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New insights into the intercalation chemistry of $Al(OH)_3$: supporting information

Gareth R. Williams,[1,2]* Saul J. Moorhouse,[1] Timothy J. Prior,[3] Andrew M. Fogg,[4] Nicholas H. Rees,[1] and Dermot O'Hare[1]*

[1] Chemistry Research Laboratory, Department of Chemistry, University of Oxford, Mansfield Road, Oxford, OX1 3TA.

[2] School of Human Sciences, London Metropolitan University, 166-220 Holloway Road, London, N7 8DB.

[3] Department of Chemistry, University of Hull, Cottingham Road, Kingston upon Hull, HU6 7RX.

[4] Department of Chemistry, University of Liverpool, Crown Street, Liverpool, L69 7ZD

* authors for correspondence. Email address: g.williams@londonmet.ac.uk (GRW) dermot.ohare@chem.ox.ac.uk (DOH) Tel: +44 (0) 207 133 2565 (GRW) +44 (0) 1865 272686 (DOH). Fax: +44 (0) 207 133 4149 (GRW) +44 (0) 1865 272690 (DOH).

Table S1: Synthesis conditions for the three-metal LDHs.

M	M′	Volume M nitrate solution / mL	Volume M′ nitrate solution / mL	M : M′ ratio in LDH
Zn	Ni	5.0	5.0	1.00 : 39.4
Zn	Ni	8.5	1.5	1.00 : 6.26
Zn	Ni	9.0	1.0	1.00 : 1.98
Zn	Ni	9.2	0.8	1.00 : 2.38
Zn	Ni	9.5	0.5	1.00 : 0.80
Zn	Ni	9.7	0.3	1.00 : 0.70
Zn	Co	2.0	8.0	1.00 : 3.79
Zn	Co	4.0	6.0	1.00 : 1.46
Zn	Co	5.0	5.0	1.00 : 0.97
Zn	Co	6.0	4.0	1.00 : 0.70
Zn	Co	8.0	2.0	1.00 : 0.24
Co	Ni	5.0	5.0	1.00 : 35.6
Co	Ni	9.0	1.0	1.00 : 5.34

Table S2: Atomic coordinates and occupancies for $ZnAl_4$-NO_3.

Atom	Site	x	y	z	Occupancy	U_{iso}
Al1	4e	0.66048	0.00742	0.66981	0.8863	0
Zn2	4e	0.66049	0.00742	0.66981	0.1137	0
Al3	4e	0.34658	0.0038	0.82421	0.8863	0
Zn4	4e	0.34657	0.0038	0.8242	0.1137	0
Al5	2a	0	0	1	0.45481	0
Zn6	2a	0	0	1	0.54519	0
O7	4e	0.68114	0.06556	0.84139	1.0	0.06673
O8	4e	0.66879	-0.0574	0.8271	1.0	0.06556
O9	4e	0.35107	0.04988	0.99689	1.0	0.06556
O10	4e	0.51492	-0.06869	0.5103	1.0	0.06556
O11	4e	-0.00838	-0.05829	0.69094	1.0	0.06556
O12	4e	0.31865	0.06462	0.65543	1.0	0.06556
O13	4e	0.36515	0.33018	0.50704	1.0	0.16292
N14	4e	-0.00824	0.20425	0.49395	1.0	0.1446
O15	4e	-0.19721	0.24691	0.38374	1.0	0.1446
O16	4e	0.10874	0.23651	0.62413	1.0	0.1446

Table S3: Indexing of $[ZnAl_4(OH)_{24}](SO_4)\cdot yH_2O$

Monoclinic cell, a = 10.23 (1) Å, b = 8.875(3) Å, c = 17.03(2) Å, β = 95.79(14) °

h	*k*	*l*	d[obs]/Å	d[calc]/Å	Residual
0	*0*	*2*	8.4351	8.4725	0.0374
0	*1*	*1*	7.8203	7.8615	0.0412
1	*1*	*0*	6.6663	6.6906	0.0244
-1	*1*	*1*	6.3462	6.3690	0.0228
1	*1*	*1*	6.0740	6.0868	0.0128
-1	*1*	*2*	5.4166	5.4288	0.0122
1	*1*	*2*	5.0849	5.0893	0.0044
0	*1*	*3*	4.7632	4.7651	0.0019
-2	*0*	*2*	4.5680	4.5730	0.0050
0	*0*	*4*	4.2399	4.2362	-0.0036
2	*0*	*2*	4.1834	4.1821	-0.0013
-1	*2*	*1*	4.0064	3.9922	-0.0142
-1	*1*	*4*	3.7006	3.6915	-0.0091
2	*2*	*0*	3.3446	3.3453	0.0007
-2	*2*	*2*	3.1784	3.1845	0.0061
-3	*0*	*3*	3.0489	3.0486	-0.0002
-1	*3*	*2*	2.7176	2.7165	-0.0011
-3	*2*	*3*	2.5145	2.5127	-0.0017
4	*1*	*2*	2.2920	2.2926	0.0006
-3	*1*	*6*	2.2160	2.2151	-0.0009
5	*0*	*1*	1.9996	1.9985	-0.0011
-4	*1*	*7*	1.8110	1.8111	0.0001
-1	*3*	*8*	1.7214	1.7214	0.0001
-3	*5*	*2*	1.5597	1.5596	-0.0001
-4	*3*	*8*	1.4838	1.4841	0.0003
-5	*2*	*8*	1.4618	1.4618	0.0000
-2	*5*	*7*	1.3998	1.3999	0.0000

Table S4: Indexing of $[CuZnAl_8(OH)_{24}](NO_3)_4 \cdot 8H_2O$

Orthorhombic cell, a = 5.311(4) Å, b = 8.847(6) Å, c = 16.99(1) Å

h	*k*	*l*	d[obs]/Å	d[calc]/Å	Residual
0	*0*	*2*	8.4576	8.4958	0.0382
0	*1*	*1*	7.8192	7.8465	0.0274
0	*1*	*3*	4.7715	4.7699	-0.0015
1	*1*	*0*	4.5416	4.5531	0.0116
0	*0*	*4*	4.2460	4.2479	0.0019
0	*1*	*5*	3.1756	3.1723	-0.0033
0	*2*	*4*	3.0558	3.0638	0.0080
1	*3*	*0*	2.5834	2.5780	-0.0054
2	*1*	*1*	2.5155	2.5152	-0.0003
0	*2*	*6*	2.3875	2.3850	-0.0026
0	*1*	*7*	2.3408	2.3408	0.0000
2	*1*	*3*	2.3194	2.3200	0.0006
2	*2*	*0*	2.2776	2.2766	-0.0011
2	*2*	*3*	2.1106	2.1123	0.0017
1	*4*	*1*	2.0270	2.0270	0.0000
2	*2*	*4*	2.0080	2.0066	-0.0015
1	*4*	*2*	1.9839	1.9851	0.0012

Table S5: Indexing of $[Ni_{0.9}Zn_{1.1}Al_8(OH)_{24}](NO_3)_4 \cdot 2H_2O$

Orthorhombic cell, a = 5.320(8) Å, b = 8.823(11) Å, c = 17.28(3) Å

h	*k*	*l*	d[obs]/Å	d[calc]/Å	Residual
0	*0*	*2*	8.6136	8.6410	0.0274
0	*1*	*1*	7.8731	7.8580	-0.0151
0	*1*	*1*	7.8597	7.8580	-0.0017
0	*1*	*3*	4.8363	4.8235	-0.0128
0	*0*	*4*	4.2994	4.3205	0.0211
1	*2*	*2*	3.1748	3.1605	-0.0143
2	*1*	*1*	2.5120	2.5196	0.0076
1	*3*	*4*	2.2115	2.2112	-0.0003
1	*2*	*7*	2.0029	1.9969	-0.0060
3	*1*	*1*	1.7306	1.7299	-0.0008
1	*4*	*8*	1.4794	1.4822	0.0028
2	*3*	*8*	1.4574	1.4567	-0.0007
1	*6*	*2*	1.3986	1.3986	0.0000

Table S6: Indexing of $[CoZnAl_8(OH)_{24}](NO_3)_4 \cdot 5.5H_2O$

Orthorhombic cell, a = 5.329(3) Å, b = 8.827(5) Å, c = 17.12(1) Å

h	*k*	*l*	d[obs]/Å	d[calc]/Å	Residual
0	*0*	*2*	8.5403	8.5611	0.0208
0	*1*	*1*	7.8977	7.8455	-0.0522
1	*1*	*0*	4.5817	4.5620	-0.0197
0	*0*	*4*	4.2776	4.2805	0.0029
0	*1*	*5*	3.1916	3.1926	0.0009
0	*2*	*4*	3.0684	3.0727	0.0043
2	*1*	*1*	2.5237	2.5230	-0.0007
1	*0*	*7*	2.2228	2.2230	0.0003
2	*2*	*4*	2.0102	2.0130	0.0028
3	*1*	*1*	1.7323	1.7325	0.0001
0	*5*	*5*	1.5696	1.5691	-0.0005
3	*1*	*6*	1.4866	1.4865	-0.0001
2	*5*	*1*	1.4657	1.4662	0.0005
2	*2*	*9*	1.4619	1.4610	-0.0008

Table S7: Indexing of the Cu/Ni/Al three-metal LDH system.

Orthorhombic cell, a = 5.380(13) Å, b = 8.892(13) Å, c = 17.10(4) Å

h	*k*	*l*	d[obs]/Å	d[calc]/Å	Residual
0	*0*	*2*	8.5363	8.5514	0.0151
0	*0*	*4*	4.2801	4.2757	-0.0044
1	*2*	*0*	3.4351	3.4271	-0.0080
1	*2*	*2*	3.1736	3.1811	0.0075
1	*4*	*0*	2.0545	2.0545	0.0000
2	*2*	*4*	2.0265	2.0265	0.0000

Table S8: Indexing of $[CoCuAl_8(OH)_{24}](NO_3)_4 \cdot 7H_2O$

Orthorhombic cell, a = 5.317(16) Å, b = 8.867(21) Å, c = 16.76(6) Å

h	*k*	*l*	d[obs]/Å	d[calc]/Å	Residual
0	*0*	*2*	8.3020	8.3800	0.0780
0	*0*	*4*	4.2056	4.1900	-0.0155
1	*2*	*2*	3.1515	3.1545	0.0030
1	*4*	*1*	2.0304	2.0309	0.0005
2	*2*	*4*	2.0007	2.0027	0.0020
2	*3*	*0*	1.9791	1.9765	-0.0025

Table S9: Indexing of $[Co_{0.3}Ni_{1.7}Al_8(OH)_{24}](NO_3)_4 \cdot 2H_2O$

Orthorhombic cell, a = 5.503(1) Å, b = 8.864(12) Å, c = 17.25(4) Å

h	***k***	***l***	**d[obs]/Å**	**d[calc]/Å**	**Residual**
0	*0*	*2*	8.6446	8.6248	-0.0198
0	*1*	*1*	7.9509	7.8838	-0.0671
0	*0*	*4*	4.3154	4.3124	-0.0030
2	*1*	*2*	2.5182	2.5135	-0.0047
1	*4*	*2*	1.9991	1.9995	0.0004
2	*4*	*6*	1.4794	1.4797	0.0002
3	*2*	*6*	1.4591	1.4600	0.0008