

Supplementary Info

Pressure-induced transformations in kaolinite

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<i>P</i> (GPa)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	α°	β°	γ°	<i>V</i> (Å ³)
kaolinite-I							
0.00*	5.1542(4)	8.9307(5)	7.3936(6)	91.879(8)	104.550(8)	89.783(9)	329.24(3)
0.05(4)	5.1539(4)	8.9279(6)	7.3832(6)	91.975(9)	104.396(7)	89.715(9)	328.86(3)
0.25(5)	5.1508(5)	8.9262(7)	7.3820(6)	91.839(7)	104.798(9)	89.823(8)	327.98(3)
0.41(4)	5.1502(4)	8.9227(8)	7.3744(6)	91.876(8)	104.865(9)	89.843(8)	327.36(3)
0.70(10)	5.1454(3)	8.9158(7)	7.3546(5)	92.020(6)	104.973(6)	89.8635	325.73(3)
0.87(5)	5.1426(3)	8.9081(7)	7.3458(5)	92.062(6)	105.022(7)	89.861(6)	324.80(3)
1.06(9)	5.1387(3)	8.9009(7)	7.3368(5)	92.146(7)	105.085(7)	89.861(6)	323.77(3)
1.34(5)	5.1339(4)	8.8901(8)	7.3246(6)	92.302(8)	105.196(8)	89.854(6)	322.34(3)
1.66(11)	5.1273(4)	8.8827(7)	7.3116(6)	92.482(8)	105.340(8)	89.852(7)	320.82(3)
2.02(9)	5.1202(4)	8.8685(7)	7.3012(5)	92.686(7)	105.470(8)	89.845(6)	319.16(3)
2.45(8)	5.1110(5)	8.8501(6)	7.2893(6)	93.057(8)	105.709(8)	89.910(7)	316.92(3)
2.95(5)	5.1005(4)	8.8332(5)	7.2800(6)	93.496(7)	106.030(7)	89.937(8)	314.61(3)
3.44(13)	5.0872(4)	8.8140(6)	7.2741(6)	94.079(7)	106.400(7)	89.933(7)	312.04(3)
kaolinite-II							
3.89(5)	5.0681(6)	8.7971(12)	7.4323(10)	101.234(11)	108.712(11)	90.117(15)	307.09(4)
4.46(15)	5.0464(4)	8.7818(9)	7.3966(8)	101.162(8)	108.715(9)	90.363(7)	303.76(4)
5.04(7)	5.0305(5)	8.7589(9)	7.3785(7)	101.676(7)	108.593(8)	90.508(10)	300.82(4)
5.57(11)	5.0168(5)	8.7404(8)	7.3444(7)	101.565(7)	108.432(8)	90.582(10)	298.38(4)
6.02(10)	5.0061(5)	8.7250(9)	7.3189(7)	101.463(8)	108.345(8)	90.631(10)	296.45(4)
6.53(18)	4.9914(5)	8.7058(8)	7.2797(7)	101.185(7)	108.140(8)	90.564(7)	294.06(4)
kaolinite-III							
7.24(5)	4.9528(3)	8.6521(7)	7.4530(9)	112.890(9)	104.076(8)	89.834(8)	283.88(3)
	4.9527(3)	4.9787(4)	6.8114(5)	97.675(9)	95.700(7)	119.663(5)	141.95(1)
7.55(4)	4.9308(3)	8.6101(6)	7.3895(7)	112.899(6)	103.693(7)	89.856(7)	279.37(2)
	4.9306(3)	4.9560(3)	6.7740(5)	97.511(7)	96.167(7)	119.684(5)	139.694(9)
7.84(7)	4.9168(3)	8.5881(6)	7.3616(6)	112.968(6)	103.615(6)	89.815(6)	276.80(2)
	4.9159(3)	4.9405(3)	6.7498(4)	97.446(6)	96.298(6)	119.669(7)	138.336(7)
5.11(13)†	4.9639(4)	8.6413(6)	7.4391(8)	112.656(7)	103.601(8)	89.918(8)	284.80(3)
	4.9632(3)	4.9801(5)	6.8380(6)	97.544(8)	96.213(7)	119.812(5)	142.39(1)
3.56(23)†	4.9985(3)	8.6859(6)	7.5118(9)	112.837(7)	103.671(8)	89.922(6)	290.57(3)
	4.9985(3)	5.0078(4)	6.8824(8)	97.319(7)	96.087(8)	119.861(7)	145.29(1)
2.08(10)†	5.0318(3)	8.7431(5)	7.5887(7)	112.770(6)	103.638(7)	90.028(7)	297.59(3)
	5.0318(3)	5.0449(3)	6.9526(5)	97.276(7)	95.975(6)	119.941(5)	148.80(1)
0.48(4)†	5.0779(5)	8.8255(9)	7.6653(12)	112.370(10)	103.745(12)	90.056(10)	306.97(3)
	5.0780(4)	5.0932(6)	7.0467(9)	97.648(10)	95.810(12)	119.952(12)	153.50(1)

Notes: For the kaolinite-III data there are two entries: the upper row correspond to values obtained by Le Bail refinement against the Bookin obtuse cell setting (α and β are obtuse) of the one-layer high-pressure Model 18 structure of Mercier and Le Page (2009); the lower value is from Le Bail refinement directly against the corresponding one-layer *P1* cell of Model 18 (Mercier and Le Page 2009).

* Ambient in-cell.

† On decompression.