

Fig. S1. Wireframe model of the minimum energy structure of $[\text{Al}_2\text{O}_6\text{H}_9\text{Cl}_2]^{1+}$ and $[\text{Al}_2\text{O}_4\text{H}_4\text{Cl}]^{1+}$.

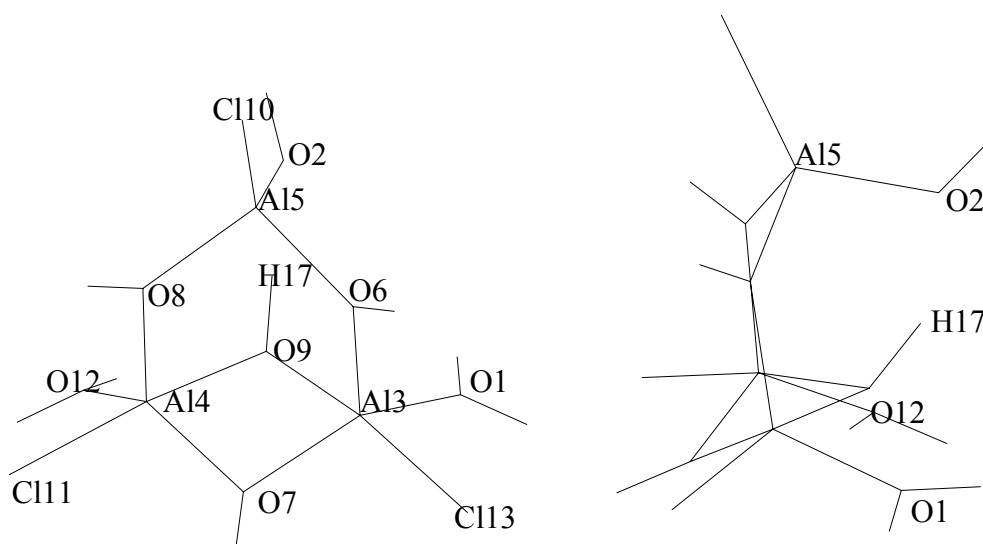


Fig. S2. Wireframe model of the minimum energy structure of $[\text{Al}_3\text{O}_7\text{H}_9\text{Cl}_3]^{1+}$ from two different angles.

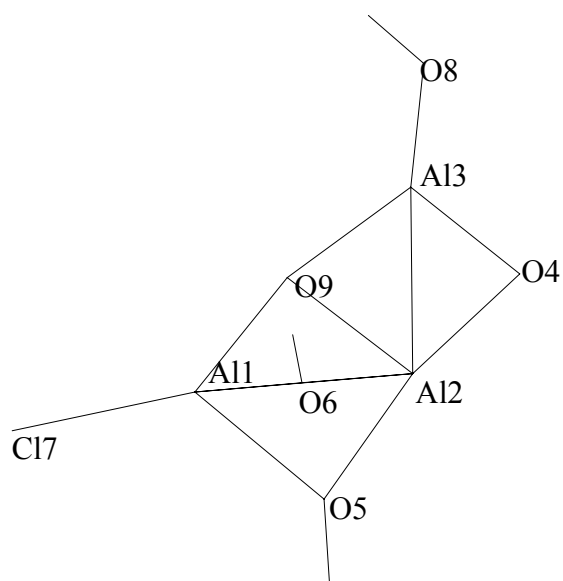


Fig. S3. Wireframe model of the minimum energy structure of [Al₃O₅H₃Cl]¹⁺.

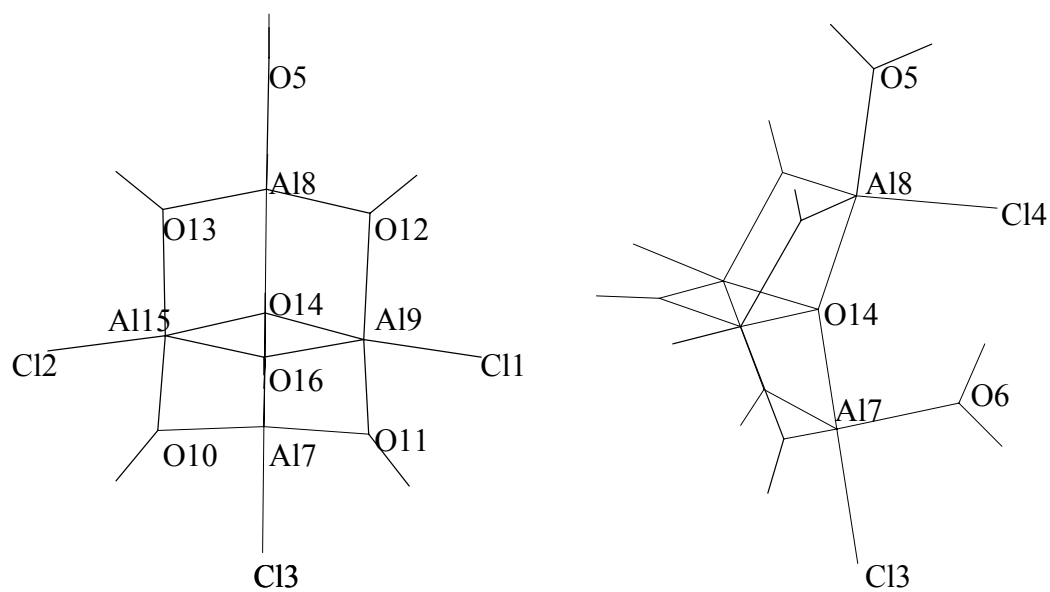


Fig. S4. Wireframe model of the minimum energy structure of [Al₄O₈H₉Cl₄]¹⁺ from two different angles.

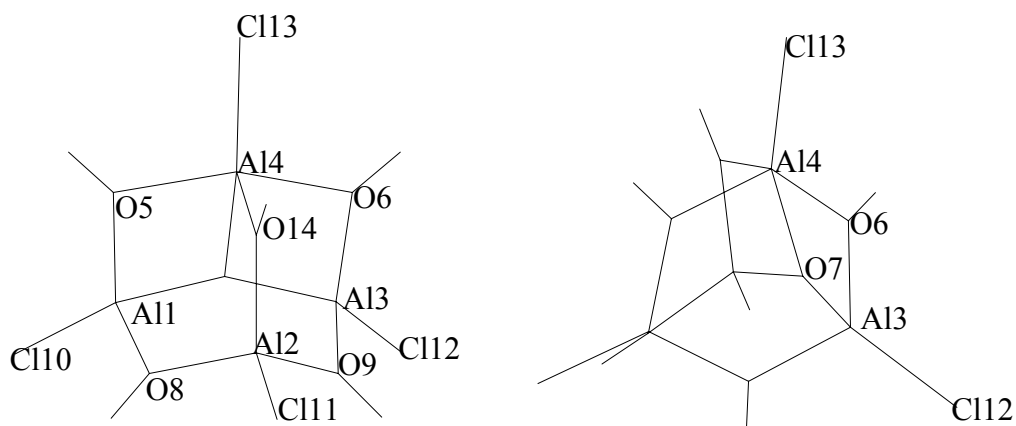


Fig. S5. Wireframe model of the minimum energy structure of $[\text{Al}_4\text{O}_6\text{H}_5\text{Cl}_4]^{1+}$ from two different angles.

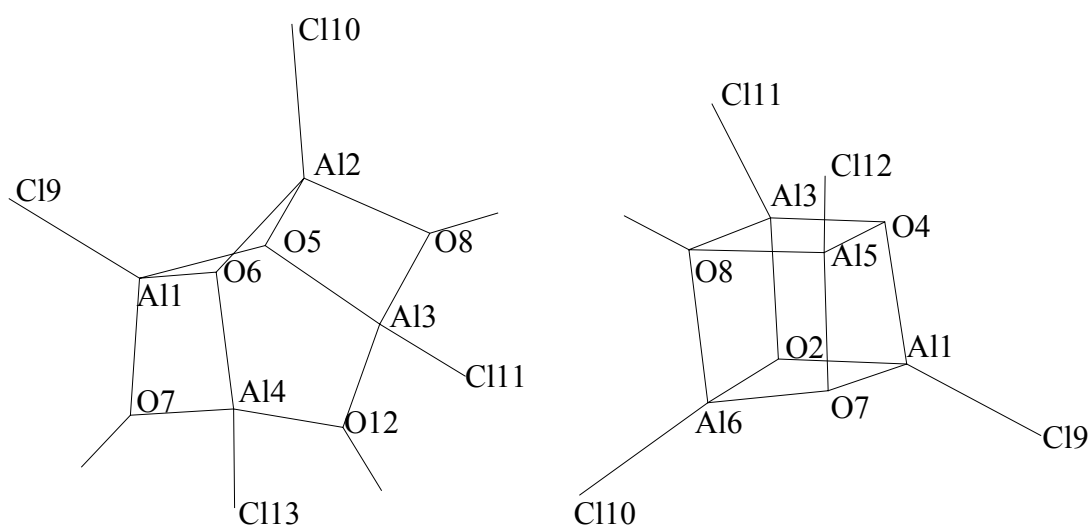


Fig. S6. Wireframe model of the minimum energy structures of $[\text{Al}_4\text{O}_5\text{H}_3\text{Cl}_4]^{1+}$ and $[\text{Al}_4\text{O}_4\text{HCl}_4]^{1+}$.

Table S1. Geometrical properties of minimum energy structures shown in Fig. S1-S6.

$[\text{Al}_2\text{O}_6\text{H}_9\text{Cl}_2]^{1+}$		$[\text{Al}_2\text{O}_4\text{H}_4\text{Cl}]^{1+}$		$[\text{Al}_3\text{O}_7\text{H}_9\text{Cl}_3]^{1+}$		$[\text{Al}_3\text{O}_5\text{H}_3\text{Cl}]^{1+}$		$[\text{Al}_4\text{O}_8\text{H}_9\text{Cl}_4]^{1+}$		$[\text{Al}_4\text{O}_6\text{H}_5\text{Cl}_4]^{1+}$		$[\text{Al}_4\text{O}_5\text{H}_3\text{Cl}_4]^{1+}$		$[\text{Al}_4\text{O}_4\text{HCl}_4]^{1+}$	
Bond	length	Bond	length	Bond	length	Bond	length	Bond	length	Bond	length	Bond	length	Bond	length
R _{Al1-07}	1.96	R _{Al1-C17}	2.06	R _{Al3-07}	1.86	R _{Al1-C17}	2.06	R _{Al8-O12}	1.84	R _{Al1-05}	1.82	R _{Al1-05}	1.83	R _{Al1-02}	1.89
R _{Al1-C19}	2.17	R _{Al1-05}	1.87	R _{Al3-09}	1.90	R _{Al1-05}	1.92	R _{Al8-O13}	1.84	R _{Al1-07}	1.79	R _{Al1-06}	1.92	R _{Al1-04}	1.89
R _{Al1-05}	1.81	R _{Al1-04}	1.88	R _{Al3-01}	1.95	R _{Al1-06}	1.96	R _{Al8-O14}	1.86	R _{Al1-08}	1.88	R _{Al1-07}	1.83	R _{Al1-07}	1.89
R _{Al1-010}	1.87	R _{Al1-03}	1.87	R _{Al3-C113}	2.17	R _{Al1-09}	1.79	R _{Al8-O5}	2.01	R _{Al1-C110}	2.08	R _{Al1-C19}	2.07	R _{Al1-C19}	2.06
R _{Al1-03}	1.95	R _{Al2-05}	1.88	R _{Al3-06}	1.86	R _{Al2-05}	1.85	R _{Al8-C14}	2.18	R _{Al2-08}	1.85	R _{Al2-05}	1.93	R _{Al3-02}	1.84
R _{Al2-06}	1.95	R _{Al2-04}	1.88	R _{Al4-07}	1.85	R _{Al2-06}	1.84	R _{Al7-06}	1.92	R _{Al2-09}	1.85	R _{Al2-06}	1.83	R _{Al3-04}	1.84
R _{Al2-03}	1.92	R _{Al2-03}	1.88	R _{Al4-09}	1.91	R _{Al2-09}	1.98	R _{Al7-010}	1.87	R _{Al2-014}	1.82	R _{Al2-08}	1.83	R _{Al3-08}	2.03
R _{Al2-010}	1.85	R _{Al2-06}	1.66	R _{Al4-012}	1.94	R _{Al2-04}	1.71	R _{Al7-011}	1.87	R _{Al2-C111}	2.09	R _{Al2-C110}	2.07	R _{Al3-C111}	2.06
R _{Al2-C18}	2.17	-	-	R _{Al4-C111}	2.17	R _{Al3-04}	1.76	R _{Al7-014}	1.92	R _{Al3-06}	1.82	R _{Al3-05}	1.81	R _{Al5-04}	1.84
R _{Al2-04}	1.87	-	-	R _{Al4-08}	1.86	R _{Al3-09}	1.79	R _{Al7-C13}	2.16	R _{Al3-07}	1.79	R _{Al3-08}	1.86	R _{Al5-07}	1.84
-	-	-	-	R _{Al5-06}	1.85	R _{Al3-08}	1.67	R _{Al9-011}	1.87	R _{Al3-09}	1.87	R _{Al3-012}	1.87	R _{Al5-08}	2.03
-	-	-	-	R _{Al5-08}	1.86	-	-	R _{Al9-012}	1.91	R _{Al3-C112}	2.08	R _{Al3-C111}	2.07	R _{Al5-C112}	2.06
-	-	-	-	R _{Al5-C110}	2.10	-	-	R _{Al9-014}	1.99	R _{Al4-05}	1.94	R _{Al4-06}	1.81	R _{Al6-02}	1.84
-	-	-	-	R _{Al5-02}	1.75	-	-	R _{Al9-016}	1.87	R _{Al4-06}	1.94	R _{Al4-07}	1.86	R _{Al6-07}	1.84
-	-	-	-	R _{H17-02}	1.68	-	-	R _{Al9-C11}	2.14	R _{Al4-07}	1.93	R _{Al4-012}	1.87	R _{Al6-08}	2.03
-	-	-	-	-	-	-	-	R _{Al15-010}	1.87	R _{Al4-014}	1.91	R _{Al4-C113}	2.07	R _{Al6-C110}	2.06
-	-	-	-	-	-	-	-	R _{Al15-013}	1.91	R _{Al4-C113}	2.12	-	-	-	-
-	-	-	-	-	-	-	-	R _{Al15-014}	1.99	-	-	-	-	-	-
-	-	-	-	-	-	-	-	R _{Al15-016}	1.87	-	-	-	-	-	-
-	-	-	-	-	-	-	-	R _{Al15-C12}	2.14	-	-	-	-	-	-