

Table 1.

Summaries of bond lengths R (Å) and bond angles A (deg.), and ranges of vibrational frequencies (cm⁻¹), together with normal mode symmetries and the number of vibrations in each group, for the AlO(OH) + 2 H₂O system:

AlO(OH)			
C _s	R(Al=O): 1.611	R(O-H): 0.955	A(O=Al-O): 177.9
(M)	R(Al-O): 1.677		A(Al-O-H): 139.2
	A' + A'' (4+1 vib.): 225–1172		A' (1 vib.): 3980
C _s	R(Al=O): 1.601	R(O-H): 0.956	A(O=Al-O): 177.4
(L)	R(Al-O): 1.671		A(Al-O-H): 135.3
	A' + A'' (4+1 vib.): 218–1170		A' (1 vib.): 3965
C _s	R(Al=O): 1.601	R(O-H): 0.955	A(O=Al-O): 177.2
(XL)	R(Al-O): 1.672		A(Al-O-H): 134.0
	A' + A'' (4+1 vib.): 207–1168		A' (1 vib.): 3958
Min. M	80 b.f.	E = -393.590173134	ZPE = 0.015479
Min. L	97 b.f.	E = -393.602188527	ZPE = 0.015469
Min. XL	142 b.f.	E = -393.607281861	ZPE = 0.015448
AlO(OH)·H₂O			
C _s	R(Al=O): 1.622	A(Al-O-H): 126.7	A(O=Al-O): 159.9
(M)	R(Al-O): 1.717	A(Al···O-H): 117.2–129.0	A(O=Al···O): 108.2
	R(Al···O): 1.944	A(H-O-H): 112.9	A(O-Al···O): 92.7
	R(O-H): 0.957–0.966		
	A' + A'' (8+4 vib.): 110–1576		A' (3 vib.): 3771–3946
C ₁	R(Al=O): 1.611	A(Al-O-H): 125.9	A(O=Al-O): 158.0
(L)	R(Al-O): 1.704	A(Al···O-H): 113.0–130.0	A(O=Al···O): 106.2
	R(Al···O): 1.925	A(H-O-H): 112.6	A(O-Al···O): 95.0
	R(O-H): 0.957–0.967		
	A (12 vib.): 94–1573		A (3 vib.): 3756–3944

C_1 R(Al=O): 1.612 A(Al-O-H): 125.3 A(O=Al-O): 158.2
 (XL) R(Al-O): 1.702 A(Al...O-H): 106.0-128.6 A(O=Al...O): 104.7
 R(Al...O): 1.931 A(H-O-H): 111.8 A(O-Al...O): 97.3
 R(O-H): 0.956-0.969

A (12 vib.): 80-1560

A (3 vib.): 3720-3936

Min. M 114 b.f. E = -470.090643990 ZPE = 0.041569
 Min. L 131 b.f. E = -470.104241123 ZPE = 0.041482
 Min. XL 215 b.f. E = -470.113694172 ZPE = 0.041569

Al(OH)₃

C_{3h} R(Al-O): 1.706 A(O-Al-O): 120.0

(M) R(O-H): 0.958 A(Al-O-H): 125.2

A' + A'' + E' + E'' (2+2+3+1 vib.): 218-924 A' + E' (1+1 vib.): 3939-3941

C_{3h} R(Al-O): 1.693 A(O-Al-O): 120.0

(L) R(O-H): 0.958 A(Al-O-H): 124.6

A' + A'' + E' + E'' (2+2+3+1 vib.): 224-931 A' + E' (1+1 vib.): 3939-3941

C_{3h} R(Al-O): 1.694 A(O-Al-O): 120.0

(XL) R(O-H): 0.956 A(Al-O-H): 124.5

A' + A'' + E' + E'' (2+2+3+1 vib.): 227-931 A' + E' (1+1 vib.): 3936-3947

Min. M 114 b.f. E = -470.186162515 ZPE = 0.041138
 Min. L 131 b.f. E = -470.203121938 ZPE = 0.041160
 Min. XL 215 b.f. E = -470.214648710 ZPE = 0.041168

AlO(OH)·2 H₂O

C_1 R(Al=O): 1.621 A(Al-O-H): 120.6 A(O=Al-O): 149.1

(M) R(Al-O): 1.755 A(Al-O...H): 114.9 A(O=Al...O): 118.8

R(Al...O): 1.896 A(Al...O-H): 120.4-122.8 A(O-Al...O): 92.1

R(O-H): 0.960-1.010 A(H-O-H): 107.8-115.4 A(O-H...O): 145.7-153.7

R(O...H): 1.596-1.819 A(H-O...H): 92.8-124.7

A (17 vib.): 54-1100 A (3 vib.): 1605-2984 A (4 vib.): 3469-3910

Min. M 148 b.f. E = -546.577171067 ZPE = 0.067889

Al(OH)₃·H₂O

C ₁	R(Al–O): 1.699–1.726	A(Al–O–H): 116.7–124.2	A(O–Al–O): 117.2–124.8
(1-M)	R(O–H): 0.957–0.973	A(Al–O···H): 103.3	A(O–H···O): 140.0–146.4
	R(O···H): 1.951–2.113	A(H–O–H): 106.6	A(H–O···H): 96.0–134.4
	A (18 vib.): 53–961	A (1 vib.): 1628	A (5 vib.): 3658–3944
C ₁	R(Al–O): 1.687–1.713	A(Al–O–H): 116.6–125.2	A(O–Al–O): 117.4–124.5
(1-L)	R(O–H): 0.958–0.972	A(Al–O···H): 103.0	A(O–H···O): 141.0–146.5
	R(O···H): 1.974–2.107	A(H–O–H): 106.5	A(H–O···H): 95.0–133.8
	A (18 vib.): 53–966	A (1 vib.): 1626	A (5 vib.): 3669–3942
C ₁	R(Al–O): 1.726–1.743	A(Al–O–H): 123.0–128.4	A(O–Al–O): 114.3–120.6
(2-M)	R(Al···O): 1.988	A(Al···O–H): 105.0–107.9	A(O–Al···O): 87.5–112.3
	R(O–H): 0.955–0.970	A(H–O–H): 108.4	
	A (18 vib.): 107–866	A (1 vib.): 1620	A (5 vib.): 3738–3968
C ₁	R(Al–O): 1.713–1.730	A(Al–O–H): 122.6–128.5	A(O–Al–O): 114.0–120.5
(2-L)	R(Al···O): 1.973	A(Al···O–H): 105.7–107.5	A(O–Al···O): 88.2–111.6
	R(O–H): 0.956–0.970	A(H–O–H): 108.4	
	A (18 vib.): 108–871	A (1 vib.): 1616	A (5 vib.): 3740–3964
Min. 1-M	148 b.f.	E = -546.658301057	ZPE = 0.066391
Min. 2-M	148 b.f.	E = -546.676546070	ZPE = 0.066521
Min. 1-L	165 b.f.	E = -546.674605541	ZPE = 0.066306
Min. 2-L	165 b.f.	E = -546.693330224	ZPE = 0.066493

Al(OH)₃·2 H₂O

C ₁	R(Al–O): 1.761–1.766	A(Al–O–H): 121.4–123.4	A(O–Al–O): 117.3–124.4
(1-M)	R(Al···O): 2.093–2.097	A(Al–O···H): 76.8–77.6	A(O–Al···O): 80.3–98.8
	R(O–H): 0.956–0.974	A(Al···O–H): 95.2–109.8	A(O···Al···O): 175.8
	R(O···H): 2.039–2.120	A(H–O–H): 107.5–108.2	A(H–O···H): 157.0–158.4
			A(O–H···O): 103.5–106.8
	A (24 vib.): 106–849	A (2 vib.): 1608–1634	A (7 vib.): 3679–3951

C_1 R(Al–O): 1.728–1.776 A(Al–O–H): 121.7–125.6 A(O–Al–O): 114.5–119.0
 (2-M) R(Al···O): 1.933 A(Al–O···H): 113.9 A(O–Al···O): 94.0–113.6
 R(O–H): 0.956–1.006 A(Al···O–H): 109.6–113.9 A(H–O···H): 90.2–124.3
 R(O···H): 1.630–1.730 A(H–O–H): 107.4–109.8 A(O–H···O): 150.0–157.6
 A (24 vib.): 46–1084 A (2 vib.): 1630–1693 A (7 vib.): 3048–3952

Min. 1-M 182 b.f. E = -623.153107181 ZPE = 0.092523
 Min. 2-M 182 b.f. E = -623.162977429 ZPE = 0.092332

Al(OH)₃·3 H₂O

C_1 (1-M) R(Al–O): 1.752–1.802 R(Al···O): 2.014–2.150
 C_1 (2-M) R(Al–O): 1.732–1.777 R(Al···O): 1.909
 C_1 (3-M) R(Al–O): 1.727–1.766 R(Al···O): 1.914
 C_1 (4-M) R(Al–O): 1.728–1.773 R(Al···O): 1.898
 Min. 1-M 216 b.f. E = -699.637331711 ZPE = 0.118782
 Min. 2-M 216 b.f. E = -699.642429553 ZPE = 0.116989
 Min. 3-M 216 b.f. E = -699.643829846 ZPE = 0.117876
 Min. 4-M 216 b.f. E = -699.647314357 ZPE = 0.118260

Al(OH)₃·4 H₂O

C_1 (1-M) R(Al–O): 1.766–1.799 R(Al···O): 1.966–2.196
 C_1 (2-M) R(Al–O): 1.770–1.829 R(Al···O): 1.935–2.112
 C_1 (3-M) R(Al–O): 1.771–1.785 R(Al···O): 2.035–2.062
 C_1 (4-M) R(Al–O): 1.754–1.768 R(Al···O): 1.893
 C_1 (5-M) R(Al–O): 1.732–1.769 R(Al···O): 1.876
 Min. 1-M 250 b.f. E = -776.120468721 ZPE = 0.144749
 Min. 2-M 250 b.f. E = -776.118149665 ZPE = 0.144772
 Min. 3-M 250 b.f. E = -776.121904919 ZPE = 0.144407
 Min. 4-M 250 b.f. E = -776.123133493 ZPE = 0.144163
 Min. 5-M 250 b.f. E = -776.125739153 ZPE = 0.142411

Al(OH)₃·5 H₂O

C ₁	(1-M)	R(Al–O): 1.789–1.843	R(Al···O): 1.939–2.037
C ₁	(2-M)	R(Al–O): 1.765–1.831	R(Al···O): 1.994–2.086
C ₁	(3-M)	R(Al–O): 1.784–1.792	R(Al···O): 1.976–2.113
C ₁	(4-M)	R(Al–O): 1.763–1.823	
C ₁	(5-M)	R(Al–O): 1.764–1.767	R(Al···O): 1.844
Min. 1-M	284 b.f.	E = -852.598067278	ZPE = 0.170318
Min. 2-M	284 b.f.	E = -852.600020003	ZPE = 0.171050
Min. 3-M	284 b.f.	E = -852.602177580	ZPE = 0.170068
Min. 4-M	284 b.f.	E = -852.600434619	ZPE = 0.167147
Min. 5-M	284 b.f.	E = -852.606911834	ZPE = 0.168756

Al(OH)₃·6 H₂O

C ₁	(1-M)	R(Al–O): 1.824–1.881	R(Al···O): 1.976–2.107
C ₁	(2-M)	R(Al–O): 1.831–1.834	R(Al···O): 2.068–2.077
C ₁	(3-M)	R(Al–O): 1.826–1.852	R(Al···O): 2.026–2.122
C ₁	(4-M)	R(Al–O): 1.752–1.848	
C ₁	(5-M)	R(Al–O): 1.757–1.829	
C ₁	(6-M)	R(Al–O): 1.766–1.839	
Min. 1-M	318 b.f.	E = -929.060247467	ZPE = 0.196325
Min. 2-M	318 b.f.	E = -929.066304583	ZPE = 0.196050
Min. 3-M	318 b.f.	E = -929.068618501	ZPE = 0.196277
Min. 4-M	318 b.f.	E = -929.078335810	ZPE = 0.194097
Min. 5-M	318 b.f.	E = -929.077051556	ZPE = 0.192450
Min. 6-M	318 b.f.	E = -929.085641007	ZPE = 0.193892

Table 2.

Summaries of bond lengths R (Å) and bond angles A (deg.), and ranges of vibrational frequencies (cm⁻¹), together with normal mode symmetries and the number of vibrations in each group, for the Al₂O₃ + H₂O systems:

AlO₃Al			
D _{3h}	R(Al–O): 1.818	R(O–O): 2.590	A(Al–O–Al): 69.3
(M)	R(Al–Al): 2.068		A(O–Al–O): 90.8
	A ₁ ' + A ₂ ' + E' + E'' (2+1+2+1 vib.): 327–783		
D _{3h}	R(Al–O): 1.797	R(O–O): 2.560	A(Al–O–Al): 69.3
(L)	R(Al–Al): 2.043		A(O–Al–O): 90.9
	A ₁ ' + A ₂ ' + E' + E'' (2+1+2+1 vib.): 344–798		
D _{3h}	R(Al–O): 1.797	R(O–O): 2.560	A(Al–O–Al): 69.3
(XL)	R(Al–Al): 2.043		A(O–Al–O): 90.9
	A ₁ ' + A ₂ ' + E' + E'' (2+1+2+1 vib.): 345–797		
Min. M	126 b.f.	E = -710.652815913	ZPE = 0.010784
Min. L	160 b.f.	E = -710.683449315	ZPE = 0.011184
Min. XL	211 b.f.	E = -710.690846898	ZPE = 0.011166
OAlOAlO			
D _{∞h}	R(Al=O): 1.610	A(Al–O–Al): 180.0	
(M)	R(Al–O): 1.687	A(O=Al–O): 180.0	
	sg _{g/u} + pi _{g/u} (1+3 vib.): 73–421		sg _{g/u} (3 vib.): 929–1234
D _{∞h}	R(Al=O): 1.599	A(Al–O–Al): 180.0	
(L)	R(Al–O): 1.678	A(O=Al–O): 180.0	
	sg _{g/u} + pi _{g/u} (1+3 vib.): 60–422		sg _{g/u} (3 vib.): 932–1230
D _{∞h}	R(Al=O): 1.599	A(Al–O–Al): 180.0	
(XL)	R(Al–O): 1.676	A(O=Al–O): 180.0	
	sg _{g/u} + pi _{g/u} (1+3 vib.): 58–421		sg _{g/u} (3 vib.): 931–1228
Min. M	126 b.f.	E = -710.733215140	ZPE = 0.011144
Min. L	160 b.f.	E = -710.754933076	ZPE = 0.010897
Min. XL	211 b.f.	E = -710.759372940	ZPE = 0.010760
OAlOAl(OH)₂			
C _{2v}	R(Al=O): 1.612	R(O–H): 0.956	A(Al–O–Al): 180.0
(1-M)	R(Al–O): 1.673–1.714	A(Al–O–H): 127.5	A(O=Al–O): 180.0

A(O–Al–O): 117.0–121.5

$A_1 + A_2 + B_1 + B_2$ (6+1+4+5 vib.): 55–1210 $A_1 + B_2$ (1+1 vib.): 3956–3957

C_s R(Al=O): 1.612 R(O–H): 0.957–0.958 A(Al–O–Al): 172.8

(2-M) R(Al–O): 1.673–1.707 A(Al–O–H): A(O=Al–O): 178.4

125.4–128.0 A(O–Al–O): 117.0–122.4

$A' + A''$ (11+5 vib.): 48–1213 A' (2 vib.): 3941–3949

Min. 1-M 160 b.f. E = -787.328788860 ZPE = 0.035315

Min. 2-M 160 b.f. E = -787.330940700 ZPE = 0.035479

(HO)AlO₂Al(OH)

C_{2v} R(Al–O): 1.691–1.756 A(Al–O–H): 128.9 A(Al–O–Al): 86.9–87.2

(1-M) R(O–H): 0.960 A(O–Al–O): 93.0–135.1

$A_1 + A_2 + B_1 + B_2$ (6+2+3+5 vib.): 95–1002 $A_1 + B_2$ (1+1 vib.): 3957–3958

C_{2h} R(Al–O): 1.691–1.755 A(Al–O–H): 128.7 A(Al–O–Al): 87.0

(2-M) R(O–H): 0.957 A(O–Al–O): 93.0–131.8

$A_g + A_u + B_g + B_u$ (6+3+2+5 vib.): 95–1001 $A_g + B_u$ (1+1 vib.): 3957

Min. 1-M 160 b.f. E = -787.393323062 ZPE = 0.036232

Min. 2-M 160 b.f. E = -787.393438626 ZPE = 0.036222

(HO)AlO(OH)₂Al(OH)

C_{2v} R(Al–O): 1.696–1.747 A(Al–O–H): 130.4 A(Al–O–Al): 84.4

(M) R(Al··O): 1.924 A(Al··O–H): 129.3 A(Al··O··Al): 75.5

R(O–H): 0.955–0.961 A(O··Al··O): 82.2 A(O–Al–O): 143.2

A(O–Al··O): 85.5–121.0

$A_1 + A_2 + B_1 + B_2$ (8+4+5+6 vib.): 93–991

$A_1 + B_1 + B_2$ (2+1+1 vib.): 3874–3973

Min. M 194 b.f. E = -863.912773482 ZPE = 0.060727

(HO)₂AlOAl(OH)₂

D_{2d} R(Al–O): 1.698–1.701 A(Al–O–H): 125.4 A(Al–O–Al): 180.0

(1-M) R(O–H): 0.957 A(O–Al–O): 115.2–122.4

$A_1 + A_2 + B_1 + B_2 + E$ (4+1+2+4+6 vib.): 9–1099

$A_1 + B_2 + E$ (1+1+1 vib.): 3953–3954

C_2 R(Al–O): 1.689–1.710 A(Al–O–H): A(Al–O–Al): 179.8

(2-M) R(O–H): 0.958 123.6–125.1 A(O–Al–O): 117.9–123.5

