Revisiting the crystal structure of dickite: X-ray diffraction, solid-state NMR and DFT calculations study

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Table S1. Crystallographic details and atomic coordinates for the four structure models of dickite

	Reference: (Dera et al., 2003) Monoclinic *C*c a = 5.161 Å, b = 8.96 Å, c = 14.46 Å, β = 96.77° Unit cell Axial Ratio: a/b = 0.576; c/a = 2.802			Reference: (Bish and Johnston, 1993) Monoclinic *C*c a = 5.147 Å, b = 8.939 Å, c = 14.390 Å, β = 96.483° Unit cell Axial Ratio: a/b = 0.576; c/a = 2.796			Reference: (Mercier and Le Page, 2008). Monoclinic *C*c a = 5.110 Å, b = 8.874 Å, c = 14.030 Å, β = 96.643° Unit cell Axial Ratio: a/b = 0.576; c/a = 2.746			Reference: this work Monoclinic *C*c a = 5.1444(2) Å, b = 8.9334(3) Å, c = 14.3896(5) Å, β = 96.544(2)° Unit cell Axial Ratio: a/b = 0.576; c/a = 2.797		
Atom	***X***	***Y***	***Z***	***X***	***Y***	***Z***	***X***	***Y***	***Z***	***X***	***Y***	***Z***
Si1	0.00000	0.90120	0.00000	0.00000	0.89920	0.00000	0.00000	0.90807	0.00000	0.00000	0.89944	0.00000
Si2	0.01230	0.57230	0.00060	0.01490	0.56920	-0.00050	0.01201	0.57893	0.00098	0.01307	0.57081	0.00068
Al1	0.09680	0.75250	-0.19090	0.09990	0.74890	-0.18850	0.09873	0.75825	-0.19726	0.09906	0.75087	-0.19114
Al2	0.09010	0.41730	-0.19030	0.09930	0.41490	-0.18780	0.09142	0.42271	-0.19578	0.09382	0.41579	-0.19032
O1	0.24520	1.00570	0.03290	0.24630	1.00540	0.03120	0.23779	1.02285	0.03849	0.24652	1.00548	0.03387
O2	0.05210	0.73940	0.04570	0.05760	0.73520	0.04600	0.07204	0.74483	0.04977	0.05582	0.73615	0.04709
O3	0.25390	0.47150	0.04670	0.25490	0.46950	0.04660	0.24590	0.46880	0.04996	0.25462	0.46897	0.04767
O4	-0.06980	0.89030	-0.11120	-0.06600	0.88800	-0.11180	-0.06287	0.89961	-0.11448	-0.06598	0.88879	-0.11135
O5	0.00630	0.58080	-0.11200	0.00740	0.57900	-0.11250	0.00010	0.58734	-0.11375	0.00762	0.58001	-0.11111
O6	0.25980	0.89390	-0.25760	0.26790	0.89140	-0.25920	0.26239	0.90162	-0.26495	0.26582	0.89228	-0.25787
O7	0.18550	0.58400	-0.25530	0.19350	0.58130	-0.25760	0.19532	0.58905	-0.26071	0.19122	0.58240	-0.25498
O8	0.26580	0.27720	-0.25520	0.26840	0.27610	-0.25780	0.26506	0.27916	-0.26047	0.26812	0.27546	-0.25509
O9	0.42640	0.77340	-0.11670	0.43120	0.77220	-0.11660	0.43086	0.77930	-0.11720	0.43022	0.77321	-0.11623
H1	0.16410	0.92700	-0.31330	0.18660	0.94560	-0.31170	0.21539	0.93488	-0.33056	0.19492	0.95250	-0.30386
H2	0.21980	0.60090	-0.31830	0.22350	0.58130	-0.32070	0.23491	0.58390	-0.32689	0.23322	0.58070	-0.31356
H3	0.18690	0.25240	-0.31480	0.21690	0.25580	-0.32290	0.20908	0.25356	-0.32725	0.22052	0.25780	-0.31536
H4	0.50980	0.68300	-0.13040	0.53310	0.68480	-0.11510	0.52568	0.68436	-0.12082	0.52832	0.67900	-0.10876
										Please note: atomic coordinates modified from those reported in the CIF file for the sake of comparison with the other crystallographic determinations of dickite		

Table S2. Hydrogen bonding interactions present in the various crystallographic descriptions of dickite. Distances are given in Å and interaction angles in degrees, and were calculated using the software package PLATON (Spek, 1990; Spek, 2003).

D–H···A	***d*(D···A)**	**<(DHA)**
Reference: (Dera et al., 2003)		
O–H···O_{intra}	2.803	100
O–H···O	2.963	163
O–H···O	3.153	138
O–H···O	2.978	152
Reference: (Bish and Johnston, 1993)		
Please note: no intra-layer O–H···O interaction is present		
O–H···O	2.910	164
O–H···O	3.144	140
O–H···O	2.906	166
Reference: (Mercier and Le Page, 2008)		
O–H···O_{intra}	3.367	140
O–H···O	2.747	164
O–H···O	2.738	165
O–H···O	2.827	161
O–H···O	3.370	139
This work		
O–H···O_{intra}	3.274	145
O–H···O	2.932	166
O–H···O	2.931	164
O–H···O	3.124	137

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References

Bish, D.L., and Johnston, C.T. (1993) Rietveld refinement and fourier transform infrared spectroscopic study of the dickite structure at low temperature Clays and Clay Minerals, 41(3), 297-304.

Dera, P., Prewitt, C.T., Japel, S., Bish, D.L., and Johnston, C.T. (2003) Pressure-controlled polytypism in hydrous layered materials. American Mineralogist, 88(10), 1428-1435.

Mercier, P.H.J., and Le Page, Y. (2008) Kaolin polytypes revisited ab initio. Acta Crystallographica Section B-Structural Science Crystal Engineering and Materials, 64, 131-143.

Spek, A.L. (1990) PLATON. Acta Cryst. A, 46, C34.

Spek, A.L. (2003) Single-crystal structure validation with the program PLATON. J. Appl. Crystallogr., 36, 7-13.