Manuscript ID: CP-ART-01-2015-000390

Table S1 (electronic supplementary information, ESI)

Description of the 72 OH harmonic stretching vibrations as obtained from the full lattice dynamics calculation of crystalline $Al(NO_3)_3 \cdot 9H_2O$ (case **C**, see Fig. 3). For each normal vibration, the capital letter (H) is used to indicate the hydrogen atoms which are that main contributors while the small letter (h) indicates somewhat less contribution. Note, however, that all hydrogen atoms participate in all normal vibrations although with very small contribution in most cases.

Vibr #	Freq. (cm^{-1})	Symm. species	Description of normal vibration
1	3627	A_u	H91
2	3627	A_g	H91
3	3627	B_g	H91
4	3627	B_u	H91
5	3433	B_u	H82,h72
6	3429	A_u	H82,h92,h61,h72
7	3411	A_u	H92,H72,h82,h71
8	3409	A_g	H82
9	3409	B_u	H92,H72,h82
10	3407	B_g	H82,h92
11	3394	B_g	H92,H72,h82
12	3390	A_g	H92,H72,h71
13	3339	A_u	H72,H92
14	3339	A_g	H72,H92
15	3339	B_g	H72,H92,h21,h31
16	3335	B_u	H72,H92
17	3307	B_g	H61,H31
18	3306	B_u	H31,H61,h81,h82
19	3295	A_g	H31,h61,h72
20	3290	A_u	H31,H61,h81,h82
21	3281	A_g	H61,h31
22	3280	B_g	H31,H61
23	3263	B_u	H61,H31
24	3259	A_u	H61,H31
25	3230	A_u	H81,h31,h61,h51,h62
26	3226	B_u	H81,h61,h31,h71,h62
27	3225	B_g	H81,h62,h51
28	3224	A_g	H81,h62,h51
29	3213	B_u	H71,h81,h21,h32
30	3212	A_u	H71,H11,h21,h52
31	3206	B_g	H11,h52,h12
32	3195	A_u	H11,H71,h12,h92
33	3189	A_g	H11,h12,h52,h31
34	3180	B_u	H11,h12
35	3178	B_g	H71,h12,h21,h72
36	3174	A_g	H71,h21,h72,h32
37	3160	B_g	H12,h71,h22,h32,h11
38	3160	A_g	H52,H41,h42,h6,h11
39	3153	B_g	H41,h52,h11
40	3145	A_u	H41,h22,h52,h42,h12
41	3139	A_u	H12,H11,h41,h52
42	3133	B_u	H41,h42,h22
43	3130	B_u	H12,H52,h11
44	3127	A_g	H12,h41,h11
45	3127	B_g	H52,H42,h41,h12,h22
46	3117	A_g	H52,H41,h22,h12
47	3109	B_u	H52,H12
48	3108	A_u	H52,h12,h41
49	3077	B_g	H42,H52,h22,h41
50	3077	A_u	H42,h22,h41
51	3067	A_g	H22,h41,h21,h52,h12
52	3065	B_u	H22,h41,21
53	3047	B_g	H22,H42,h21,h12
54	3044	A_u	H22,H42,h21
55	3037	A_g	H42,h41,h21
56	3032	B_u	H42,h22,h41
57	3013	B_g	H21,h62,h71,h32,h22
58	3005	A_g	H21,h71,h22,h32,h42
59	3004	B_g	H62,h81,h21,h51
60	2993	A_g	H62,h81,h51,h42
61	2986	B_u	H62,h81,h51
62	2984	B_u	H21,h71,h22
63	2983	A_u	H21,h71,h22
64	2983	A_u	H62,h81,h51
65	2906	B_g	H32,h21,h22
66	2900	B_g	H51,h62
67	2882	A_u	H51,h62
68	2881	A_u	H32,h21
69	2880	B_u	H32,h21
70	2875	B_u	H51,h62
71	2874	A_g	H32,h21
72	2868	A_g	H51,h62,h32