Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information

DFT study on the interaction between monomeric aluminum and chloride ion in aqueous solution

Xiaoyan Jin,[a] *Wenjing Yang,*[a] *Zhaosheng Qian,*[b] *Yingjie Wang*[a] *and Shuping Bi**[a]

[a]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

[b]College of Chemistry and Life Science, Zhejiang Normal University, Jinhua, Zhejiang 321004, China

Contents

1. Optimized geometries using GP, PCM and SM models for all aqueous Al-Cl complexes.

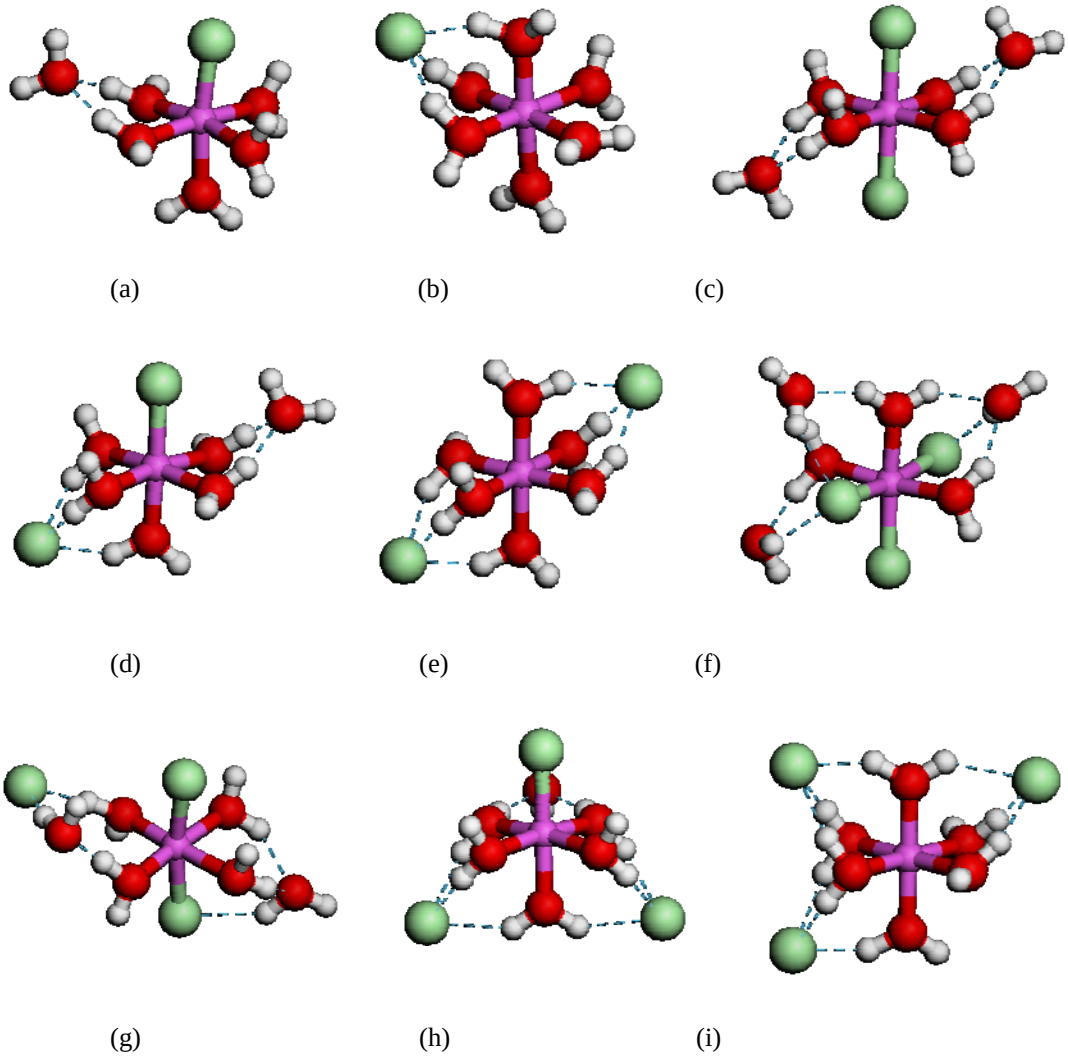


Fig. S1 Optimized geometries of hexa-aqua-aluminum $Al(H_2O)_6^{3+}$ in the presence of chloride ions using GP model. (a) only one Cl^- locates in the inner-coordination shell; (b) only one Cl^- locates in the outer-coordination shell; (c) two Cl^- locate in the inner-coordination shell; (d) one Cl^- locates in the inner-coordination shell and one Cl^- locates in the outer-coordination shell; (e) two Cl^- locate in the outer-coordination shell; (f) three Cl^- locate in the inner-coordination shell; (g) two Cl^- locate in the inner-coordination shell and one Cl^- locates in the outer-coordination shell; (h) two Cl^- locate in the outer-coordination shell and one Cl^- locates in the inner-coordination shell; (i) three Cl^- locate in the outer-coordination shell.

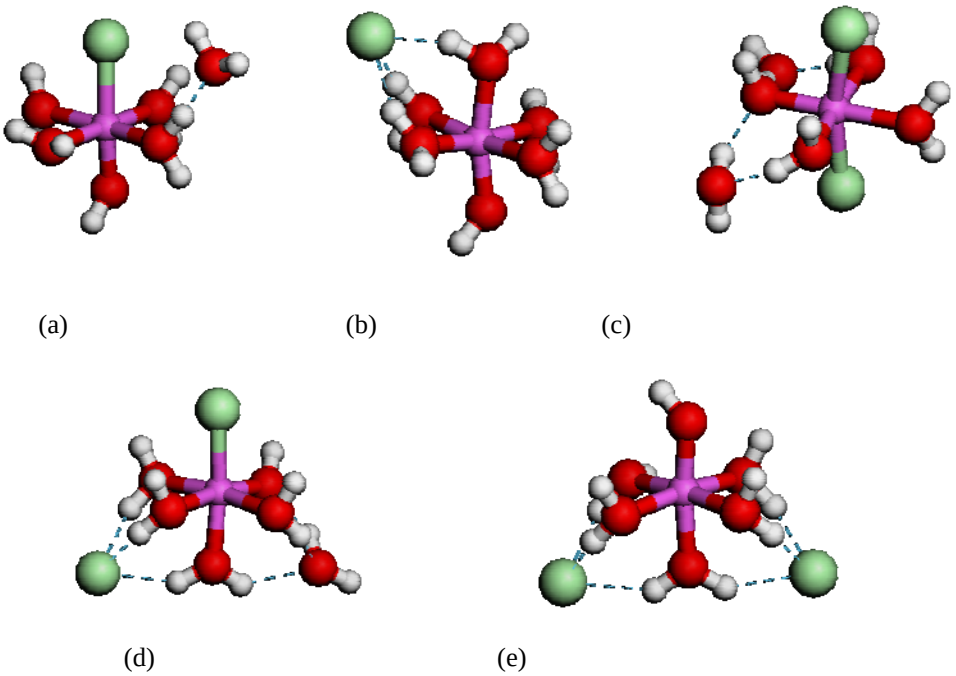


Fig. S2 Optimized geometries of the first hydrolysis product $Al(H_2O)_4(OH)^{2+}$ in the presence of chloride ions using GP model. (a) Only one Cl^- locates in the inner-coordination shell; (b) only one Cl^- locates in the outer-coordination shell; (c) two Cl^- locate in the inner-coordination shell; (d) one Cl^- locates in the inner-coordination shell and one Cl^- locates in the outer-coordination shell; (e) two Cl^- locate in the outer-coordination shell.

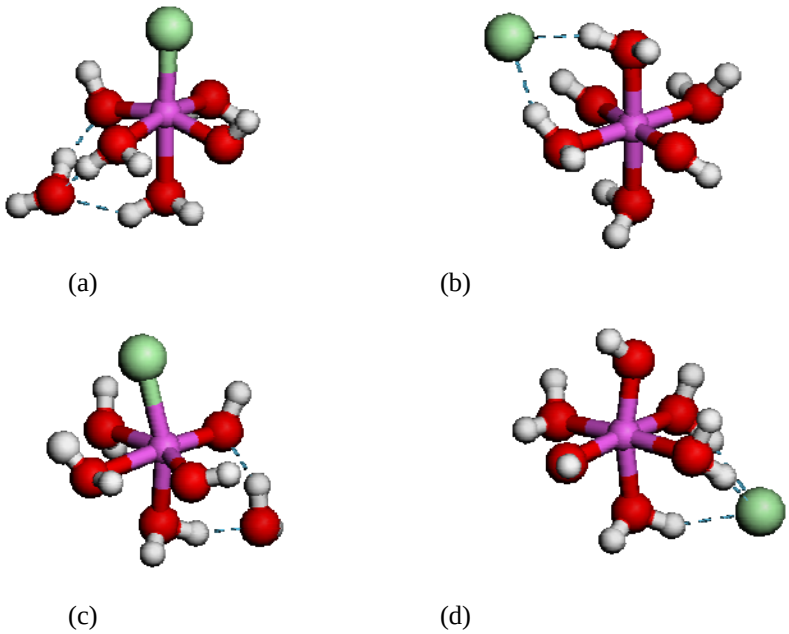
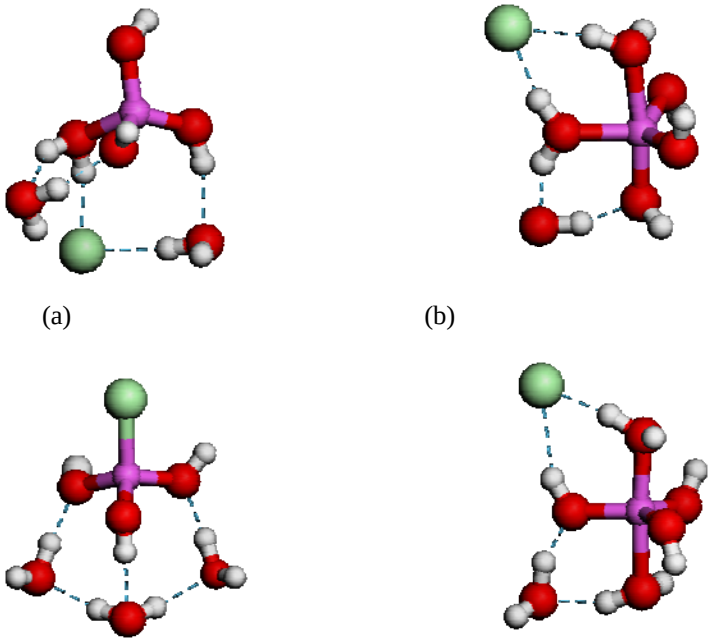


Fig. S3 Optimized geometries of the second hydrolysis product $Al(H_2O)_4(OH)_2^+$ in the presence of chloride ions using GP model. (a) One Cl^- locates in the inner-coordination shell of *trans* structure; (b) one Cl^- locates in the outer-coordination shell of *trans* structure; (c) one Cl^- locates in the inner-coordination shell of *cis* structure; (d) one Cl^- locates in the outer-coordination shell of *cis* structure.



(a) (b)

(c) (d)

Fig. S4 Optimized geometries of the third hydrolysis product $Al(H_2O)_2(OH)_3^0$ in the presence of chloride ions using GP model. (a) One inner-sphere Cl^- in the structure with two equatorial and one axial OH^- moves to the outer sphere; (b) one Cl^- locates in the outer-coordination shell of the structure with two equatorial and one axial OH^-; (c) one inner-sphere Cl^- in the structure with three equatorial OH^-; (d) one Cl^- locates in the outer-coordination shell of the structure with three equatorial OH^-.

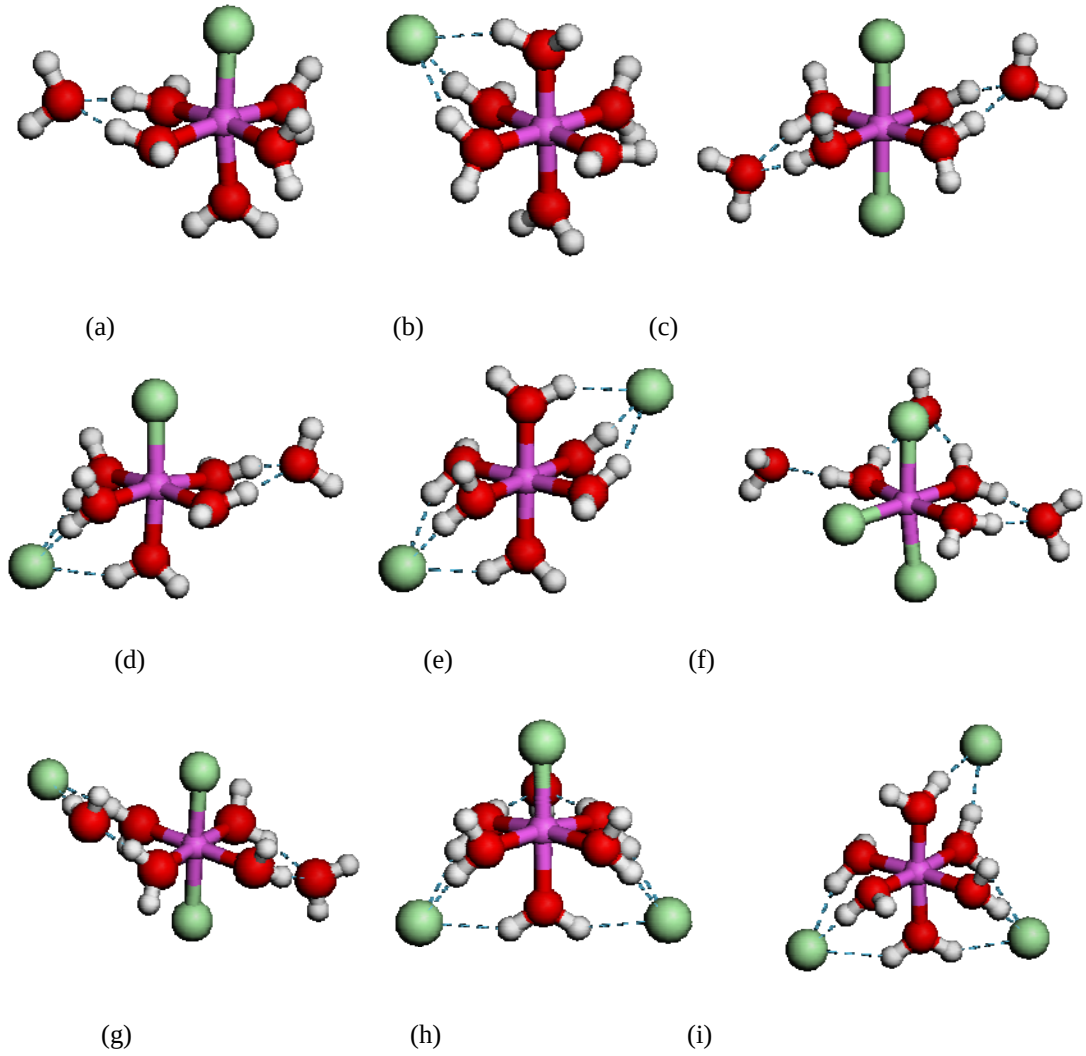


Fig. S5 Optimized geometries of hexa-aqua-aluminum $Al(H_2O)_6^{3+}$ in the presence of chloride ions using PCM model. (a) only one Cl^- locates in the inner-coordination shell; (b) only one Cl^- locates in the outer-coordination shell; (c) two Cl^- locate in the inner-coordination shell; (d) one Cl^- locates in the inner-coordination shell and one Cl^- locates in the outer-coordination shell; (e) two Cl^- locate in the outer-coordination shell; (f) three Cl^- locate in the inner-coordination shell; (g) two Cl^- locate in the inner-coordination shell and one Cl^- locates in the outer-coordination shell; (h) two Cl^- locate in the outer-coordination shell and one Cl^- locates in the inner-coordination shell; (i) three Cl^- locate in the outer-coordination shell.

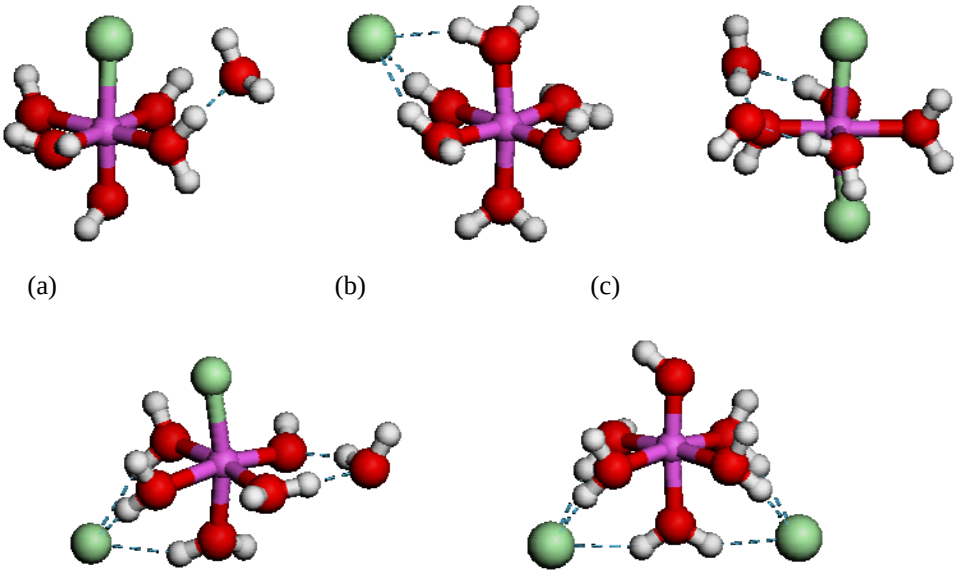


Fig. S6 Optimized geometries of the first hydrolysis product $Al(H_2O)_4(OH)^{2+}$ in the presence of chloride ions using PCM model. (a) Only one Cl^- locates in the inner-coordination shell; (b) only one Cl^- locates in the outer-coordination shell; (c) two Cl^- locate in the inner-coordination shell; (d) one Cl^- locates in the inner-coordination shell and one Cl^- locates in the outer-coordination shell; (e) two Cl^- locate in the outer-coordination shell.

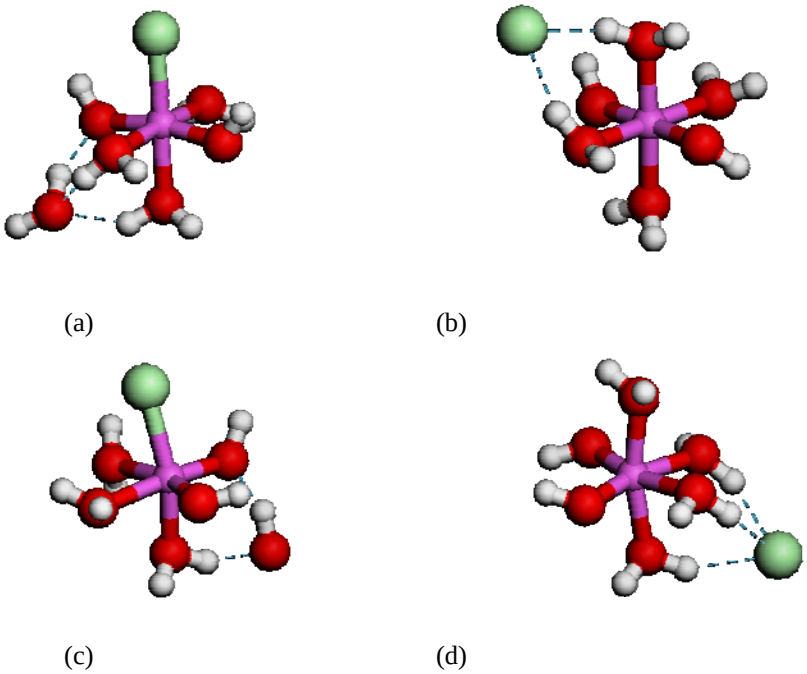


Fig. S7 Optimized geometries of the second hydrolysis product $Al(H_2O)_4(OH)_2^+$ in the presence of chloride ions using PCM model. (a) One Cl^- locates in the inner-coordination shell of *trans* structure; (b) one Cl^- locates in the outer-coordination shell of *trans* structure; (c) one Cl^- locates in the inner-coordination shell of *cis* structure; (d) one Cl^- locates in the outer-coordination shell of *cis* structure.

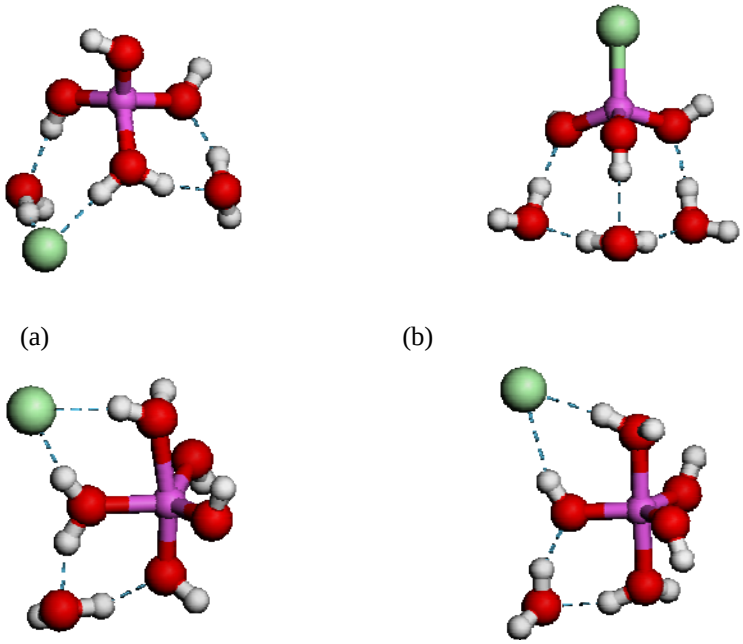


Fig. S8 Optimized geometries of the third hydrolysis product $Al(H_2O)_2(OH)_3^0$ in the presence of chloride ions using PCM model. (a) One inner-sphere Cl^- in the structure with two equatorial and one axial OH^- moves to the outer sphere; (b) one inner-sphere Cl^- in the structure with three equatorial OH^- (c) one Cl^- locates in the outer-coordination shell of the structure with two equatorial and one axial OH^-; (d) one Cl^- locates in the outer-coordination shell of the structure with three equatorial OH^-.

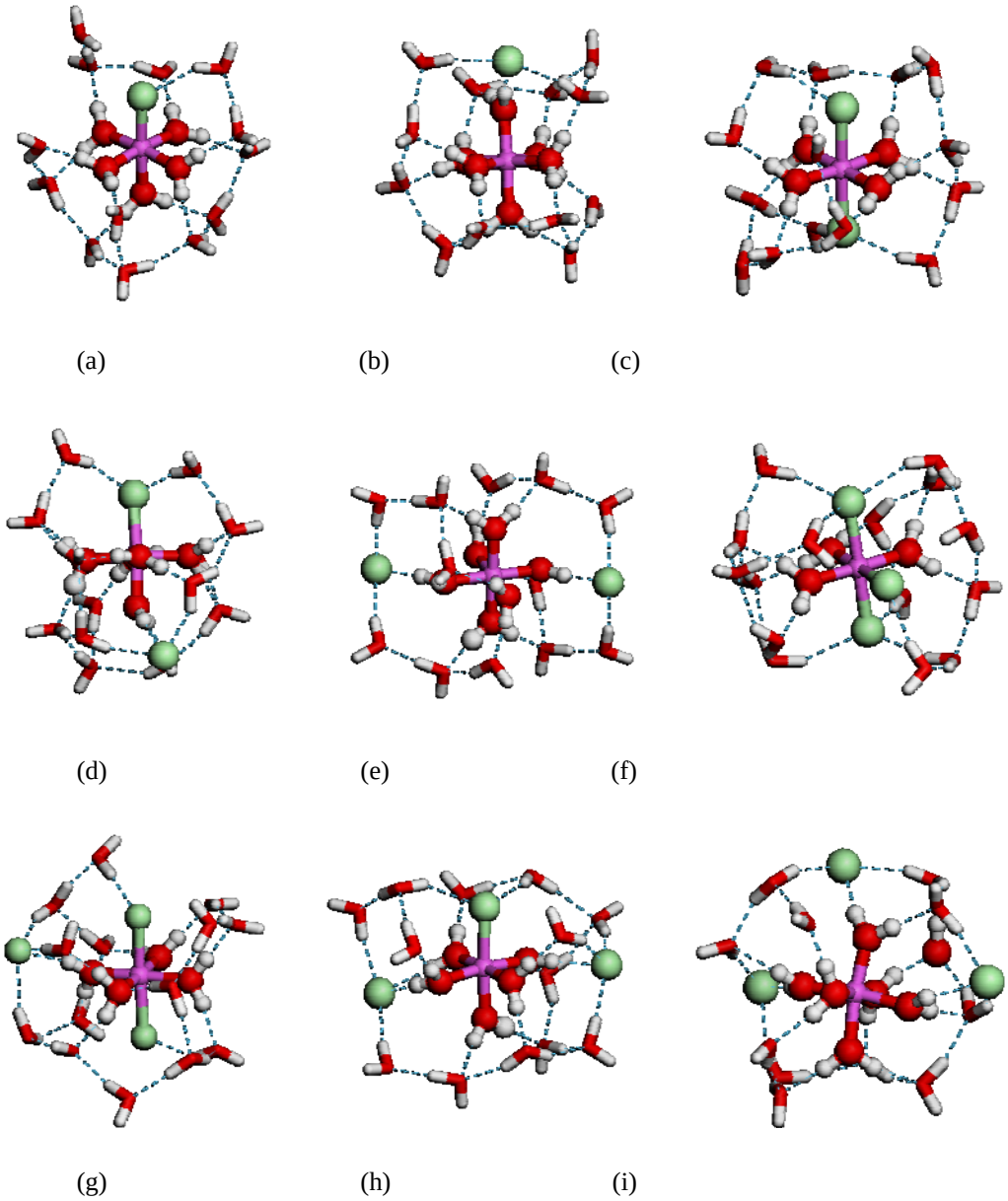


Fig. S10 Optimized geometries of hexa-aqua-aluminum $Al(H_2O)_6^{3+}$ in the presence of chloride ions using SM model. (a) only one Cl^- locates in the inner-coordination shell; (b) only one Cl^- locates in the outer-coordination shell; (c) two Cl^- locate in the inner-coordination shell; (d) one Cl^- locates in the inner-coordination shell and one Cl^- locates in the outer-coordination shell; (e) two Cl^- locate in the outer-coordination shell; (f) three Cl^- locate in the inner-coordination shell; (g) two Cl^- locate in the inner-coordination shell and one Cl^- locates in the outer-coordination shell; (h) two Cl^- locate in the outer-coordination shell and one Cl^- locates in the inner-coordination shell; (i) three Cl^- locate in the outer-coordination shell.

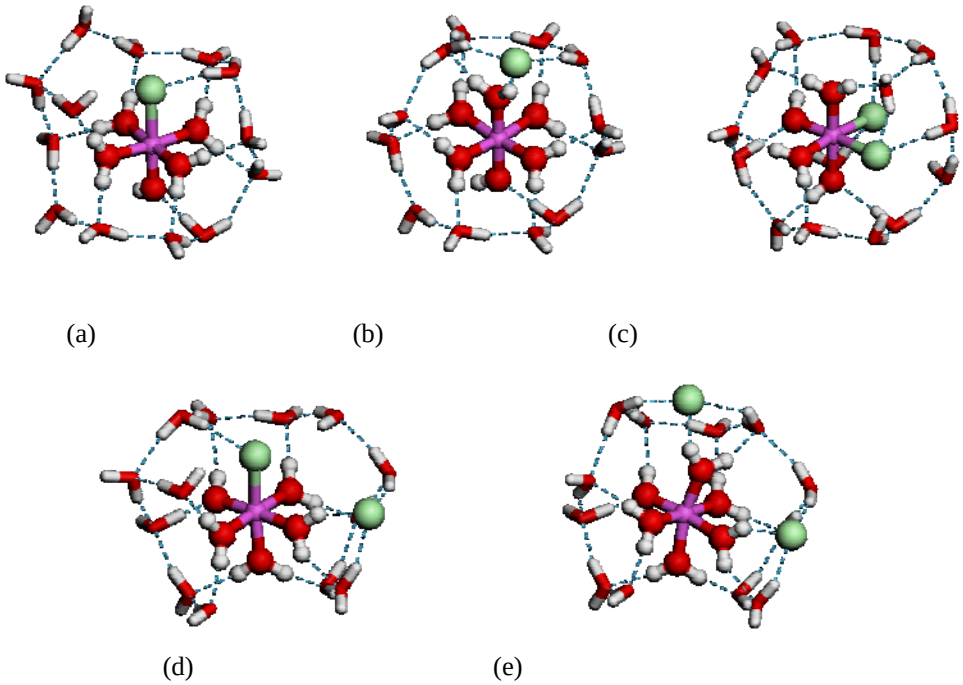


Fig. S11 Optimized geometries of the first hydrolysis product $Al(H_2O)_4(OH)^{2+}$ in the presence of chloride ions using SM model. (a) Only one Cl^- locates in the inner-coordination shell; (b) only one Cl^- locates in the outer-coordination shell; (c) two Cl^- locate in the inner-coordination shell; (d) one Cl^- locates in the inner-coordination shell and one Cl^- locates in the outer-coordination shell; (e) two Cl^- locate in the outer-coordination shell.

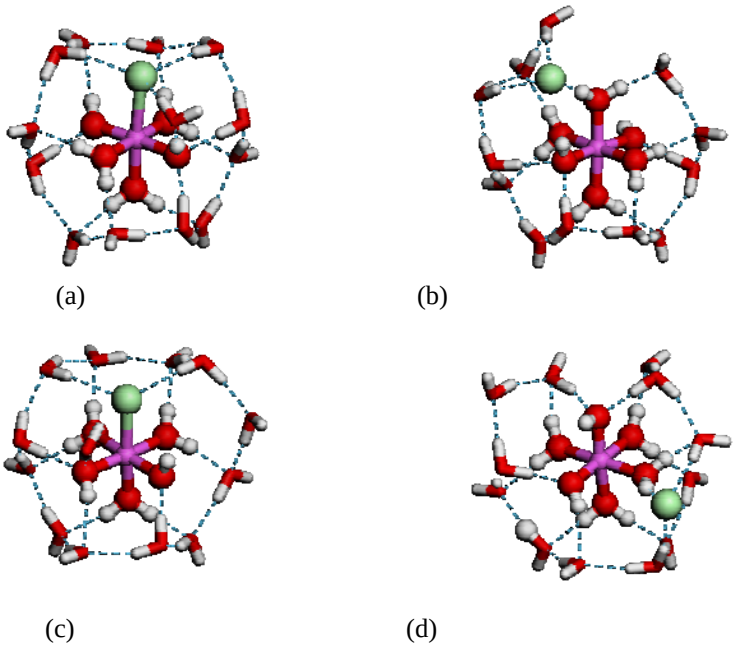
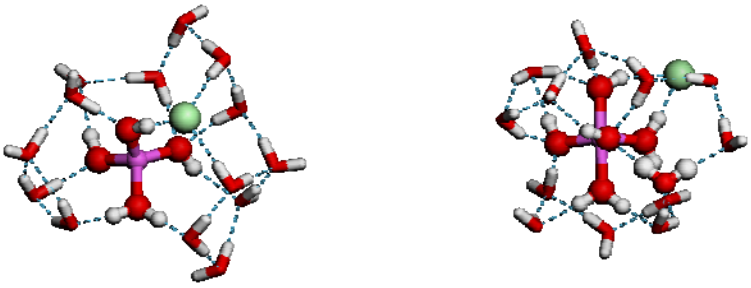
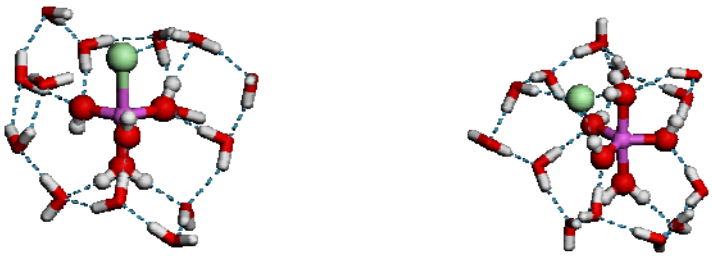


Fig. S12 Optimized geometries of the second hydrolysis product $Al(H_2O)_4(OH)_2^+$ in the presence of chloride ions using SM model. (a) One Cl^- locates in the inner-coordination shell of *trans* structure; (b) one Cl^- locates in the outer-coordination shell of *trans* structure; (c) one Cl^- locates in the inner-coordination shell of *cis* structure; (d) one Cl^- locates in the outer-coordination shell of *cis* structure.



(a) (b)



(c) (d)

Fig. S13 Optimized geometries of the third hydrolysis product $Al(H_2O)_2(OH)_3^0$ in the presence of chloride ions using SM model. (a) One inner-sphere Cl^- in the structure with two equatorial and one axial OH^- moves to the outer sphere; (b) one Cl^- locates in the outer-coordination shell of the structure with two equatorial and one axial OH^-; (c) one inner-sphere Cl^- in the structure with three equatorial OH^- move to the outer-coordination shell; (d) one Cl^- locates in the outer-coordination shell of the structure with three equatorial OH^-.

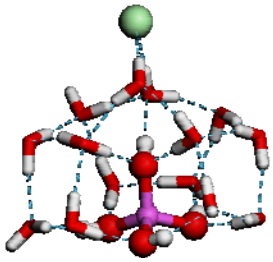
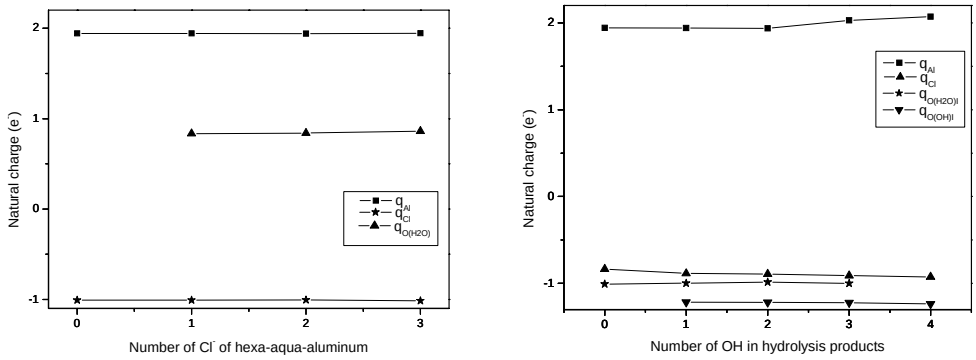


Fig. S14 Optimized geometry of $Al(OH)_4^-$ in the presence of chloride ion using SM-PCM model.

2. The change in the atomic natural charge.



(A) (B)

Fig. S15 (A). Natural charge of hexa-aqua-aluminum as a function of the number of chloride ions. (B). Natural charge of various hydrolysis products in the presence one chloride ion. Note: all atomic charge is average.

3. The computational energies (a.u.) of all the clusters.

Table S1 The absolute energies (a. u.) of various aqueous aluminum clusters in the presence of chloride ions

Cluster[a]	I/O[b]	E(GP)[c]	E(PCM)[d]	E(SM)[e]	E(SM-PCM)[f]
$[Al(H_2O)_5Cl](H_2O)^{2+}$	I	-1160.935016	-1161.275368	-2078.484213	-2078.742702
$[Al(H_2O)_6]Cl^{2+}$	O	-1160.902032	-1161.269686	-2078.478142	-2078.748240
$[Al(H_2O)_4Cl_2](H_2O)_2^{+}$	2I	-1621.582706	-1621.699508	-2539.023078	-2539.143127
$[Al(H_2O)_5Cl](H_2O)Cl^{+}$	1I+1O	-1621.569788	-1621.701147	-2539.033886	-2539.164064
$[Al(H_2O)_6]Cl_2^{+}$	2O	-1621.555496	-1621.697824	-2539.036018	-2539.173032
$[Al(H_2O)_3Cl_3](H_2O)_3^{0}$	3I	-2082.058182	-2082.114860	-2999.479681	-2999.545506
$[Al(H_2O)_4Cl_2](H_2O)_2Cl^{0}$	2I+1O	-2082.063171	-2082.125791	-2999.484412	-2999.565378
$[Al(H_2O)_5Cl](H_2O)Cl_2^{0}$	1I+2O	-2082.073276	-2082.123889	-2999.505074	-2999.581245
$[Al(H_2O)_6]Cl_3^{0}$	3O	-2082.066054	-2082.124457	-2999.486781	-2999.587848
$[Al(OH)(H_2O)_4Cl](H_2O)^{+}$	I	-1160.727199	-1160.850743	-2078.183168	-2078.302372
$[Al(OH)(H_2O)_5]Cl^{+}$	O	-1160.710956	-1160.848981	-2078.174413	-2078.310757
$[Al(OH)(H_2O)_3Cl_2](H_2O)_2^{0}$	2I	-1621.218249	-1621.264796	-2538.609011	-2538.708454
$[Al(OH)(H_2O)_4Cl](H_2O)Cl^{0}$	1I+1O	-1621.222749	-1621.271992	-2538.637594	-2538.717361
$[Al(OH)(H_2O)_5]Cl_2^{0}$	2O	-1621.220072	-1621.271722	-2538.633789	-2538.726076
cis-$[Al(OH)_2(H_2O)_3Cl](H_2O)^{0}$	I	-1160.359414	-1160.409093	-2077.768717	-2077.846037
cis-$[Al(OH)_2(H_2O)_4]Cl^{0}$	O	-1160.362266	-1160.412322	-2077.785583	-2077.863235
trans-$[Al(OH)_2(H_2O)_3Cl](H_2O)^{0}$	I	-1160.360776	-1160.408860	-2077.777301	-2077.845671
trans-$[Al(OH)_2(H_2O)_4]Cl^{0}$	O	-1160.355496	-1160.415154	-2077.790928	-2077.861319
trans-$[Al(OH)_3(H_2O)Cl](H_2O)_2^{-}$	I	-1159.884264	-1159.985224	-2077.285021	-2077.418191
trans-$[Al(OH)_3(H_2O)_2](H_2O)Cl^{-}$	O	-1159.876246	-1159.984030	-2077.295468	-2077.421097
cis-$[Al(OH)_3(H_2O)Cl](H_2O)_2^{-}$	I	-1159.879216	-1159.983615	-2077.298551	-2077.420969
cis-$[Al(OH)_3(H_2O)_2](H_2O)Cl^{-}$	O	-1159.878368	-1159.980210	-2077.294241	-2077.412070

[a] Twelve water molecules in the second solvation sphere for SM and SM-PCM models were omitted for simplicity.
[b] I/O denotes Cl^- in inter-coordination shell or in outer-coordination shell.
[c] The energy for gas phase cluster only involving first solvation sphere.
[d] The energy using PCM method only involving first solvation sphere.
[e] The energy for gas phase cluster in supermolecular model.
[f] The energy using PCM method in supermolecular model.
[g] tetra=tetracoordinate.

4. The free energy (a. u.) of the related species for the pK_a computation.

Table S2 The free energy (a. u.) of the related species for the pK_a computation.

	GP		PCM		SM		SM-PCM	
	With Cl^-	Without Cl^-	With Cl^-	Without Cl^-	With Cl^-	Without Cl^-	With Cl^-	Without Cl^-
Hexa-aqua-aluminum	-1160.939903	-700.155711	-1161.309394	-700.900582	-2078.552792	-1617.891459	-2078.822577	-1618.394544
The first hydrolysis product	-1160.749267	-700.107726	-1160.888762	-700.461618	-2078.246403	-1617.701128	-2078.382676	-1617.959907
The second hydrolysis product	-1160.394666	-699.908885	-1160.455531	-700.034998	-2077.863676	-1617.403406	-2077.936570	-1617.517758
The third hydrolysis product	-1159.927763	-699.531151	-1160.027546	-699.581986	-2077.372126	-1617.008087	-2077.493792	-1617.077978
The forth hydrolysis product	-	-699.062024	-	-699.165789	-2076.806914	-1616.528135	-2077.053240	-1616.635099
H_2O	-76.454816		-76.467652		-		-	
H_3O^+	-76.714912		-76.895985		-		-	

5. The computed pK_a using GP, PCM and SM models.

Table S3 The computed pK_a using GP, PCM and SM models.

	GP		PCM		SM	
	With Cl^-	Without Cl^-	With Cl^-	Without Cl^-	With Cl^-	Without Cl^-
pK_{a1}	-33.7	-99.3	-5.3	3.1	19.5	-33.8
pK_{a2}	8.0	-129.2	-4.8	0.6	74.2	18.2
pK_{a3}	101.4	-76.8	-6.7	10.2	178.9	78.6
pK_{a4}	-	17.6	-	2.9	317.5	178.0

6. Cartesian coordinates of all the optimized geometries using SM-PCM model.

$\{[Al(H_2O)_5Cl]\cdot(H_2O)_{13}\}^{2+}$ (I)

Al	0.16033400	-0.08641600	0.03287100
O	0.99794500	1.10253300	1.27828900
O	0.89861100	-1.58999300	0.96401500
O	-1.34325500	-0.14363100	1.27648200
O	-0.77098000	-1.29999400	-1.09005000
O	-0.73664000	1.39017500	-0.82419400
O	3.27147300	0.49534900	2.42234300
O	0.14501900	3.64690600	1.49106400
O	-0.88264500	-3.60481900	1.32351100
O	3.48681300	-2.05834000	1.32953700
O	-2.17859100	2.27462700	2.22149400
O	-3.23521000	-2.01957000	1.26718400
O	-4.55798700	-0.59344700	-0.70045400
O	-0.06275100	-3.82587300	-1.34974500
O	0.36412300	3.78216600	-1.24540100
O	-3.35367700	1.89457000	-0.24775300
O	4.47342500	-2.02831400	-1.16711400
O	2.90649000	3.17421000	-1.83745600
H	1.86021000	0.88993900	1.74685600
H	0.78121000	2.06178400	1.37586200
H	0.31936400	-2.35499100	1.20417400
H	1.85903100	-1.83589000	1.05059300
H	-1.61239000	0.65012700	1.79296400
H	-2.05445600	-0.83361100	1.31678100
H	-1.45963600	-1.06095100	-1.77652600
H	-0.46333400	-2.23549300	-1.25817800
H	-0.30602100	2.23976100	-1.10971700
H	-1.70447200	1.55656600	-0.70073700
H	3.51185000	-0.41608800	2.15798200
H	3.31439700	0.51905200	3.39322100
H	-1.78921900	-3.23900200	1.30502500
H	-0.84715000	-4.21319500	2.08286400
H	-1.44913900	2.92011300	2.11422800
H	-2.57941000	2.44129300	3.09309200
H	0.21232900	3.98781900	0.57303500
H	0.59642600	4.29023800	2.06698900
H	3.97242800	-2.09413800	0.46639100
H	3.74999800	-2.84453900	1.83971900
H	-3.82541000	-1.68249700	0.55579100
H	-3.79211900	-2.10837000	2.06212500

H	-4.32573900	0.33326500	-0.47946000
H	-5.52685400	-0.62347300	-0.79015000
H	1.30296100	3.69420400	-1.55174500
H	-0.07856100	4.40680300	-1.84705400
H	5.34531200	-1.64877600	-1.37066800
H	3.82337700	-1.40670200	-1.53395100
H	-0.38291700	-4.19143800	-0.50647300
H	-0.44930200	-4.37237700	-2.05476100
H	-3.21345200	2.19321100	0.67531900
H	-3.77130100	2.63950200	-0.71873600
H	3.32037500	3.38261600	-2.69217500
H	2.86376000	2.20378800	-1.79126000
Cl	1.96462500	0.07212800	-1.42223200
H	-2.84900700	-1.33424300	-3.52520400
O	-2.71141300	-0.74878900	-2.76169800
H	-3.52211000	-0.79921200	-2.21601700

$\{[Al(H_2O)_6]\cdot(H_2O)_{12}Cl\}^{2+}(O)$

Al	-0.33228600	-0.25467400	-0.41758200
O	-0.97718200	1.28812200	0.52668200
O	1.46398600	0.35265700	-0.23093500
O	-0.20230200	-1.24273000	1.21724300
O	0.25515800	-1.77657300	-1.40262900
O	-2.14741200	-0.80541300	-0.61619600
O	-0.43901800	0.72026000	-2.09186200
O	-0.40330400	3.82846000	0.08334500
O	-3.30668800	1.09461800	1.84606400
O	3.94934200	-2.57043400	0.20075600
O	2.24860900	4.04498300	0.32604300
O	-2.45327400	-1.45809700	2.66272800
O	2.23795500	-1.58667900	2.26981000
O	-0.88352600	-4.09437100	-0.91115500
O	2.77774600	-2.08706200	-2.16104300
O	-3.87123600	1.20300000	-0.93883700
O	-3.10288200	-3.02449500	0.46535800
O	2.28099200	0.55546100	-2.73386900
O	-1.90566200	2.93090500	-2.06285400
H	-0.69067800	2.23793900	0.42040000
H	-1.77644700	1.26161500	1.11047100
H	1.89770700	0.75461200	0.57765000
H	1.97131000	0.58511800	-1.04700900
H	-0.94466400	-1.32195700	1.86830700
H	0.67179700	-1.43380700	1.65231400
H	-0.18671500	-2.66422400	-1.25914200
H	1.19822900	-1.93759300	-1.68052800
H	-2.85563900	-0.14220200	-0.83036200
H	-2.56065200	-1.65395900	-0.30130200
H	0.35636700	0.73736700	-2.66069400
H	-0.94622000	1.57071800	-2.19433500
H	0.57318200	4.00540000	0.14901800
H	-0.83147800	4.44236300	0.70774600
H	3.41026200	-2.24935900	0.94956400
H	4.86033600	-2.28704900	0.38427800

H	-2.92460700	-0.60540600	2.57025200
H	-2.45345100	-1.67928900	3.61206200
H	-3.88889800	1.22436500	1.07362600
H	-3.57810600	1.75368300	2.51226600
H	2.54728000	3.35865900	0.95466900
H	2.67643200	4.87169500	0.60589600
H	2.30458600	-2.08063700	3.10839200
H	2.53743500	-0.67010900	2.46313300
H	-1.70545200	-3.96934800	-0.40071200
H	-1.11910600	-4.66112600	-1.66626600
H	-3.38583100	1.93647400	-1.36783900
H	-4.71332500	1.10901300	-1.42048800
H	2.68998300	-0.32846300	-2.83081000
H	2.84497300	1.19519000	-3.20406900
H	3.30300700	-2.27305700	-1.33924200
H	2.96294800	-2.81060600	-2.78580400
H	-3.07217600	-2.74808900	1.40308400
H	-4.00394400	-3.35525500	0.29409000
H	-1.42673300	3.52449200	-1.44720900
H	-2.08224900	3.44280500	-2.87391200
Cl	2.85234400	1.48175900	2.16069900

{[Al(H$_2$O)$_4$Cl$_2$]·(H$_2$O)$_{14}$}$^+$ (2I)

Al	0.04624600	-0.07844200	-0.01173400
O	0.80366900	-1.30735800	1.25133600
O	-1.27424000	0.52346900	1.22613900
O	-0.68262000	1.13384000	-1.29381600
O	1.40280500	-0.58094200	-1.27740100
O	-0.53209400	-1.63124300	3.49346100
O	3.50693600	-1.65053300	1.10911200
O	-2.06916600	3.04851300	1.10068300
O	-3.25691800	-0.83434500	2.33990100
O	4.81227400	0.66749900	-0.00725200
O	0.10598300	4.37050200	-0.02264700
O	0.95121600	2.90449300	-2.45658500
O	-3.27530100	0.91421700	-1.93879600
O	2.61132100	-2.98165900	-1.12754600
O	3.19768900	1.19598800	-2.12552800
O	-4.76174400	-0.52647500	0.09592900
O	0.44350200	-4.51888400	-0.72636600
H	0.32275100	-1.51676200	2.10578400
H	1.78288400	-1.36307200	1.36603800
H	-1.55215800	1.48508900	1.20343100
H	-2.00256600	-0.01149700	1.64117700
H	-0.15669700	1.80517800	-1.79945400
H	-1.64490200	1.13257900	-1.54338100
H	1.80824400	-1.48521800	-1.29943100
H	2.06616100	0.07157800	-1.63085700
H	-1.48176800	-1.61882800	3.29993900
H	-0.31135500	-0.74417500	3.85400900
H	-1.38356900	3.61573400	0.68297900
H	-2.30976600	3.48709700	1.93331600
H	4.39843900	-0.10179200	0.43152400
H	4.79924100	1.37613600	0.65646200

H	3.42065700	-2.30683100	0.38568700
H	3.99774100	-2.09086900	1.82552800
H	-3.88211300	-0.78493200	1.57422700
H	-3.70872600	-0.38932700	3.07801700
H	0.23166100	4.24815200	-0.97709800
H	0.69050900	3.68781400	0.35297400
H	1.83428900	2.49527900	-2.35311400
H	0.86479100	3.12783900	-3.39993300
H	1.90307100	-3.65670600	-0.96981100
H	3.14613100	-3.30061700	-1.87555700
H	-4.24785300	-0.02635900	-0.56852100
H	-5.01228300	-1.35595000	-0.34298300
H	-3.73756700	1.69983100	-2.28107100
H	-3.23610800	0.25834300	-2.67584500
H	3.86388200	1.09649900	-1.39796600
H	3.66407700	0.99698900	-2.95711400
H	0.35519200	-5.08083400	0.06187600
H	-0.21899300	-3.81108100	-0.62501300
Cl	-1.34398500	-1.81807000	-0.76225700
H	-3.37678100	-1.72820600	-4.02523900
O	-2.72957800	-1.11006200	-3.64593800
H	-2.25734100	-1.60898700	-2.95794800
Cl	1.47391100	1.62157800	0.86004400
O	0.34937400	0.93343100	4.00268500
H	1.07825300	1.13510700	4.61308200
H	0.65778700	1.21929800	3.12544600

{[Al(H$_2$O)$_5$Cl]·(H$_2$O)$_{13}$Cl}$^+$ (1I+1O)

Al	-0.24755400	0.35293300	-0.41409600
O	-1.31637000	-0.36236000	0.99253700
O	-0.35607800	2.12693300	0.31707200
O	1.31674100	0.02544800	0.70587900
O	0.91370500	1.05808900	-1.73805500
O	0.03835000	-1.40113900	-1.14965500
O	-1.61065500	0.66430500	3.34831000
O	-1.73003400	-3.03237800	1.13999900
O	2.03558700	3.44492500	0.24658400
O	-2.30156500	2.98986100	1.88228600
O	0.99351200	-3.29240900	2.10034100
O	3.72726000	1.13881200	0.30384500
O	4.13053200	-1.15056800	-1.21979900
O	1.09644900	3.61670000	-2.38124000
O	-1.82841900	-3.27907100	-1.60431700
O	2.11944700	-2.88178200	-0.31723000
O	-4.29370700	2.06065900	0.31490500
O	-3.94208600	-1.93298200	-2.56296900
H	-1.44988500	0.04611100	1.90691100
H	-1.53306600	-1.32648100	1.03868500
H	0.47510200	2.65046700	0.41728900
H	-1.08090900	2.51433700	0.88313600
H	1.24254800	-0.18305700	1.67474000
H	2.19423500	0.46393800	0.57364800
H	1.46504900	0.50414800	-2.36349800
H	0.91702800	2.00474900	-2.05117700

H	-0.67029900	-2.02791000	-1.44403600
H	0.82613300	-1.93913100	-0.86465600
H	-1.75654900	1.61888100	3.22893000
H	-0.71854700	0.53253700	3.72527800
H	2.77628100	2.80847300	0.23068100
H	2.28000700	4.13490000	0.88905700
H	0.04376700	-3.31032700	1.88216100
H	1.10077000	-2.52587200	2.69919800
H	-1.88595900	-3.33770800	0.22047900
H	-2.47464600	-3.36358700	1.67331100
H	-3.13158700	2.73218200	1.40987000
H	-2.36750400	3.94109600	2.07637100
H	4.07342200	0.44205400	-0.29549900
H	4.33248800	1.15364400	1.06769900
H	3.55401700	-1.82032500	-0.79226600
H	5.00194200	-1.56890300	-1.33511600
H	-2.64194100	-2.91848600	-2.03918800
H	-1.56227100	-4.07060500	-2.10495200
H	-4.96023500	1.45347800	0.67872800
H	-3.78712000	1.54076400	-0.33416200
H	1.56475200	3.91097700	-1.57898800
H	1.64688800	3.88627100	-3.13583000
H	1.82682100	-3.07137300	0.61381600
H	2.21230800	-3.74805900	-0.75374600
H	-4.26626700	-1.99955400	-3.47728300
H	-3.57911000	-1.03564100	-2.47408700
Cl	-2.14408100	0.67383600	-1.73473000
H	2.25416700	-0.92900300	-3.91105500
O	2.55977300	-0.23007800	-3.30897900
H	3.22548800	-0.64055000	-2.71877700
Cl	1.30004400	-0.53350000	3.71187500

$\{[Al(H_2O)_6]\cdot(H_2O)_{12}Cl_2\}^+$ (2O)

Al	-0.00096300	-0.00149300	0.00125900
O	-1.86530600	0.28454300	0.27430100
O	-0.30203500	-0.64537400	-1.79061200
O	0.15912600	1.76520200	-0.69348500
O	1.86485600	-0.29252600	-0.26921500
O	0.30388200	0.64987700	1.79119300
O	-0.15743200	-1.76637600	0.70135400
O	-4.49339800	-2.73937000	0.04229900
O	-4.15290400	3.01409300	-0.15916900
O	2.14333500	0.26978300	-2.86462600
O	0.18389800	-3.15521100	-2.28348900
O	-1.55338500	3.69871700	-0.09015000
O	2.39151100	2.76327100	-1.70981400
O	4.50290200	2.72638700	-0.04961400
O	4.15119900	-2.99493200	0.12910700
O	-2.14660100	-0.26982400	2.86801900
O	-0.19024500	3.16327700	2.28804100
O	1.55650000	-3.69555500	0.08346100
O	-2.39090900	-2.76869700	1.71591700
H	-2.62413600	0.17908500	-0.36918700
H	-2.19826700	0.21806300	1.20238600

H	0.22455100	-0.20261700	-2.48471600
H	-0.22518100	-1.63345800	-1.97375200
H	-0.52746100	2.47424500	-0.55517600
H	1.00144000	2.18347600	-1.02598500
H	2.20042600	-0.22808800	-1.19586400
H	2.62268000	-0.18370600	0.37467200
H	-0.20501200	0.20018500	2.49345200
H	0.21582600	1.63649700	1.97158900
H	0.52733700	-2.47573700	0.55572500
H	-0.99898400	-2.18620100	1.03354600
H	-5.38473300	-2.88559800	0.40043800
H	-4.53768500	-1.88889500	-0.44245800
H	2.39000900	1.21547100	-2.82130800
H	2.65643400	-0.13268500	-3.58708900
H	-2.52035900	3.47720900	-0.13520900
H	-1.44169000	4.53868000	-0.56985800
H	-4.80324700	3.63461500	-0.52789900
H	-4.32574400	2.15200500	-0.58924100
H	0.68133600	-3.56798100	-1.54892700
H	-0.48047800	-3.80188300	-2.57493600
H	3.19844000	2.78595700	-1.13118600
H	2.32482500	3.63652600	-2.13481100
H	5.39324600	2.86066300	-0.41480600
H	4.54216600	1.87919200	0.44167000
H	-2.39568600	-1.21475900	2.82635800
H	-2.66461500	0.13601700	3.58494100
H	2.52258100	-3.46865700	0.12062800
H	1.45257100	-4.53656100	0.56319400
H	4.82151400	-3.61704300	0.45680300
H	4.32974400	-2.14084600	0.57286800
H	-0.68308100	3.57197600	1.54829200
H	0.47414200	3.81096500	2.57770800
H	-3.19389000	-2.79674700	1.13234000
H	-2.32488400	-3.63980900	2.14527700
Cl	-4.34448400	0.08565600	-1.39134900
Cl	4.34027300	-0.08732800	1.40287900

{[Al(H$_2$O)$_3$Cl$_3$]·(H$_2$O)$_{15}$}^{0} (3I)

Al	0.09888800	-0.03743400	0.04742900
O	-1.68955200	0.51849600	-0.19275000
O	-0.54113800	-1.04914600	1.56384100
O	1.85559000	-0.68423300	0.41779500
O	2.24922100	4.04773100	-1.97470400
O	3.55257600	-0.65870300	-2.67864100
O	-3.89473200	-0.89723500	0.37555600
O	-3.06096300	2.73514100	-0.35694700
O	2.55952400	-3.21655300	-2.00679000
O	-3.19688900	-3.37937100	-0.48304300
O	1.09380600	-2.49971200	3.00945400
O	-2.85020100	-0.22414400	2.80937100
O	4.11070300	0.60863100	-0.16235400
O	2.79448700	-3.16790700	0.69796600
O	-2.57648400	2.60625200	2.40450100
O	3.38664400	3.14182900	0.38135000

H	-2.46297700	-0.07555300	-0.00095700
H	-2.04807500	1.44390600	-0.33417100
H	0.04682900	-1.64772500	2.11345300
H	-1.31440700	-0.75227200	2.09893600
H	2.67491600	-0.14912500	0.22889700
H	2.14565800	-1.62757200	0.53354700
H	1.68680400	4.83944700	-2.00408300
H	1.64093000	3.29104000	-2.02973400
H	-3.79421700	-1.83424900	0.08361300
H	-4.50759500	-0.44579300	-0.23951400
H	2.98985400	-2.37909700	-2.28600000
H	1.61168800	-3.00289900	-2.02869600
H	3.90815000	-0.22186200	-1.88248800
H	2.73081400	-0.17223900	-2.84749600
H	-3.15470200	2.83020800	0.61325600
H	-3.87553000	2.32108200	-0.69602200
H	-3.15629700	-4.11906300	0.14610400
H	-2.27231900	-3.16839300	-0.70484600
H	1.68541400	-2.98026000	2.40815400
H	1.61549000	-1.75334100	3.37941700
H	3.94842200	1.57838400	-0.01508400
H	4.89110800	0.37417600	0.36940600
H	-2.75386500	1.68309500	2.66593100
H	-1.61511900	2.61588000	2.26912100
H	-3.48412500	-0.52856700	2.12647200
H	-3.13509800	-0.61426900	3.65425000
H	2.78611400	-3.37521400	-0.27029200
H	3.72482900	-3.22882600	0.97820600
H	3.06979400	3.58593000	-0.43447100
H	2.56865700	2.92175600	0.85834800
Cl	0.56386600	1.81654400	1.51164800
H	2.06921500	0.27460300	4.65508400
O	2.20335300	-0.09001100	3.76452500
H	1.77002700	0.53658300	3.15976800
Cl	-0.39655500	-1.95878800	-1.33810700
O	-2.84303400	-0.31347700	-3.23766200
H	-2.10213700	-0.66761900	-2.71960200
H	-2.43091300	0.24485200	-3.91791700
Cl	0.78608200	1.13899900	-1.82201300
H	-4.17973700	0.45396000	-2.28383000
O	-4.79228500	0.81867500	-1.60638500
H	-5.65581700	0.92075700	-2.03998300

{[Al(H$_2$O)$_4$Cl$_2$]·(H$_2$O)$_{14}$Cl}^{0} (2I+1O)

Al	-0.09681300	-0.31477800	-0.47584800
O	1.62344400	0.51128200	-0.37694200
O	-0.74862600	0.89265100	0.94663200
O	-1.80283900	-1.14166200	-0.69698200
O	0.66218400	-1.53990300	-1.78242300
O	4.67433900	-1.08730200	0.04962400
O	2.06966600	3.87062700	0.03998100
O	-3.71055600	-2.62304700	2.34861700
O	3.35585900	-3.08920000	1.43154500
O	-0.61725400	3.59703600	0.64418800

O	-3.44784600	0.09473600	2.02250600
O	-4.69684000	1.50833800	-0.02120300
O	-2.57847200	-3.55636700	0.09669200
O	2.87786600	1.63785400	-2.41866700
O	-3.27714200	3.89398500	-0.36625700
O	-0.18637200	-4.06587600	-1.46942300
O	3.32899400	-1.13402500	-2.31937700
H	2.17066300	0.71694100	0.41763000
H	1.97071300	1.05162500	-1.13907200
H	-0.79664800	1.85609700	0.71726500
H	-0.23711600	0.87121200	1.80907800
H	-2.50852600	-0.75658100	-1.27138900
H	-2.07677700	-2.04703400	-0.38700800
H	0.39574800	-2.49511400	-1.71546300
H	1.62889600	-1.47854500	-1.97389000
H	4.28581700	-1.82608800	0.56773200
H	4.45908600	-0.28528000	0.55674600
H	-3.65411300	-1.64294500	2.25087700
H	-3.33777200	-2.82631500	3.22128900
H	0.30095400	3.74331400	0.32023100
H	-0.65340000	4.02856600	1.51663100
H	2.41861200	3.71921600	-0.85042700
H	2.55951400	3.25343500	0.61853400
H	3.34647300	-3.98817200	1.06317600
H	2.43169600	-2.78142200	1.39478300
H	-3.99434900	0.57020100	1.35736000
H	-2.54105400	0.25050300	1.71433900
H	-4.21008100	2.35220600	-0.12908400
H	-4.48739500	0.99432200	-0.81959100
H	3.20030100	0.75215300	-2.67906200
H	2.40148700	1.98449300	-3.19125200
H	-0.90256800	-4.06156900	-0.80980400
H	-0.54116900	-4.54471800	-2.23770500
H	-2.94959400	-3.33823800	0.99099500
H	-3.31937300	-3.92624500	-0.41521600
H	-2.33197500	3.84784200	-0.13229200
H	-3.61217400	4.70255900	0.05356400
H	3.86001200	-1.15041100	-1.48112100
H	3.79341900	-1.70585000	-2.95421200
Cl	-0.70032100	1.22387800	-2.08661700
Cl	0.38656300	-1.80763100	1.24995400
Cl	3.48935500	1.52294300	1.79809500
O	0.65158600	1.14219200	3.19470100
H	0.63073100	0.40237700	3.82488100
H	1.59103900	1.23864700	2.93342800
H	-3.27020000	0.49585800	-2.92432200
O	-3.72994500	-0.06350200	-2.27212100
H	-4.33183300	-0.63368100	-2.78466500

{[Al(H$_2$O)$_5$Cl]·(H$_2$O)$_{13}$Cl$_2$}^{0} (1I+2O)

Al	0.20460300	-0.05092900	0.15166400
O	-1.53930500	-0.58863500	-0.40547500
O	-0.49860700	0.86175300	1.66936500
O	1.93213700	0.65640900	0.57077100

O	0.90458600	-0.92619400	-1.41873000
O	-0.01693900	1.54220300	-0.94710400
O	-3.52837500	2.89394400	0.09815000
O	-4.18344800	-2.46802700	-1.15454800
O	3.20425000	0.25947300	2.81143600
O	-1.08609300	3.43455800	1.48746800
O	-1.75965000	-3.83123400	-0.41676200
O	3.70949900	-2.32036100	2.09020900
O	5.04384300	-2.16111700	-0.33734000
O	3.67286800	3.51160900	-0.89711900
O	-2.59665400	-0.72074400	-2.76242500
O	0.35006100	-3.37573100	-2.10875400
O	1.02169000	3.96237500	-0.47739600
O	-2.32609300	2.09307700	-2.26418600
H	-2.33498000	-0.39976800	0.14515500
H	-1.85408100	-0.67141700	-1.36172700
H	-1.04402100	0.43428700	2.38689900
H	-0.70567900	1.83884500	1.63131800
H	2.37518300	0.55119900	1.46976100
H	2.63232800	0.61254700	-0.12382000
H	1.75064300	-0.61236600	-1.80082700
H	0.75134100	-1.89291900	-1.66300300
H	0.42489800	2.41602400	-0.78620700
H	-0.83676900	1.70985900	-1.47532600
H	-4.28037000	3.51153600	0.12477400
H	-3.86264100	2.04687200	0.46385500
H	3.51871100	-0.66645400	2.67613600
H	3.99108700	0.80141000	2.98592000
H	-2.59671600	-3.39615300	-0.67175800
H	-1.38760700	-3.28441600	0.29277800
H	-4.96956900	-3.01560500	-1.32163800
H	-4.43910600	-1.84176800	-0.44976100
H	-0.41229900	3.85126400	0.92334100
H	-1.92621000	3.45584100	0.98923300
H	4.21014700	-2.29522200	1.24536500
H	2.79165400	-2.51122200	1.84020700
H	6.01415400	-2.12791900	-0.34211100
H	4.75202900	-1.37922900	-0.84354100
H	-2.87550800	0.20354100	-2.87856600
H	-3.39182800	-1.24933000	-2.56723300
H	2.00315800	3.86034900	-0.53481700
H	0.79098000	4.63699300	-1.13988000
H	4.32509400	3.60717000	-0.18354800
H	3.79374400	2.60899100	-1.24776600
H	-0.43802900	-3.63636500	-1.57564300
H	1.01728300	-4.06543800	-1.95779400
H	-2.87350100	2.48440200	-1.54795600
H	-2.27851100	2.76184500	-2.96943600
Cl	-4.25679700	-0.07120800	1.01041800
Cl	3.75840800	0.39112100	-1.86482200
Cl	0.43786300	-1.97567600	1.43322500
H	-2.04459000	-0.97937900	3.84356500
O	-2.20809700	-0.11406800	3.43240600

H	-2.98671600	-0.23227200	2.85271600

$\{[Al(H_2O)_6]\cdot(H_2O)_{12}Cl_3\}^0$ (3O)

Al	0.09888800	-0.03743400	0.04742900
O	-1.68955200	0.51849600	-0.19275000
O	-0.54113800	-1.04914600	1.56384100
O	1.85559000	-0.68423300	0.41779500
O	2.24922100	4.04773100	-1.97470400
O	3.55257600	-0.65870300	-2.67864100
O	-3.89473200	-0.89723500	0.37555600
O	-3.06096300	2.73514100	-0.35694700
O	2.55952400	-3.21655300	-2.00679000
O	-3.19688900	-3.37937100	-0.48304300
O	1.09380600	-2.49971200	3.00945400
O	-2.85020100	-0.22414400	2.80937100
O	4.11070300	0.60863100	-0.16235400
O	2.79448700	-3.16790700	0.69796600
O	-2.57648400	2.60625200	2.40450100
O	3.38664400	3.14182900	0.38135000
H	-2.46297700	-0.07555300	-0.00095700
H	-2.04807500	1.44390600	-0.33417100
H	0.04682900	-1.64772500	2.11345300
H	-1.31440700	-0.75227200	2.09893600
H	2.67491600	-0.14912500	0.22889700
H	2.14565800	-1.62757200	0.53354700
H	1.68680400	4.83944700	-2.00408300
H	1.64093000	3.29104000	-2.02973400
H	-3.79421700	-1.83424900	0.08361300
H	-4.50759500	-0.44579300	-0.23951400
H	2.98985400	-2.37909700	-2.28600000
H	1.61168800	-3.00289900	-2.02869600
H	3.90815000	-0.22186200	-1.88248800
H	2.73081400	-0.17223900	-2.84749600
H	-3.15470200	2.83020800	0.61325600
H	-3.87553000	2.32108200	-0.69602200
H	-3.15629700	-4.11906300	0.14610400
H	-2.27231900	-3.16839300	-0.70484600
H	1.68541400	-2.98026000	2.40815400
H	1.61549000	-1.75334100	3.37941700
H	3.94842200	1.57838400	-0.01508400
H	4.89110800	0.37417600	0.36940600
H	-2.75386500	1.68309500	2.66593100
H	-1.61511900	2.61588000	2.26912100
H	-3.48412500	-0.52856700	2.12647200
H	-3.13509800	-0.61426900	3.65425000
H	2.78611400	-3.37521400	-0.27029200
H	3.72482900	-3.22882600	0.97820600
H	3.06979400	3.58593000	-0.43447100
H	2.56865700	2.92175600	0.85834800
Cl	0.56386600	1.81654400	1.51164800
H	2.06921500	0.27460300	4.65508400
O	2.20335300	-0.09001100	3.76452500
H	1.77002700	0.53658300	3.15976800
Cl	-0.39655500	-1.95878800	-1.33810700

O	-2.84303400	-0.31347700	-3.23766200
H	-2.10213700	-0.66761900	-2.71960200
H	-2.43091300	0.24485200	-3.91791700
Cl	0.78608200	1.13899900	-1.82201300
H	-4.17973700	0.45396000	-2.28383000
O	-4.79228500	0.81867500	-1.60638500
H	-5.65581700	0.92075700	-2.03998300

$\{[Al(OH)(H_2O)_4Cl]\cdot(H_2O)_{13}\}^+$ (I)

Al	-0.34449500	0.16421200	-0.14682200
O	-0.96908400	1.51501500	-1.19561600
O	-1.42355700	-1.17007700	-1.06933100
O	1.10914100	-0.25903800	-1.37852800
O	0.80969200	1.38487000	0.80931400
O	-1.79507100	0.50976000	1.12792000
O	-3.50007400	2.21193300	-1.45702900
O	2.02139300	3.96292100	-1.09510500
O	-0.67222100	-3.75622500	-1.18997800
O	-4.08706500	-0.67180000	-1.27218000
O	3.16182000	1.52004400	-1.48244400
O	1.96868000	-2.81763900	-1.58038200
O	4.14066100	-2.61319900	0.02298300
O	-2.01695100	-3.60827700	1.40662800
O	-0.09164700	3.93356400	0.85594100
O	4.54315100	0.14999500	0.49932800
O	-3.69632300	-1.44945100	1.35838400
O	-2.75889100	3.05638700	0.95847400
H	-2.54016300	1.92988800	-1.46677200
H	-0.47773200	1.66757000	-2.01546200
H	-1.23849800	-2.14046200	-1.11090600
H	-2.36041500	-0.98428800	-1.31357300
H	1.87821000	0.35972200	-1.42723600
H	1.42507000	-1.19039100	-1.49411600
H	0.52541700	2.32561700	0.89362400
H	1.48103600	1.15383900	1.50727100
H	-2.48555500	-0.16876700	1.31422400
H	-2.19215500	1.41277500	1.16621000
H	-3.98254000	1.36982700	-1.44633100
H	0.29555600	-3.60479200	-1.22756900
H	-0.89673300	-4.27576500	-1.98121100
H	2.78061300	2.41644700	-1.30700500
H	3.60982900	1.58098600	-2.34470500
H	1.25384400	4.06358900	-0.50326300
H	2.54278500	4.77721200	-1.00902900
H	-4.24527900	-1.00264200	-0.36388700
H	-4.70005800	-1.15048300	-1.85574900
H	2.72604600	-2.81957500	-0.94100000
H	2.34080500	-3.08810100	-2.43813900
H	4.29967000	-1.66967300	0.22977600
H	4.10843200	-3.06832300	0.88011300
H	-1.05826500	3.76894700	0.80730900
H	0.05053700	4.49908600	1.63488400
H	-3.19655400	-2.30301600	1.38209700
H	-4.32976600	-1.47331600	2.09624300

H	-1.79597100	-3.98312500	0.53769100
H	-1.21587200	-3.08969300	1.61010000
H	4.14751000	0.71247400	-0.20266800
H	5.47467300	0.42091700	0.57213900
H	-3.21982200	2.88492600	0.09457100
H	-3.40705500	3.45054400	1.56637500
Cl	0.42233800	-1.54898400	1.30942800
O	2.72472100	0.72826800	2.53915500
H	2.48825800	-0.09206700	3.00051200
H	3.46583200	0.49169300	1.94361700

{[Al(OH)(H_2O)$_5$]·(H_2O)$_{12}$Cl }$^+$ (O)

Al	0.44777300	0.12219200	-0.34699200
O	2.00975200	0.77091300	-0.93334100
O	-0.60964300	1.16881900	-1.59961900
O	0.39089100	-1.41249100	-1.63318100
O	-1.18085500	-0.60279500	0.28931300
O	1.38196000	-1.05056300	0.92815300
O	0.30945500	1.49956100	1.00951300
O	2.62865300	3.35693900	-0.74001800
O	4.24215200	-1.61705800	-0.70587300
O	-3.16600200	0.36953900	-2.13543400
O	-0.30038600	3.86804000	-1.45988000
O	2.20415900	-3.39750400	-1.05130100
O	-2.24580100	-2.34890600	-2.15712400
O	-2.24269000	-3.05986800	0.47626500
O	-3.75741100	1.74220700	0.44652700
O	3.80332000	-0.06527000	1.64369200
O	0.59496200	-3.67373400	1.28891800
O	-1.69969000	3.29109800	0.85157600
O	2.77087800	2.50273600	1.70330600
H	2.43840600	2.42021800	-1.00043000
H	2.55152700	0.23376700	-1.51629500
H	-1.55576700	0.98076500	-1.79567900
H	-0.42187000	2.12464700	-1.74322400
H	1.01670400	-2.16488000	-1.52199200
H	-0.45509000	-1.75239100	-1.99061700
H	-1.39335900	-1.55868700	0.20258400
H	-1.76006100	-0.36237200	1.09689000
H	2.25564600	-0.79321500	1.29994100
H	1.03809100	-1.86941500	1.33686100
H	-0.42431400	2.16471600	1.05351100
H	1.13270200	1.88923300	1.38397200
H	1.83831800	3.84853700	-1.00409900
H	-3.04504900	-0.59999100	-2.16585900
H	-3.67947600	0.60887500	-2.91537700
H	3.01039300	-2.84537700	-0.89939300
H	2.45841300	-4.08178400	-1.68127100
H	4.24709400	-1.01392000	0.06161800
H	5.14970300	-1.67794800	-1.02110800
H	-0.87564500	3.93120700	-0.66748400
H	-0.58692900	4.54881400	-2.07861300
H	-2.43095700	-2.79059900	-1.29817500

H	-2.53264800	-2.95456600	-2.85040600
H	-1.56966500	-3.59419500	0.92375300
H	-2.78021500	-2.61267400	1.17326500
H	3.57786700	0.89572300	1.63516200
H	4.29360500	-0.22590000	2.45789300
H	-2.52701100	2.73039800	0.69634400
H	-1.91131200	3.88400000	1.58191900
H	-3.77823700	1.26798700	-0.39839800
H	-3.80111500	1.03813700	1.13104500
H	1.19242400	-3.87355000	0.54306800
H	0.82035800	-4.28417600	2.00034700
H	2.81939900	2.99088900	0.82198500
H	2.98740900	3.13075100	2.40123100
Cl	-3.18764800	-0.70322500	2.32270600

{[Al(OH)(H_2O)$_3$$Cl_2$]·($H_2O$)$_{14}$}^{0} (2I)

Al	0.45438100	-0.65148500	0.16428100
O	0.87834700	1.30310900	0.37536200
O	-1.05226800	-0.34127300	-0.83364700
O	1.65903400	-0.57304600	-1.40881900
O	-4.27156100	1.93363200	-0.68419900
O	-1.32719000	4.54661900	-1.28663900
O	-1.88265000	-2.48221900	-2.28289000
O	-3.58482900	-0.60186400	0.11604200
O	2.68491200	1.88550100	-1.57624600
O	3.78932000	-2.14667800	-1.87163700
O	4.61810200	-0.83818000	0.37533900
O	-3.59558200	-3.01340900	-0.45272300
O	-0.90125500	3.67189000	1.17777100
O	4.53450300	1.62669300	0.11146700
O	-2.12323500	-3.62066000	1.58460200
O	-2.98968000	2.07892200	2.00615300
H	-4.99517000	2.52347300	-0.91488100
H	1.31254300	1.71987700	-0.40246400
H	-1.53506200	-1.64730200	-1.86555800
H	-1.11847600	0.49902700	-1.31073700
H	2.09024400	0.27792900	-1.66080900
H	2.28750000	-1.29860200	-1.64272800
H	3.05191600	-0.97385100	0.95585700
H	-4.10165600	0.14673400	-0.23036900
H	-1.11701200	-3.07139800	-2.24747800
H	-0.76926100	5.29868300	-1.49966000
H	2.82157300	2.51961800	-2.28487600
H	-1.16908700	4.32023400	-0.32860600
H	-1.66636900	3.07357300	-2.04042100
H	-2.02869500	-2.80500500	2.10443900
H	-2.63592500	-0.42092100	-0.12181300
H	4.30555700	-1.76062600	-1.13154000
H	4.34651300	-2.12648400	-2.65431700
H	4.69368900	0.22011300	0.26031000
H	5.32259900	-1.12490900	0.96465500
H	-1.68463900	3.21935500	1.56368600
H	-0.25748000	2.95680400	1.07700100
H	-3.06837300	-3.35095400	0.35621200

H	-1.23593800	-3.70926400	1.18576900
H	-2.93421300	-2.94160600	-1.23911800
H	-3.77363200	-2.00717900	-0.22701600
H	3.52681800	1.86687400	-0.95887400
H	5.35418400	2.11892400	0.01136100
H	-3.53029600	1.96908500	1.20822600
H	-2.59291200	1.21091400	2.17062200
O	2.73354400	2.25142400	1.94256600
H	3.53490400	2.07833600	1.36913100
H	1.51280000	1.53652900	1.12308500
H	-3.54340100	2.09888300	-1.32386900
O	-2.00958100	2.16906200	-2.25734000
H	-2.04019200	2.10415900	-3.21701900
Cl	-0.65618500	-0.67187400	2.19779000
Cl	0.45819200	-2.97633700	-0.11691700
H	1.97097900	-1.55361700	1.98811200
O	2.11433000	-0.90112600	1.29297600
H	2.93077800	1.93432000	2.82810300

{[Al(OH)(H_2O)$_4$Cl]·(H_2O)$_{13}$Cl}^{0} (1I+1O)

Al	0.27365300	0.23664500	-0.13559000
O	-0.01889700	1.76558100	-1.32157100
O	-0.82035100	-0.86826000	-1.32153100
O	1.79677500	-0.27204600	-1.02358400
O	1.30210000	1.45097700	0.96558800
O	-1.34433700	0.87974400	0.70890200
O	-2.45785100	2.37453500	-1.98661900
O	2.43196900	3.12239100	-1.90397200
O	-0.39937600	-3.57403700	-1.51753500
O	-3.30250900	-0.31884200	-2.17300400
O	3.94922800	0.94944400	-1.21689500
O	2.31497900	-3.32246600	-1.55139900
O	3.25231400	-2.81347600	0.88582700
O	-2.39125600	-3.37939100	0.64929900
O	1.46830600	4.11660200	0.51470600
O	4.76339500	-0.32077100	1.10162900
O	-4.43913700	-1.64943600	-0.28610200
O	-3.15934000	2.98399500	0.65907500
H	-0.92248000	2.06427900	-1.65646300
H	0.72069500	2.21920000	-1.76108700
H	-0.71244400	-1.84326800	-1.37494000
H	-1.72275700	-0.63735900	-1.65995500
H	3.04786400	0.39936200	-1.15690200
H	1.82302000	-1.14656000	-1.42693300
H	1.28545000	2.43294900	0.91434900
H	1.83666400	1.14928300	1.74935300
H	-2.06862100	0.42132600	1.22222000
H	-1.62896700	1.81237200	0.68498500
H	-2.90921000	1.51618200	-2.10688500
H	0.58540300	-3.62924600	-1.50433200
H	-0.69324000	-4.07262600	-2.28657000
H	3.09160800	2.41519500	-1.68888100
H	4.43748200	0.58935300	-1.96524400
H	1.90289700	4.03651400	-0.35491400

H	2.72210400	3.53965600	-2.72104600
H	-3.81958000	-0.81921900	-1.44821400
H	-3.64716800	-0.62279700	-3.01864700
H	2.74611900	-3.20568000	-0.66031400
H	2.89717600	-3.88743700	-2.06788000
H	3.84968600	-2.04732900	0.93695000
H	2.40251900	-2.48521900	1.23438600
H	-3.30223300	3.78510800	1.17255400
H	1.99498500	4.72469100	1.04172100
H	-3.81864300	-2.33962700	0.02647600
H	-4.52240900	-1.03861900	0.47864700
H	-1.68554200	-3.62194700	0.03062100
H	-1.93445800	-2.86601700	1.32936800
H	4.57123000	0.21404600	0.29427600
H	5.70610400	-0.23619500	1.27591300
H	-2.86030400	2.75854700	-1.18417100
H	-3.64778200	2.25578300	1.12918600
Cl	0.38567100	-1.45311800	1.48160600
O	2.78337800	0.51898500	2.94236700
H	2.25807300	-0.24199100	3.22184400
H	3.54827600	0.15938200	2.45447000
Cl	-3.96944200	0.39566400	2.02470500

$\{[Al(OH)(H_2O)_5]\cdot(H_2O)_{12}Cl_2\}^0$ (2O)

Al	0.20124800	0.39011100	-0.27846100
O	-0.24298600	2.17137300	-0.89539200
O	-0.83715700	-0.38528900	-1.73159000
O	1.72173300	0.29184100	-1.25863500
O	0.25193200	-1.38231200	0.50808800
O	1.19213900	1.07349400	1.25157600
O	-1.43379000	0.62568300	0.76638200
O	-2.81007600	2.56061100	-1.54061100
O	1.68323700	4.04948700	-0.77775200
O	0.30467900	-2.67525000	-2.70254400
O	-3.43099700	-0.12652500	-2.25615900
O	3.52127200	2.13708600	-1.29408500
O	2.90502100	-2.33194500	-1.88137300
O	4.03250000	-1.98815800	0.56240400
O	-1.29176500	-3.37235300	-0.55974100
O	0.97403100	3.65131900	1.90533700
O	3.92799300	0.84756600	1.07258000
O	-3.91429700	-2.13306100	-0.55087300
O	-3.46364500	2.38594300	1.21851400
H	-1.15330100	2.41208100	-1.21906200
H	0.38637600	2.92937200	-0.96566900
H	-0.43073200	-1.10837000	-2.25991500
H	-1.79748100	-0.29315100	-1.96407000
H	2.83745100	1.39417300	-1.40559700
H	2.08332700	-0.57723600	-1.48062700
H	0.79998000	-1.70550800	1.27543700
H	-0.29156300	-2.13782400	0.18114800
H	1.03945600	1.99425800	1.59456700
H	2.17058800	0.94306400	1.20997000
H	-1.94838100	-0.05890200	1.24782900

H	-1.94685000	1.45401700	0.88345500
H	-3.16181100	1.70883100	-1.86270600
H	1.25237700	-2.66770700	-2.43366100
H	0.27769400	-2.98590500	-3.62410200
H	2.47670600	3.51987600	-1.03822200
H	4.09334500	2.13506000	-2.07874900
H	1.30526600	4.04368800	1.07451700
H	1.69304100	4.86617100	-1.30586000
H	-3.75360000	-0.84939500	-1.65306500
H	-3.76348000	-0.33010600	-3.14751500
H	3.36311000	-2.28773300	-1.00323800
H	3.60070700	-2.39767500	-2.55570800
H	4.08076100	-1.02693400	0.72417800
H	3.41784100	-2.31251500	1.25504800
H	-3.51680300	3.10728700	1.86946000
H	1.52368000	4.01333400	2.62015900
H	-3.07806500	-2.63518000	-0.55174900
H	-3.97772100	-1.74226000	0.34626500
H	-0.81657800	-3.41062800	-1.41584500
H	-1.23568300	-4.26436500	-0.17303000
H	4.05811000	1.39720800	0.26769200
H	4.48192100	1.23185800	1.77369600
H	-3.25115700	2.69510500	-0.68196400
H	-3.89806900	1.60944300	1.62768400
Cl	-3.85670400	-0.62090400	2.22261200
Cl	1.84168700	-2.72797500	2.70681500

{[*cis*-Al(OH)$_2$(H$_2$O)$_3$Cl]·(H$_2$O)$_{13}$}^{0} (I)

Al	0.09494900	0.14751900	-0.04599500
O	-0.56080800	1.57091400	0.89254400
O	1.70873000	-0.10128800	0.77598800
O	0.59612700	-1.25829700	-1.36901600
O	-1.52745900	0.25667700	-1.24507800
O	0.87487100	1.43463700	-1.39336800
O	0.84792000	3.79497600	1.14670500
O	-4.55771800	1.56857100	0.87846500
O	3.15726300	-2.37223700	0.64487000
O	3.42287300	2.41430500	0.98908300
O	-4.19382700	-1.22594400	0.81190600
O	0.87861600	-4.09166200	0.83319500
O	-0.91236200	-3.56401200	-1.57386100
O	3.36196500	-1.51140800	-1.73031200
O	-2.78881700	2.75354900	-0.97792000
O	-3.22491100	-1.95294800	-1.51684600
O	3.66881100	1.19809100	-1.55985200
O	-0.25653400	3.97032100	-1.17071000
H	0.34415000	2.93800900	1.23402100
H	-1.02195600	1.30225700	1.69139700
H	2.65641600	-1.55264400	0.88971200
H	2.13420600	0.71640700	1.06385700
H	0.13332800	-2.12057700	-1.43218700
H	1.54846200	-1.38818100	-1.55915000
H	-2.07639400	1.04957900	-1.08423300
H	-2.11278500	-0.50787000	-1.42307700

H	1.84823500	1.47754100	-1.47160400
H	0.50720100	2.34228900	-1.43812900
H	1.78181600	3.53211900	1.17631700
H	2.50739400	-3.09624700	0.74133800
H	-4.39706900	-0.27037500	0.86413100
H	-3.34455200	-1.32521500	1.27717000
H	-3.90250600	2.08420400	0.37297500
H	-4.68627700	2.03409400	1.70997600
H	3.74587900	2.02274000	0.15781700
H	4.11019300	2.28584900	1.65011600
H	0.34605600	-4.21254400	0.03423100
H	0.34986700	-3.45073300	1.33526100
H	-1.79393400	-3.15188800	-1.44848900
H	-0.96970300	-4.06829700	-2.39175000
H	-1.93937400	3.24300900	-0.90671200
H	-3.24961400	3.13044400	-1.73473400
H	3.67549500	0.21046500	-1.61892600
H	4.19200300	1.52032900	-2.30063900
H	3.40038100	-1.95459300	-0.80430500
H	3.81650000	-2.08735600	-2.35254300
H	-3.69847000	-1.74247900	-0.65514900
H	-3.90536500	-2.04124500	-2.19187800
H	0.21349400	4.07367200	-0.27805000
H	-0.09038500	4.76816800	-1.68178300
Cl	-1.04098000	-1.49268400	1.28531300
H	0.47066500	-0.95378400	3.77219000
O	1.31248500	-0.49889900	3.66996200
H	1.41117000	-0.43203600	2.70439300

{[*cis*-Al(OH)$_2$(H$_2$O)$_4$]·(H$_2$O)$_{12}$Cl}^{0} (O)

Al	0.38536700	0.18807300	0.34081700
O	0.74729800	-1.10568900	-0.87455000
O	1.08250100	1.56604100	-0.71135100
O	-1.47917500	0.45501800	-0.18870800
O	0.00181500	1.50090900	1.74532400
O	-0.31326200	-1.15080300	1.66557300
O	2.14440900	-0.09109300	1.26417500
O	3.18937000	-1.82063100	-1.66404900
O	-0.97678400	-3.64146700	-0.93451400
O	-0.27127000	3.93240900	-1.08221900
O	4.81629700	0.49912500	-1.68243200
O	-3.49576800	-2.37045500	-0.41364600
O	-2.86155600	2.63999600	-1.23445900
O	-2.51261400	1.22859700	2.74902400
O	0.62980600	4.08117300	1.39663200
O	0.83990800	-3.67548500	1.25268200
O	-3.02380500	-1.39426500	1.94656200
O	3.45651100	2.06840500	0.18270800
O	3.26926400	-2.58537600	0.75864500
H	2.25436300	-1.49960500	-1.54792200
H	0.06038300	-1.71777200	-1.16065600
H	0.20542600	3.07180800	-1.10529100
H	1.19866400	1.18362200	-1.58922200
H	-1.87717600	0.06516500	-1.02562600

H	-1.86129100	1.35393900	-0.17976900
H	-0.85266000	1.42716200	2.22786300
H	0.23203400	2.46217600	1.65738200
H	0.06952900	-2.04777200	1.57698800
H	-1.28538600	-1.25878900	1.78831500
H	2.79156000	0.62554200	1.09205900
H	2.60208500	-0.95232000	1.15035300
H	3.74497300	-1.03125000	-1.80829900
H	-1.19899600	3.70101000	-1.25605100
H	-2.71060500	-2.89352100	-0.65560900
H	-3.58383800	-1.70884300	-1.13534400
H	-0.31333300	-3.83891200	-0.24859200
H	-0.78661500	-4.21202400	-1.68547900
H	4.48547400	1.17639700	-1.05988900
H	5.16465800	0.97313300	-2.44270500
H	-3.71628200	2.98883600	-0.96219500
H	-3.06264600	1.90411500	-1.86335000
H	-2.86231600	0.36019200	2.46006500
H	-2.83643200	1.37293000	3.64261400
H	1.77240300	-3.40348500	1.06215800
H	0.88316000	-4.34964300	1.93843100
H	2.53575800	2.05327200	-0.23069600
H	3.56435700	2.92902200	0.60060500
H	0.23188500	4.23337800	0.49651900
H	0.35934000	4.81156800	1.95987600
H	-3.27586100	-1.71338400	1.01790900
H	-3.43642600	-2.01197100	2.55876000
H	3.35689500	-2.36224000	-0.23956400
H	4.12862600	-2.88405300	1.07189500
Cl	-3.11382600	-0.13787700	-2.58466600

{[*trans*-Al(OH)$_2$(H$_2$O)$_3$Cl]·(H$_2$O)$_{13}$}^{0} (I)

Al	-0.12381800	0.06009000	-0.18389900
O	0.49877300	-1.38089700	-1.36804200
O	0.76257400	1.29355900	-1.14814000
O	-1.71857900	0.21139500	-1.30924900
O	-0.69427100	1.51704400	1.03085800
O	-0.93235100	-1.14996500	0.93670100
O	3.15630600	-1.57219600	-1.79351400
O	-1.06031300	-3.62650100	-1.59026600
O	-0.27976700	3.67936000	-1.67592800
O	3.72611100	1.15476500	-1.54967900
O	-3.29040700	-1.97481600	-1.58836500
O	-3.00961700	2.59280400	-1.29555100
O	-3.40899200	1.72144800	1.29654100
O	0.70858000	3.89111000	0.82135100
O	-0.09856600	-3.78628200	0.87502100
O	-3.62583900	-0.95751800	1.14525000
O	3.30302700	2.60361800	0.78137600
O	2.72407600	-3.22842000	0.66572100
H	1.45820400	-1.50700800	-1.57035200
H	0.00719500	-2.22047000	-1.51607800
H	1.69341900	1.18733500	-1.37593700
H	-2.35438100	-0.53665200	-1.42299900

H	-2.19570200	1.06679100	-1.42501700
H	-1.63847500	1.66511600	1.26560400
H	-0.20773500	2.37375100	1.02458400
H	-0.39122700	-2.84563600	0.96503800
H	-0.73170400	-0.99839800	1.87581400
H	3.47009000	-0.65341200	-1.64369200
H	3.47164900	-1.82038200	-2.67889700
H	-1.23666100	3.52618600	-1.62160100
H	0.12074200	2.76771700	-1.60015100
H	-2.62612500	-2.69524200	-1.64399800
H	-3.85710400	-2.06060200	-2.37326700
H	-0.75073100	-3.94344400	-0.70038500
H	-0.89841100	-4.33998500	-2.23036800
H	3.70215200	1.75017800	-0.76571400
H	4.21183600	1.62826700	-2.24366700
H	-3.36862700	2.48598800	-0.38943500
H	-3.76633200	2.77316300	-1.87898700
H	-3.65217300	0.75806900	1.27701600
H	-3.88468400	2.12362900	2.04241000
H	0.87503300	-3.72793100	0.80805100
H	2.48772300	3.13742400	0.72577600
H	2.98833800	1.76924400	1.17853200
H	0.34741100	4.06223800	-0.08382100
H	0.50929000	4.67235000	1.36317700
H	-3.96011800	-1.34327100	0.32171300
H	-2.64299000	-1.09637800	1.08128600
H	3.00764700	-3.00167200	-0.23415300
H	2.60139900	-2.34618100	1.06498200
Cl	2.02503400	-0.21212600	1.39290000
O	-0.07194800	-0.71174900	3.71755300
H	0.12934600	-1.49165200	4.25836100
H	0.75538300	-0.50821300	3.24445900

{[*trans*-Al(OH)$_2$(H$_2$O)$_4$]·(H$_2$O)$_{12}$Cl}^{0} (O)

Al	-0.41576400	-0.18706500	-0.38477600
O	-1.69875500	-0.93965200	0.97169200
O	0.30074800	0.87421000	0.94889100
O	0.84000800	-1.61191200	-0.07385200
O	0.82692500	0.54658500	-1.77580600
O	-1.29986000	-1.19381800	-1.62332300
O	-1.65305200	1.31085200	-0.82541700
O	-3.43030000	0.95061100	2.08944900
O	-2.90189700	-3.37484500	0.40570300
O	2.21470000	2.88585300	0.59199400
O	-1.39018800	2.54903800	2.19216300
O	-0.20090900	-4.12226700	-0.00552100
O	4.37016200	1.21451100	0.49249100
O	3.44267500	-0.30181100	-1.91480200
O	1.14046100	3.36370500	-1.64944700
O	-3.81119800	-1.96262000	-1.57994900
O	4.23171900	-2.46054900	-0.53760600
O	-1.19905200	3.98064800	-0.42254400
O	-4.39326500	0.78273200	-0.49015100
H	-2.29107000	-0.35797400	1.48893100

H	-2.13867400	-1.80761600	0.84733100
H	0.84229900	0.37191900	1.57470900
H	1.52889900	-1.54676400	0.65146000
H	0.50056800	-2.53886700	-0.10976600
H	1.74314000	0.18036000	-1.80670300
H	0.90340200	1.52051900	-1.85654300
H	-2.87016300	-1.65376900	-1.72964900
H	-0.87539500	-1.21412900	-2.48378700
H	-1.57470400	2.26278600	-0.59832000
H	-2.59303800	1.10014200	-0.97854700
H	-2.71566000	1.66066800	2.17201300
H	-3.84371400	0.86706900	2.95453300
H	3.07583200	2.40452500	0.60609700
H	1.55334900	2.19765200	0.82695600
H	-1.16884000	-4.00154700	0.05647300
H	0.05141300	-4.62870800	0.77321700
H	-3.39007800	-2.96315500	-0.37260900
H	-3.53847400	-3.88509700	0.91508600
H	-1.34224600	3.33323200	1.62812600
H	-0.69535400	1.93808300	1.82142200
H	4.23753700	0.78121000	-0.36511000
H	4.12907400	0.52374800	1.13812400
H	3.68757400	-1.16620200	-1.49053300
H	3.90882500	-0.27603100	-2.75638000
H	-4.27087100	-1.16285600	-1.28671300
H	-0.34473400	3.96020100	-0.91705700
H	-1.72080200	4.69683400	-0.79691800
H	1.70074900	3.26187300	-0.79573900
H	1.64985100	3.88211300	-2.27989300
H	3.91208800	-3.35908200	-0.66411100
H	3.95357100	-2.20518900	0.37366800
H	-4.25817600	0.88161500	0.47753300
H	-5.14267400	1.33769500	-0.72728900
Cl	2.92294400	-1.28785800	2.02119700

{[*cis*-Al(OH)$_3$(H$_2$O)Cl]·(H$_2$O)$_{14}$}$^-$ (I)

Al	-0.72627900	-0.46080000	-0.56670800
O	-0.55630800	-2.19889600	0.03774200
O	0.74175200	0.04107200	-1.42395700
O	-2.17892100	-0.55821500	-1.57024300
O	-1.03845900	0.62097500	0.78497800
O	4.37424000	-0.38532900	-0.26011600
O	2.56059300	-4.29606000	-1.27083800
O	-0.27931900	2.66261100	-2.38708200
O	2.95608400	1.67064900	-0.79982000
O	-4.40759700	-2.06138800	-1.03301800
O	-3.06510200	2.24494300	-1.68213100
O	-3.24242600	1.77362800	1.01882200
O	0.59997300	4.74673900	-0.78786900
O	1.47030200	-3.20832000	1.13909500
O	-4.63250000	-0.57254000	1.52337000
O	2.34284600	3.47267800	1.10727600
O	2.96311700	-1.23793500	2.16713600
H	5.31342800	-0.19792700	-0.17715300

H	-1.38422700	-2.57645300	0.45984400
H	0.13463600	1.79950100	-2.20464100
H	1.29321300	-0.60164300	-1.88828700
H	-2.53716600	0.28468000	-1.87803800
H	-2.30192600	1.31947400	0.98394000
H	-0.35777900	0.81067700	1.47169000
H	3.89773000	0.50283300	-0.41418900
H	-1.22694000	2.54384100	-2.20349400
H	1.74750300	-4.59359500	-1.69065600
H	-3.62218200	-1.55285000	-1.34948400
H	2.00308400	-3.65006300	0.45300900
H	2.77713200	-3.44615900	-1.70530800
H	2.78995700	2.34347400	-0.08839200
H	2.09965500	1.21580000	-0.94053600
H	-3.22274500	2.20249800	-0.70902200
H	-3.82426500	2.68828400	-2.06974600
H	-4.18010300	0.29500100	1.40832500
H	-3.15704900	2.48964000	1.65666300
H	2.04251500	-2.51773900	1.57269900
H	0.28224600	-2.59061400	0.50472200
H	1.61523600	3.94893400	0.66834400
H	1.93500800	2.89776200	1.79068200
H	0.29012700	3.99375300	-1.34132700
H	1.25900100	5.18772800	-1.33188000
H	-4.79419800	-1.48072100	-0.36048700
H	-5.28788900	-0.43560600	2.21288500
H	3.48793500	-0.87630200	1.43425100
H	2.41500100	-0.48845000	2.49414600
O	-2.86781800	-3.00501200	1.03930400
H	-3.20467400	-2.29389800	1.60526000
H	-3.45139700	-2.92656300	0.24948300
H	3.64247100	-1.29133300	-1.54150100
O	3.09662000	-1.73557900	-2.23793700
H	3.50564300	-1.50545600	-3.07741500
Cl	1.10388300	1.21763100	2.96794800

{[*cis*-Al(OH)$_3$(H$_2$O)$_2$]·(H$_2$O)$_{13}$Cl }$^-$ (O)

Al	0.40230300	0.31484000	0.11573500
O	2.04958900	1.03101400	0.47382900
O	-0.51555300	0.64443900	-1.40135300
O	1.52899500	-1.09558800	-0.80736900
O	-0.31844900	-1.16451400	1.00570600
O	-1.77107200	3.47635600	0.20719400
O	2.30164200	3.58933600	-0.85763000
O	-1.51350500	-1.67566900	-2.75604600
O	-3.27099400	1.36891700	-1.04723700
O	4.03052200	-0.29409100	-1.83097700
O	0.47090900	-3.23908100	-1.90557200
O	0.76068300	-3.65981600	1.05364200
O	-3.87917300	-2.48688200	-1.49142700
O	1.48494300	3.38466700	2.06696700
O	3.46125600	-3.21489800	1.03072000
O	-4.37645300	-0.70655900	0.46456500
O	-0.46598000	1.50720400	1.26173700

H	-1.86365100	4.16466700	0.87215200
H	1.99853400	1.69775500	1.17986000
H	-1.22062400	-0.82253800	-2.37561700
H	-0.35443800	1.48606500	-1.84793700
H	2.32510200	-0.79979200	-1.29256200
H	0.05459000	-2.07566100	1.02176500
H	-1.03056300	-1.05159900	1.72892000
H	-3.09955900	2.19581300	-0.57111700
H	-0.34022400	-2.79832600	-2.27806400
H	2.31056300	2.64581300	-0.61714600
H	3.99341200	0.63273700	-2.09029800
H	1.66182400	3.79071100	1.20360700
H	1.51107400	3.69261500	-1.41281000
H	-4.05484700	0.10139800	0.01208100
H	-2.36849800	1.01850100	-1.19776900
H	0.19440700	-3.71529800	-1.11170300
H	1.15140100	-1.89184100	-1.28170700
H	1.73983300	-3.53355900	1.09674700
H	0.51138300	-4.16861600	1.83134200
H	0.67234000	2.85311600	1.94025200
H	-4.05495000	-1.90683300	-0.70421100
H	-3.87652200	-0.74240800	1.30251100
H	-2.37117800	-1.89450600	-2.33545500
H	-4.68505700	-2.43861300	-2.01311300
H	3.76767400	-3.47961700	0.15711300
H	3.64629100	-2.25002300	1.07222100
H	-1.28332700	2.70199100	0.65876900
H	-1.04678500	1.10129200	1.92848000
O	4.08402500	-0.49293900	0.94691300
H	4.34397900	-0.28787900	-0.90634300
H	4.61617600	-0.09799400	1.64399600
H	-0.89252600	3.67991700	-1.28253200
O	-0.30605500	3.57513900	-2.06994200
H	-0.80680500	3.88286500	-2.83032700
Cl	-2.33453500	-0.60370400	3.02425700
H	3.26547800	0.10361800	0.83223000

{[*trans*-Al(OH)$_3$(H$_2$O)Cl]·(H$_2$O)$_{14}$}$^-$ (I)

Al	0.05377100	-0.05458900	-0.09760800
O	-2.49895500	1.17109800	-2.61239800
O	1.43304700	-0.34198500	1.02119500
O	1.31883000	0.86717800	-1.39471400
O	-0.25518100	-1.34945100	-1.26617600
O	-0.96398300	1.42213600	-0.24941300
O	-4.42088800	0.61220700	0.95147100
O	-0.98203400	-4.04663900	0.80131400
O	3.94916600	3.19942200	0.91793200
O	-3.05299100	3.28750900	1.25535900
O	1.73254400	-3.24757700	0.65800300
O	3.96237400	0.55397400	0.75171200
O	3.65827700	-0.56406500	-1.92431300
O	1.99550800	3.56005100	-0.89611700
O	-2.36083100	-3.10909700	-1.46047400
O	3.44005200	-3.15849400	-1.34953900

O	-0.95097500	4.08844100	-0.42097300
O	-4.33583500	-0.88012300	-1.60234700
H	-2.87474500	2.04976000	-2.72062100
H	-1.91892000	1.24727500	-1.82474800
H	1.24969600	-0.45754600	1.96691200
H	2.15133300	0.39048000	-1.59927700
H	1.52761800	1.81297200	-1.23812300
H	-1.61919500	-2.46606200	-1.43500700
H	-0.05672200	-1.12859200	-2.17887300
H	-0.04026000	4.40488900	-0.38300400
H	-1.67120400	1.45020800	0.40526000
H	-4.10310100	1.52871400	0.94764800
H	-3.67710800	0.09956200	1.30701200
H	4.00721500	2.20174900	0.89702700
H	3.80010400	3.43240500	1.83883100
H	0.81481900	-3.59683000	0.59336200
H	1.63320800	-2.28423000	0.77838000
H	-1.52339500	-3.94135500	-0.01074400
H	-1.25020400	-3.26611200	1.30909100
H	-2.36809000	3.76478100	0.74329100
H	-2.79214400	3.37670700	2.17661000
H	4.18389400	0.22216400	-0.13086300
H	3.03517900	0.22357700	0.90198300
H	3.58319100	-1.53928300	-1.71971400
H	4.00999900	-0.50921600	-2.81762200
H	-3.15107700	-2.54123600	-1.43182000
H	-0.83649800	3.10757100	-0.47133800
H	2.70180500	3.51191200	-0.20147900
H	2.38693100	4.03225900	-1.63722100
H	2.71741800	-3.26990800	-0.66316500
H	4.21163600	-3.57584400	-0.95531400
H	-4.51564000	-0.41729700	-0.76593400
H	-3.75013800	-0.26328100	-2.07474800
Cl	-1.54044600	-0.87674000	1.64375000
O	0.69581400	-0.75557900	3.84998400
H	-0.18276400	-0.78153900	3.42577700
H	0.89421100	-1.67646900	4.04953400

{[*trans*-Al(OH)$_3$(H$_2$O)$_2$]·(H$_2$O)$_{13}$Cl }$^-$ (O)

Al	0.40761000	0.35070100	-0.00281500
O	1.62104100	1.65090900	0.25790400
O	-0.82928500	0.34301300	-1.32300400
O	1.75730800	-0.47702200	-1.25718600
O	0.37012500	-1.12366700	0.99368800
O	-3.01455300	2.61842900	-0.10231400
O	0.98992000	4.11396700	-1.10199100
O	-1.17867100	-2.26466200	-2.36254300
O	-3.63286300	0.30621900	-0.98794700
O	4.47439900	-0.10951900	-1.36728200
O	1.48315600	-3.22635400	-1.61690000
O	1.90871200	-3.11842900	1.01391700
O	-3.24467500	-3.57474800	-1.10473100
O	0.54658700	4.02216600	1.74897100
O	4.44737400	-1.85687300	1.25242000

O	-4.17626500	-1.65866200	0.78936300
O	-0.89945400	1.32032000	1.25650000
H	-3.65962300	3.09784200	0.42525200
H	1.38566200	2.29029600	0.94761600
H	-1.06032100	-1.33727600	-2.06205800
H	-0.79370600	1.06037300	-1.96736100
H	2.71200300	-0.24810600	-1.31531300
H	1.66830800	-1.41686100	-1.51055200
H	1.27397100	-2.29904400	1.06899200
H	-0.32862900	-1.18488700	1.67349100
H	-3.43159300	1.73794700	-0.39605900
H	-0.33706900	-2.70158300	-2.16033100
H	1.38418900	3.24543200	-0.90080000
H	4.89348600	0.40737700	-2.06093400
H	0.56386900	4.27899200	0.80826900
H	0.19963800	3.90660900	-1.62774500
H	-3.90574100	-0.38636100	-0.33154400
H	-2.68062900	0.14018100	-1.15236300
H	1.64453600	-3.39385500	-0.65191800
H	2.09741900	-3.77610400	-2.11106500
H	3.59670500	-2.33772100	1.25292200
H	1.59508500	-3.74501200	1.67344100
H	-0.17238900	3.38267200	1.82997200
H	-3.81726100	-2.43249800	0.31577400
H	-3.58286700	-1.49746100	1.55109200
H	-2.49425100	-3.10943500	-1.54430900
H	-3.94012500	-3.59258800	-1.76851100
H	4.67638900	-1.76386900	0.31954500
H	4.18869200	0.17769300	1.44377700
H	-1.65343300	1.75409600	0.80437300
H	-1.30506200	0.71069400	1.94800500
O	4.20834800	1.02283300	0.96273800
H	4.52674000	0.43296100	-0.52411500
H	3.26590800	1.28031500	0.81741500
H	-2.08338400	3.11817600	-1.55171800
O	-1.44991400	3.18803700	-2.29887100
H	-1.96473100	3.45304000	-3.06589000
Cl	-2.04770900	-0.77757800	3.04925800

{[$Al(OH)_4$]·$(H_2O)_{14}Cl$ }$^{2-}$ (I)

Al	-1.57321600	1.10947800	0.10010700
O	-0.13832800	0.09295800	-0.30326800
O	-1.11546000	2.54008200	1.05804600
O	-2.21940900	1.60319500	-1.48795900
O	-2.79288300	0.19138200	1.01812600
O	1.74585300	-1.26159900	1.40139500
O	-0.40061000	-1.96369500	-2.05096400
O	2.48836000	1.14084200	2.48716500
O	-0.25244500	-2.82924600	2.34123400
O	1.74152700	1.10859600	-1.95173100
O	2.80818300	2.69545400	0.16958300
O	-1.55807500	-3.65246700	-0.08017200
O	2.29947900	-1.50619900	-2.84361000
O	0.52642900	4.28334700	-0.23560700

O	-0.05639200	1.58377400	3.62354600
O	-2.91134000	-0.74836100	-2.73526100
O	0.01510800	3.06802100	-2.79596400
O	-1.68296500	-0.58562600	3.36439600
O	-3.85575700	-2.04467500	-0.52368900
H	0.41370800	-0.33292900	0.37667200
H	-0.76226200	2.36861700	1.94517600
H	-1.61297000	2.12838000	-2.03312100
H	-3.21897100	-0.56515300	0.58515000
H	2.12703400	-0.45773200	1.82810700
H	2.44879000	-1.66009800	0.84271600
H	-0.31694700	-1.20524000	-1.41701800
H	-0.69765700	-2.69675800	-1.47328000
H	2.58150600	1.72894100	1.70507500
H	1.64118400	1.38034200	2.91264300
H	1.05095900	0.75970200	-1.32874100
H	2.07766600	0.29619700	-2.38623400
H	-1.14402300	-3.40149800	0.76831100
H	-2.40914300	-3.17519500	-0.11621000
H	0.55232200	-2.33062700	2.05973800
H	0.05978000	-3.53817000	2.92921900
H	2.64709300	2.08610600	-0.57674100
H	2.07415700	3.34311000	0.08430300
H	1.39522800	-1.81670300	-2.63781500
H	2.85426300	-1.86287900	-2.11912800
H	-0.10095400	3.69983800	0.26170000
H	0.34893100	4.07501300	-1.17039000
H	-2.70602700	0.14998300	-2.37442900
H	-2.05051600	-1.21033900	-2.72028500
H	-2.16521400	-0.32789600	2.53644700
H	-1.21503800	-1.40812400	3.12412800
H	-0.61380900	0.76492400	3.63264000
H	-0.18143600	2.01301900	4.48606000
H	0.05350500	3.40650200	-3.70573300
H	0.70584100	2.37124000	-2.72458200
H	-3.66861800	-1.61243000	-1.39290300
H	-4.78005600	-2.34284400	-0.54893300
Cl	3.99607600	-2.63392900	-0.37035600