Proofs to Professor D. O'Hare, address given below:

Preferential Anion Exchange Intercalation of Pyridinecarboxylates and Toluates Isomers in the Layered Double Hydroxide $[LiAl_2(OH)_6]Cl{\cdot}H_2O$

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SUPPLEMENTARY DATA

Appendix: XRD patterns of the intercalation compounds:

Compound: $LiAl_2(OH)_6{\cdot}(2\text{-PA})\cdot 0.6Al(OH)_3{\cdot}2.5H_2O$

Cell: 5.0800 5.0800 30.2298 90.000 90.000 120.000
Space group: P63/M
Wavelength: 1.54180

N	h	k	l	2Thobs	2Thcalc	Dif	Iobs	Explanation
1	0	0	2	5.91	5.85	0.06	100.0	
2	0	0	4	11.72	11.71	0.01	89.1	
3	0	0	6	17.60	17.60	0.00	51.6	
4				18.27			34.7	Gibbsite
5	0	1	1	20.34	20.40	-0.06	10.1	
6	0	1	2	21.03	21.03	-0.01	12.9	
7	0	1	4	23.47	23.40	0.07	11.0	
8	0	1	6	26.88	26.90	-0.03	11.4	
9	0	0	12	35.61	35.64	-0.03	24.0	
10	1	1	5	38.40	38.44	-0.04	17.8	

Compound: $LiAl_2(OH)_6 \cdot (3\text{-PA}) \cdot 0.6Al(OH)_3 \cdot 3.5H_2O$
Cell: 5.0800 5.0800 30.9219 90.000 90.000 120.000
Space group: P63/M
Wavelength: 1.54180

N	h	k	l	2Thobs	2Thcalc	Dif	Iobs	Explanation
1	0	0	2	5.77	5.72	0.05	100.0	
2	0	0	4	11.49	11.45	0.04	39.8	
3	0	0	6	17.23	17.21	0.02	14.2	
4				18.34			2.2	Gibbsite
5	0	1	1	20.30	20.39	-0.09	2.2	
6	0	0	8	23.03	23.01	0.02	45.5	
7	0	0	10	28.82	28.87	-0.05	1.4	
8	0	0	12	34.80	34.82	-0.02	7.3	
9	1	1	0	35.39	35.34	0.05	2.2	
10	1	1	3	36.32	36.43	-0.11	3.2	
11	1	1	4	37.15	37.26	-0.11	0.6	
12	0	1	11	38.09	37.98	0.11	0.9	
13	1	1	5	38.36	38.31	0.05	4.3	

Compound: $LiAl_2(OH)_6 \cdot (4\text{-PA}) \cdot 0.2Al(OH)_3 \cdot 3H_2O$
Cell: 5.0800 5.0800 29.6700 90.000 90.000 120.000
Space group: P63/M
Wavelength: 1.54180

N	h	k	l	2Thobs	2Thcalc	Dif	Iobs
1	0	0	2	6.01	5.96	0.05	100.0
2	0	0	4	11.99	11.93	0.06	39.7
3	0	0	6	18.02	17.94	0.08	17.9
4	0	1	1	20.30	20.41	-0.11	2.7
5	0	0	8	24.08	23.99	0.09	41.8
6	1	1	3	36.46	36.52	-0.07	15.6
7	1	1	5	38.43	38.56	-0.13	5.8

Compound: $LiAl_2(OH)_6 \cdot (o\text{-TA}) \cdot 1.4Al(OH)_3 \cdot 2.5H_2O$
Cell: 5.0801 5.0801 31.5000 90.000 90.000 120.000
Space group: P63/M
Wavelength: 1.54180

N	h	k	l	2Thobs	2Thcalc	Dif	Iobs	Explanation
1	0	0	2	5.61	5.61	0.00	100.0	
2	0	0	4	11.22	11.24	-0.02	143.0	
3	0	0	6	16.88	16.89	-0.01	41.4	
4				18.29			79.7	Gibbsite
5	0	1	0	20.21	20.18	0.03	3.4	
6	0	0	8	22.59	22.58	0.01	68.2	
7	0	1	4	23.18	23.16	0.02	13.9	
8	0	0	10	28.26	28.33	-0.07	4.1	
9	1	1	2	35.70	35.81	-0.11	4.4	
10	1	1	4	37.25	37.19	0.06	22.0	

Compound: $LiAl_2(OH)_6 \cdot (m\text{-}TA) \cdot 0.25Al(OH)_3 \cdot 2.5H_2O$
Cell: 5.0800 5.0800 34.5000(Phase 1)/31.8155 (Phase 2) 90.000 90.000 120.000
Space group: P63/M
Wavelength: 1.54180

N	h	k	l	2Thobs	2Thcalc	Dif	Iobs	Explanation
1	0	0	2	5.11	5.12	-0.02	100.0	Phase 1
2	0	0	2	5.50	5.56	-0.05	28.9	Phase 2
3	0	0	4	10.23	10.26	-0.03	8.7	Phase 1
4	0	0	4	11.10	11.12	-0.02	16.6	Phase 2
5	0	0	6	15.38	15.41	-0.03	3.3	Phase 1
6	0	0	6	16.75	16.72	0.03	6.8	Phase 2
7				18.24			2.2	Gibbsite
8	0	1	0	20.16	20.18	-0.02	2.6	Phase 1&2
9	0	0	8	20.64	20.60	0.05	5.5	Phase 1
10	0	0	8	22.37	22.35	0.02	41.6	Phase 2
11	1	1	2	35.94	35.80	0.14	10.1	Phase 1&2
12	1	1	3	36.14	36.22	-0.08	6.2	Phase 1
13	1	1	5	38.21	38.15	0.06	8.6	Phase 1&2
14	1	1	6	38.65	38.76	-0.10	8.9	Phase 1

Compound: $LiAl_2(OH)_6 \cdot (p\text{-}TA) \cdot 0.37Al(OH)_3 \cdot 2.5H_2O$
Cell: 5.0839 5.0839 33.2708 90.000 90.000 120.000
Space group: P63/M
Wavelength: 1.54180

N	h	k	l	2Thobs	2Thcalc	Dif	Iobs
1	0	0	2	5.31	5.31	-0.01	100.0
2	0	0	4	10.62	10.64	-0.02	32.0
3	0	0	6	15.93	15.98	-0.06	8.3
4	0	1	1	20.31	20.35	-0.04	1.9
5	0	1	2	20.91	20.87	0.04	6.0
6	0	0	8	21.31	21.37	-0.06	25.3
7	0	0	10	26.70	26.80	-0.09	9.8
8	0	0	12	32.19	32.29	-0.10	1.2
9	1	1	1	35.43	35.42	0.01	0.6
10	1	1	3	36.23	36.26	-0.02	2.3
11	0	0	14	37.73	37.86	-0.12	6.7
12	0	1	12	38.24	38.37	-0.13	0.7
13	0	1	12	38.44	38.37	0.07	1.7