crystals

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Supplementary Materials

The Crystal Structure of Mg–Al–CO_3 Layered Double Hydroxide

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Table S1. Powder X-ray diffraction data for quintinite sample **91002**.

d_{calc} (Å)	I_{meas} (%)	*h*	*k*	*l*
7.56	46	0	0	2
4.571	1	0	1	0
3.779	100	0	0	4
?	2	-	-	-
2.5998	11	1	1	1
2.5195	22	0	0	6
2.4916	8	1	1	2
2.3379	8	1	1	3
2.2856	2	0	2	0
2.1638	9	1	1	4
1.9882	9	1	1	5
1.8896	5	0	0	8
1.8224	21	1	1	6
1.5364	4	1	1	8
1.5237	23	0	3	0

Table S2. Anisotropic displacement parameters (Å²) for quintinite samples **91002** and **C7029**.[1]

Sample	Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
91002	Mg	0.0049(5)	0.0049(4)	0.0110(7)	0	0	0.0024(2)
	Al	0.0063(5)	0.0063(5)	0.0195(11)	0	0	0.0031(3)
	O1	0.0091(8)	0.0250(10)	0.0108(8)	-0.0029(9)	0.0037(9)	0.0097(8)
C7029	Mg	0.0066(4)	0.0066(4)	0.0170(6)	0	0	0.0033(2)
	Al	0.0077(5)	0.0077(5)	0.0218(9)	0	0	0.0038(2)
	O1	0.0095(7)	0.0306(10)	0.0154(6)	-0.0012(10)	0.0017(9)	0.0121(7)

[1] O2, O3, C1 and C2 atoms have only isotropic displacement parameter.