.77819447	1.34787230
O	-0.11650460	3.01244355	2.26697510
O	-0.11603797	2.91629653	-2.21274273
O	-0.11650460	-3.46947980	1.47536510
O	-0.11603797	0.45814315	3.63195824
O	-0.11650460	0.45703625	-3.74234019
O	-0.11603797	-3.37443968	-1.41921551
O	3.11586053	-3.01119319	-2.26886527
O	3.11668216	-2.91718081	2.21106207
O	3.11586053	3.47049156	-1.47333716
O	3.11668216	-0.45624551	-3.63188372
O	3.11586053	-0.45929830	3.74220244
O	3.11668216	3.37342635	1.42082160
H	0.08558477	2.01999430	0.79637986
H	0.08558477	2.01999430	-0.79637986
H	0.08558477	-1.69968233	1.35117645
H	0.08558477	-0.32031196	2.14755630
H	0.08558477	-0.32031196	-2.14755630
H	0.08558477	-1.69968233	-1.35117645
H	2.91441523	-2.01999430	-0.79637986
H	2.91441523	-2.01999430	0.79637986
H	2.91441523	1.69968233	-1.35117645
H	2.91441523	0.32031196	-2.14755630
H	2.91441523	0.32031200	2.14755630
H	2.91441523	1.69968236	1.35117642
H	-0.08146865	2.35005594	2.98429241
H	-0.95024317	3.49385178	2.43327337
H	-0.08146865	-3.75950101	0.54306194
H	-0.95024317	-3.85420244	1.80912771
H	-0.08146865	1.40944507	-3.52735435
H	-0.95024317	0.36035066	-4.24240108

H	0.72797803	3.40829410	-2.20252575
H	-0.79563257	3.61766261	-2.24041578
H	0.72797803	0.20329620	4.05293215
H	-0.79563257	0.13142568	4.25319561
H	0.72797803	-3.61159030	-1.85040641
H	-0.79563257	-3.74908828	-2.01277983
H	3.08082458	-2.34880559	-2.98618259
H	3.94959911	-3.27482774	-2.70464710
H	3.08082458	3.76051278	-0.54103401
H	3.94959911	3.97970697	-1.48376046
H	3.08082458	-1.41170713	3.52721663
H	3.94959911	-0.70487916	4.18840758
H	2.26792793	-3.40105029	2.21500872
H	3.51673047	-3.13900617	3.07436031
H	2.26792793	-0.21772867	-4.05290031
H	3.51673047	-1.09297104	-4.25563924
H	2.26792793	3.61877900	1.83789153
H	3.51673047	4.23197724	1.18127886

$Al(OH)(H_2O)_5^{2+}•12H_2O$

Al	0.02710000	-0.12830000	0.07690000
O	1.33120000	-0.86080000	1.04070000
O	-1.42010000	-0.83420000	1.14150000
O	-0.04210000	1.57720000	1.06840000
O	-1.43070000	0.69790000	-0.99710000
O	1.24870000	0.74460000	-1.20500000
O	-0.06340000	-1.65990000	-1.11210000
O	2.41660000	-3.27480000	1.18000000
O	3.87480000	0.73240000	1.20240000
O	-3.84560000	0.52000000	1.21830000
O	-1.64740000	-3.38890000	1.60350000
O	2.30790000	2.91850000	1.34790000
O	-2.42500000	2.97550000	1.17930000
O	-1.38350000	3.42510000	-1.37540000
O	-3.80380000	-0.64280000	-1.32070000
O	3.63150000	-0.48940000	-1.33870000
O	1.39980000	3.52400000	-1.18570000
O	-2.39740000	-3.11850000	-1.13520000
O	2.32960000	-2.89790000	-1.34660000

H	1.89600000	-2.44530000	1.34370000
H	2.02780000	-0.31400000	1.42740000
H	-2.29110000	-0.40390000	1.28170000
H	-1.44310000	-1.77930000	1.46780000
H	0.76740000	2.06190000	1.36040000
H	-0.85620000	2.07760000	1.29720000
H	-1.42730000	1.62640000	-1.32140000
H	-2.22890000	0.22030000	-1.31820000
H	2.14520000	0.33620000	-1.33750000
H	1.31380000	1.71480000	-1.34080000
H	-0.84730000	-2.25560000	-1.17130000
H	0.77250000	-2.18010000	-1.26260000
H	2.12280000	-3.96970000	1.78070000
H	-3.55200000	1.45720000	1.23090000
H	-4.51020000	0.41920000	1.91530000
H	3.00440000	2.20890000	1.32110000
H	2.55430000	3.53410000	2.05320000
H	4.01010000	0.26020000	0.35360000
H	4.63340000	0.53360000	1.76850000
H	-2.08530000	-3.70180000	0.79250000
H	-1.94480000	-3.92890000	2.34730000
H	-2.25760000	3.38010000	0.30020000
H	-2.65690000	3.69250000	1.78780000
H	-0.42760000	3.65960000	-1.33320000
H	-1.76930000	3.93280000	-2.10410000
H	3.32630000	-1.43310000	-1.36400000
H	4.28380000	-0.38210000	-2.04570000
H	-3.07310000	-2.41790000	-1.24740000
H	-2.58650000	-3.80340000	-1.79260000
H	-4.14150000	-0.27590000	-0.47520000
H	-4.48990000	-0.50720000	-1.99040000
H	1.82660000	3.56020000	-0.29780000
H	1.93110000	4.06910000	-1.78430000
H	2.42860000	-3.25180000	-0.40320000
H	2.54400000	-3.61030000	-1.96500000

***trans*-$Al(OH)_2(H_2O)_4^+ \cdot 12H_2O$**

Al	0.00010000	0.00040000	-0.00010000
O	0.97060000	-1.23840000	-1.23130000
O	0.57370000	1.45500000	-0.92770000
O	-1.58000000	-0.16150000	-1.19380000

O	-0.97000000	1.23930000	1.23090000
O	-0.57360000	-1.45400000	0.92780000
O	1.58120000	0.16130000	1.19250000
O	3.74730000	-1.13490000	-1.07580000
O	-0.14460000	-3.76200000	-1.20910000
O	-0.74850000	3.70240000	-1.19690000
O	3.81240000	1.54770000	-1.26790000
O	-2.68860000	-2.67820000	-1.03880000
O	-3.23570000	2.02710000	-1.50630000
O	-3.74640000	1.13370000	1.07820000
O	0.14470000	3.76250000	1.20840000
O	0.74910000	-3.70160000	1.19620000
O	-3.81550000	-1.54880000	1.26600000
O	2.68840000	2.67770000	1.03890000
O	3.23560000	-2.02770000	1.50850000
H	1.95310000	-1.27590000	-1.22500000
H	0.61190000	-2.15180000	-1.34000000
H	1.18820000	1.27950000	-1.64920000
H	-2.10390000	-0.99300000	-1.19630000
H	-2.10600000	0.59910000	-1.52170000
H	-1.95260000	1.27510000	1.22720000
H	-0.61230000	2.15330000	1.33880000
H	0.26500000	-2.82620000	1.25820000
H	-1.18740000	-1.27840000	1.64990000
H	2.10410000	0.99340000	1.19830000
H	2.10600000	-0.59930000	1.52230000
H	3.88650000	-0.15360000	-1.15470000
H	4.29230000	-1.55190000	-1.75620000
H	-1.68010000	3.48780000	-1.36220000
H	-0.26500000	2.82660000	-1.25850000
H	-1.82480000	-3.16280000	-1.03350000
H	-3.23850000	-3.09230000	-1.71690000
H	0.25320000	-3.93700000	-0.29050000
H	0.05480000	-4.51730000	-1.77720000
H	3.43290000	2.07760000	-0.53410000
H	4.43230000	2.11270000	-1.74480000
H	-3.67500000	1.83840000	-0.65000000
H	-3.92530000	2.19100000	-2.16270000
H	-3.88670000	0.15250000	1.15680000
H	-4.29090000	1.55100000	1.75890000
H	1.68050000	-3.48620000	1.36160000

H	1.82460000	3.16230000	1.03270000
H	3.23820000	3.09300000	1.71630000
H	-0.25270000	3.93750000	0.28950000
H	-0.05410000	4.51820000	1.77600000
H	-3.43430000	-2.07890000	0.53310000
H	-4.43630000	-2.11380000	1.74190000
H	3.67530000	-1.83890000	0.65230000
H	3.92480000	-2.19300000	2.16500000

***trans*-$Al(OH)_3(H_2O)_2 \bullet 13H_2O$**

Al	-0.15770000	0.56150000	-0.60530000
O	-0.56810000	2.08140000	0.68140000
O	1.41490000	1.39260000	-1.00320000
O	-0.08080000	-0.56410000	0.77570000
O	0.34930000	-0.92230000	-1.94070000
O	-1.64510000	0.81230000	-1.50000000
H	0.12710000	2.23470000	1.35360000
H	-2.15150000	1.63450000	-1.37050000
H	0.75460000	-1.03120000	0.94250000
H	1.75060000	1.19330000	-1.88630000
H	-0.32080000	-1.64970000	-1.94700000
H	-3.30160000	-1.79680000	-1.81590000
O	-3.69990000	-0.94930000	-1.56280000
H	-2.94770000	-0.30600000	-1.63970000
H	-1.42500000	-3.85940000	-1.91170000
O	-1.50860000	-2.95410000	-1.58990000
H	-1.57820000	-2.99540000	-0.59250000
H	-3.59120000	2.49120000	0.09370000
O	-3.55960000	2.84660000	-0.81720000
H	-4.37390000	2.55820000	-1.24780000
H	1.58020000	3.11920000	-0.76100000
O	1.75140000	4.02970000	-0.40930000
H	0.96510000	4.54530000	-0.63000000
O	4.86170000	-0.18990000	-1.11540000
H	5.81400000	-0.30320000	-1.01840000
H	4.53150000	0.27340000	-0.31080000
H	3.71500000	-1.42790000	-1.49510000
O	2.94670000	-2.05450000	-1.52500000
H	1.22320000	-1.34370000	-1.80070000
H	-1.08420000	-3.22310000	1.62750000
O	-1.63630000	-2.64670000	1.06390000

H	-1.09440000	-1.79960000	1.00010000
O	2.43950000	-1.94240000	1.29450000
H	2.82960000	-1.04810000	1.38760000
H	2.67660000	-2.22510000	0.39160000
H	-3.94520000	-0.92410000	0.17480000
O	-3.86450000	-0.86360000	1.16230000
H	-3.23200000	-1.57370000	1.38580000
H	-3.41550000	1.83760000	2.50410000
O	-3.06490000	1.56680000	1.64700000
H	-3.34970000	0.60070000	1.50460000
O	1.81150000	2.95100000	2.03360000
H	1.86530000	3.51090000	2.81740000
H	1.86350000	3.54360000	1.23610000
O	3.26600000	0.74520000	0.86230000
H	3.13550000	1.44340000	1.52890000
H	2.58680000	0.97300000	0.17000000
H	1.30710000	-3.15470000	2.15720000
O	0.61180000	-3.80000000	2.39850000
H	0.75820000	-4.02790000	3.32360000
H	-1.42250000	1.90690000	1.15370000
H	3.19970000	-2.78510000	-2.10280000

$Al(OH)_4^-•14H_2O$

Al	0.03580000	-0.07010000	-1.50260000
O	-0.00890000	-0.28950000	0.31270000
O	1.56620000	0.67900000	-1.97920000
O	-0.14360000	-1.73260000	-2.10220000
O	-1.32290000	0.96650000	-1.98790000
O	0.20150000	1.72450000	2.47350000
O	-1.98080000	-1.72510000	1.41310000
O	2.52340000	2.43700000	1.57010000
O	-2.17100000	2.68520000	1.65230000
O	1.70920000	-2.01040000	1.41890000
O	3.80180000	0.03250000	1.25520000
O	-3.86970000	0.33810000	1.25950000
O	-0.35420000	-3.02310000	3.13170000
O	3.86200000	-0.65460000	-1.42380000
O	1.55050000	3.45860000	-0.88690000
O	-2.54850000	-2.63320000	-1.26220000
O	2.34350000	-3.14010000	-0.96680000
O	-1.09510000	3.41270000	-0.97600000
O	-3.91690000	-0.38510000	-1.49710000

H	0.06180000	0.50030000	0.87550000
H	1.67530000	1.61910000	-1.76530000
H	0.60890000	-2.32460000	-1.94990000
H	-2.22320000	0.60790000	-1.93250000
H	1.12380000	2.04140000	2.18450000
H	0.32230000	1.09250000	3.19210000
H	-1.27060000	-1.17380000	0.97470000
H	-2.72000000	-1.08930000	1.54910000
H	3.04010000	1.60230000	1.41660000
H	2.32410000	2.82260000	0.69200000
H	1.08430000	-1.35430000	0.99300000
H	1.16260000	-2.46380000	2.09270000
H	-3.34330000	1.15570000	1.34510000
H	-4.01240000	0.20420000	0.30050000
H	-1.31080000	2.36070000	2.02480000
H	-2.50130000	3.34960000	2.26830000
H	3.19560000	-0.67350000	1.54670000
H	3.94340000	-0.17130000	0.29670000
H	-1.05850000	-2.56240000	2.60400000
H	-0.58510000	-3.95880000	3.11040000
H	3.06230000	-0.14000000	-1.71400000
H	3.56040000	-1.57940000	-1.42680000
H	-1.65620000	-2.41060000	-1.65020000
H	-2.40700000	-2.57640000	-0.29590000
H	-1.24860000	2.53470000	-1.43630000
H	-1.52060000	3.30670000	-0.10600000
H	0.54720000	3.51770000	-0.89810000
H	1.88020000	4.20920000	-1.39350000
H	2.58380000	-4.07290000	-0.94240000
H	2.13980000	-2.86850000	-0.03410000
H	-3.46870000	-1.28630000	-1.48040000
H	-4.62780000	-0.43210000	-2.14590000

7. Cartesian coordinates of the solution phase structures optimized using the supermolecule density functional calculations at B3LYP/6-31+G(d,p) with PCM calculation

$Al(H_2O)_6^{3+}•12H_2O$

Al	0.00015200	0.00103400	-0.00607300
O	-1.12725000	-1.09196300	1.09451100
O	-0.38422900	1.52491600	1.09290000

O	1.50754900	-0.42793300	1.09754800
O	1.12808100	1.09351600	-1.10640300
O	0.38441200	-1.52268700	-1.10461600
O	-1.50912600	0.42776100	-1.10720400
O	-3.66541800	-0.36944100	1.34998100
O	-0.56230600	-3.68514800	1.26166100
O	1.51789800	3.35718900	1.34338400
O	-2.91421300	2.32771500	1.26598200
O	2.15085400	-2.98723300	1.34639300
O	3.47455600	1.35270200	1.26548200
O	3.66976200	0.36622900	-1.33743700
O	0.56016400	3.68851300	-1.26010600
O	-1.51569700	-3.35720800	-1.34347500
O	2.91565000	-2.32897300	-1.25783300
O	-2.15504100	2.98921000	-1.34040400
O	-3.47618600	-1.35782400	-1.25708200
H	-2.07242900	-0.85690800	1.31136200
H	-0.95052500	-2.05371900	1.28376500
H	0.29242300	2.22490700	1.31118800
H	-1.30579400	1.85120300	1.28362600
H	1.77597400	-1.36459300	1.31274200
H	2.25368100	0.20427100	1.28723300
H	2.07455400	0.85950600	-1.31785100
H	0.95162100	2.05594100	-1.29301100
H	-0.29134000	-2.22506500	-1.31840500
H	1.30615500	-1.85098500	-1.29056700
H	-1.78035000	1.36422200	-1.31957600
H	-2.25594300	-0.20536000	-1.29005100
H	-3.66675600	0.61243800	1.38520800
H	-4.22494500	-0.68372600	2.08752200
H	2.36673400	2.86337600	1.37587800
H	1.53154700	3.99761500	2.08200200
H	1.30092000	-3.47922100	1.37902500
H	2.70075300	-3.31625900	2.08473000
H	-0.95502500	-3.96570700	0.40803400
H	-0.94267900	-4.26042900	1.95562200
H	-2.96170200	2.80706100	0.41172900
H	-3.21745300	2.94717400	1.95981000
H	3.91467600	1.15043000	0.41278900
H	4.16165000	1.31163800	1.96070700
H	3.66812100	-0.61591900	-1.37043200

H	4.23673900	0.67606000	-2.07105700
H	-2.36563300	-2.86522700	-1.37421400
H	-1.52943600	-3.99904200	-2.08076200
H	-1.30493000	3.48069000	-1.37321000
H	-2.70638400	3.32222300	-2.07592800
H	0.95507600	3.96630600	-0.40679100
H	0.93764600	4.26685100	-1.95289500
H	2.95864400	-2.80849100	-0.40341200
H	3.22700000	-2.94674100	-1.94961900
H	-3.91395800	-1.15581700	-0.40311200
H	-4.16628300	-1.31685400	-1.94939100

$Al(OH)(H_2O)_5^{2+}•12H_2O$

Al	-0.03496200	-0.11918400	-0.11301800
O	-1.33191900	-0.88526300	-1.10631500
O	1.40808800	-0.80770500	-1.20181800
O	0.00119700	1.54403000	-1.14108900
O	1.36072000	0.70093900	1.00842100
O	-1.29838500	0.70545400	1.14841800
O	0.06919800	-1.66466000	1.06533300
O	-2.28553200	-3.33336300	-1.33459100
O	-3.89479200	0.68192100	-1.15392800
O	3.72975100	0.59380700	-1.27932700
O	1.88931100	-3.38300000	-1.40516100
O	-2.31690300	2.89359100	-1.26679400
O	2.29205000	2.98411500	-1.19492200
O	1.34722000	3.36703400	1.37812700
O	3.77061100	-0.47605200	1.27404400
O	-3.63627300	-0.58418600	1.33763700
O	-1.41944600	3.41419600	1.28104900
O	2.45493800	-2.92865400	1.28490900
O	-2.28121100	-2.98162000	1.27025600
H	-1.84136500	-2.43520800	-1.37131500
H	-2.08207000	-0.33472900	-1.37483000
H	2.27335900	-0.33943600	-1.30763500
H	1.53810700	-1.78453100	-1.38062200
H	-0.82119100	2.06947100	-1.32137900
H	0.80730100	2.09846100	-1.28934200
H	1.37769900	1.65910900	1.26069200
H	2.22473300	0.27784700	1.23989900
H	-2.18637800	0.28291000	1.28942600

H	-1.35887200	1.67536500	1.32817400
H	0.88922100	-2.19919400	1.21395000
H	-0.74504100	-2.21664400	1.20294100
H	-1.71768000	-3.96462900	-1.80745600
H	3.42828500	1.52977000	-1.30013000
H	4.36369600	0.48178200	-2.01387800
H	-3.01628300	2.19309800	-1.26605200
H	-2.52946600	3.51418400	-1.99001800
H	-4.03799100	0.21460900	-0.30393300
H	-4.69119200	0.53895500	-1.69730500
H	2.27326600	-3.52753500	-0.51674500
H	2.53754500	-3.71460900	-2.05361200
H	2.16807200	3.40889900	-0.31850000
H	2.44906400	3.69980800	-1.84170500
H	0.39499500	3.61418500	1.40773500
H	1.77876100	3.79141500	2.14484400
H	-3.31922100	-1.51948400	1.37127400
H	-4.23600300	-0.45573600	2.09717600
H	3.10201000	-2.19313600	1.36392300
H	2.63957100	-3.55201200	2.01336900
H	4.11970600	-0.12867500	0.42467700
H	4.40490400	-0.22158200	1.97266100
H	-1.86256600	3.52816700	0.41041000
H	-1.95666400	3.89033700	1.94381300
H	-2.35271800	-3.33405600	0.33747800
H	-2.43008700	-3.72245700	1.88724700

***trans*-$Al(OH)_2(H_2O)_4^+ \cdot 12H_2O$**

Al	0.00258000	-0.00255000	0.00060400
O	-0.80868600	-1.33417500	1.23446000
O	-0.67719100	1.36967100	1.00475400
O	1.61120400	-0.04760300	1.16978400
O	0.81967600	1.32810100	-1.23420800
O	0.68476200	-1.37370000	-1.00239700
O	-1.60798100	0.04499100	-1.16540900
O	-3.52372200	-1.41560500	1.18797400
O	0.51479500	-3.72471700	1.12569800
O	0.46976100	3.69485400	1.32597400
O	-4.38342000	1.14183900	1.06262200
O	2.97957300	-2.40147900	1.00286400
O	3.03083300	2.28079500	1.43850900

O	3.53439800	1.44056800	-1.13201200
O	-0.48809600	3.72679200	-1.13754800
O	-0.46408800	-3.69589100	-1.33232200
O	4.28304200	-1.15258600	-1.15898400
O	-2.95399700	2.40881600	-1.00748800
O	-3.03181200	-2.28840900	-1.38090000
H	-1.79409800	-1.42705000	1.27380600
H	-0.38263500	-2.22479100	1.30129200
H	-1.08095700	1.08615900	1.84123500
H	2.21506200	-0.82724800	1.12656900
H	2.10289100	0.76824500	1.42352300
H	1.80531900	1.42763200	-1.24868500
H	0.39571000	2.21946500	-1.30057800
H	-0.02853600	-2.78499400	-1.30497700
H	1.10145500	-1.09054900	-1.83200300
H	-2.20477900	0.83024000	-1.11528500
H	-2.11522500	-0.76916000	-1.39339100
H	-3.84056200	-0.47289000	1.14187800
H	-4.00334000	-1.83944700	1.92387400
H	1.42108300	3.49714500	1.39640000
H	0.03545700	2.78377700	1.29911000
H	2.17577100	-2.97215200	0.96939500
H	3.50243400	-2.70665400	1.76795100
H	0.12102400	-3.95106200	0.23528900
H	0.36403800	-4.47965000	1.72376000
H	-3.93101600	1.70074000	0.39465700
H	-5.33904200	1.25415100	0.90964000
H	3.45199800	2.16641500	0.55712900
H	3.74901800	2.41582300	2.08389500
H	3.85912200	0.49911000	-1.12074700
H	4.01706100	1.89723400	-1.84609700
H	-1.41678100	-3.49686900	-1.37942700
H	-2.14941000	2.97851300	-0.98377600
H	-3.48132000	2.70873400	-1.77176600
H	-0.09772500	3.95468400	-0.24610800
H	-0.33361300	4.47897000	-1.73801200
H	3.90263300	-1.66420300	-0.41276200
H	5.23772800	-1.34688100	-1.16494400
H	-3.45664200	-2.16858300	-0.50232900
H	-3.74806600	-2.42980300	-2.02733300

***trans*-$Al(OH)_3(H_2O)_2 \bullet 13H_2O$**

Al	-0.12181500	0.60771500	-0.60560800
O	-0.50566100	2.13581100	0.64902100
O	1.48694300	1.35760500	-0.97123500
O	-0.14892200	-0.53614400	0.77572700
O	0.29875300	-0.88810600	-1.93715500
O	-1.60654300	0.92591200	-1.53054000
H	0.22266300	2.34485800	1.28429300
H	-2.10734800	1.73555600	-1.31772900
H	0.67059200	-1.04067200	0.92755100
H	1.85955300	1.14978500	-1.84837400
H	-0.37711700	-1.61243500	-1.91421700
H	-3.19880100	-1.69575700	-1.85430800
O	-3.63716400	-0.84449900	-1.67329300
H	-2.88482600	-0.19120700	-1.67830400
H	-1.43440500	-3.75669900	-1.98859100
O	-1.59349100	-2.86839800	-1.62162300
H	-1.65762500	-2.96033900	-0.63427600
H	-3.47238200	2.65938300	0.15633300
O	-3.42012800	3.04869300	-0.74178900
H	-4.30529600	2.94551200	-1.13191700
H	1.93659000	3.04717600	-0.73966400
O	2.28819900	3.90921900	-0.40266700
H	1.70658500	4.60251900	-0.76074500
O	4.84397800	-0.45934700	-1.11660300
H	5.73146500	-0.82924300	-0.96127900
H	4.57673900	-0.01303400	-0.28530700
H	3.56646000	-1.59028900	-1.48865000
O	2.73739300	-2.13516500	-1.47473400
H	1.17741700	-1.32305600	-1.82093500
H	-1.22674500	-3.16287500	1.64694900
O	-1.75541500	-2.57671800	1.06788800
H	-1.17711600	-1.75324600	0.98629700
O	2.26876700	-2.05576000	1.28262300
H	2.72638100	-1.21441700	1.48640000
H	2.51486500	-2.24301600	0.35137300
H	-3.95643900	-0.83141200	0.08304600
O	-3.95075700	-0.80811700	1.07253300
H	-3.30454200	-1.50564300	1.30766700
H	-3.32597700	1.93377700	2.53070000
O	-3.01855800	1.65984200	1.64793100

H	-3.34837800	0.72884200	1.49801500
O	1.75127900	2.88579500	2.04140600
H	1.70986800	3.43317100	2.84608800
H	2.01951000	3.47921400	1.29746000
O	3.30318100	0.59872300	0.93815600
H	3.20146600	1.26890300	1.63592600
H	2.64254300	0.87447400	0.25030400
H	1.11133600	-3.24857800	2.15248300
O	0.39557900	-3.86583100	2.40858600
H	0.50276100	-4.02527900	3.36231700
H	-1.33506000	1.97378800	1.16230700
H	2.91938600	-2.94817100	-1.98218100

$Al(OH)_4^-•14H_2O$

Al	0.03970200	-0.03787300	-1.46107200
O	0.00845900	-0.29065500	0.32939100
O	1.50450400	0.83175000	-1.97624700
O	0.01213600	-1.68643200	-2.13582600
O	-1.37344100	0.89253400	-2.01318000
O	0.05322800	1.68354000	2.43705900
O	-1.89920200	-1.87301900	1.38001400
O	2.42335900	2.56688000	1.60531700
O	-2.36950700	2.58259400	1.61134400
O	1.82806100	-1.95433500	1.41870900
O	3.77611500	0.16091700	1.27027000
O	-3.84867800	0.14785700	1.26522900
O	-0.12210100	-3.14285000	3.07004700
O	3.81757500	-0.45143200	-1.43115000
O	1.40444700	3.49943800	-0.82886200
O	-2.35870600	-2.76462500	-1.28120900
O	2.46469000	-2.94703900	-1.05103300
O	-1.28914000	3.35264500	-0.91393400
O	-3.85752600	-0.51123500	-1.47993900
H	0.01146500	0.46168500	0.95138700
H	1.57517500	1.75811600	-1.68196200
H	0.77822800	-2.23950200	-1.89978300
H	-2.25453000	0.49311400	-1.89700500
H	0.95076700	2.06845300	2.22242600
H	0.12590200	1.26006900	3.31172300
H	-1.20144900	-1.28350300	0.98014200
H	-2.65257400	-1.25806400	1.53080900

H	2.94061400	1.73890900	1.44981700
H	2.17579300	2.92524900	0.72491100
H	1.16697700	-1.32989400	1.01059200
H	1.30189500	-2.46769700	2.07050200
H	-3.36435900	0.99434700	1.36288700
H	-3.96634500	0.01230200	0.30105700
H	-1.50564700	2.33738200	2.02442900
H	-2.78578100	3.23832800	2.20063800
H	3.18317900	-0.55826100	1.56587700
H	3.88591500	-0.01803900	0.30393300
H	-0.88329200	-2.76438300	2.57120300
H	-0.24627000	-4.10843000	3.06322800
H	2.99132300	0.04455200	-1.68233300
H	3.53934200	-1.38872600	-1.41810600
H	-1.48516600	-2.46502900	-1.64785400
H	-2.25192200	-2.67667800	-0.31019100
H	-1.38113300	2.47155900	-1.37071100
H	-1.71264800	3.21918400	-0.04135100
H	0.40950600	3.55663500	-0.82722100
H	1.73529100	4.30195000	-1.27080800
H	2.77730000	-3.86535400	-1.13750900
H	2.28400400	-2.79013500	-0.09181800
H	-3.42565200	-1.40599800	-1.50545200
H	-4.62621100	-0.54205200	-2.07752000