

Tables 3a–3d for deposit.

TABLE 3a. Anisotropic displacement parameters ( $\text{\AA}^2$ ) for cavansite at RT

Site	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
V	0.00849(16)	0.00949(16)	0.01330(17)	0	0.00076(11)	0
Ca	0.01036(19)	0.01118(19)	0.0167(2)	0	0.00069(14)	0
Si1	0.00635(17)	0.00920(18)	0.00869(18)	0.00054(13)	– 0.00063(12)	0.00008(13)
Si2	0.00691(17)	0.00834(17)	0.00772(17)	0.00053(12)	0.00091(12)	0.00042(13)
O1	0.0093(5)	0.0098(5)	0.0193(5)	–0.0007(4)	0.0002(4)	–0.0007(4)
O2	0.0154(5)	0.0091(5)	0.0168(5)	0.0015(4)	0.0052(4)	0.0021(4)
O3	0.0122(5)	0.0212(6)	0.0099(5)	0.0039(4)	–0.0014(4)	–0.0003(4)
O4	0.0082(4)	0.0113(5)	0.0172(5)	–0.0015(4)	0.0026(4)	–0.0001(4)
O5	0.0103(5)	0.0122(5)	0.0111(5)	0.0019(4)	–0.0039(4)	–0.0013(4)
O6	0.0231(9)	0.0287(10)	0.0192(8)	0	–0.0052(7)	0
O7	0.0340(9)	0.0489(11)	0.0498(10)	–0.0273(9)	0.0089(7)	0.0048(7)
O8	0.0146(9)	0.0319(11)	0.0658(16)	0	–0.0048(10)	0
O9	0.066(2)	0.109(3)	0.058(2)	0	0.0091(17)	0

Table 3b. Anisotropic displacement parameters ( $\text{\AA}^2$ ) for cavansite at 75 °C

Site	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
V	0.0098(2)	0.0118(2)	0.0150(2)	0	0.00105(14)	0
Ca	0.0119(2)	0.0135(2)	0.0173(2)	0	0.00026(17)	0
Si1	0.0071(2)	0.0116(2)	0.0104(2)	0.00078(15)	–0.00049(15)	–0.00016(15)
Si2	0.0082(2)	0.0101(2)	0.0097(2)	0.00080(15)	0.00136(15)	0.00053(15)
O1	0.0107(6)	0.0122(6)	0.0220(7)	–0.0010(5)	0.0014(5)	–0.0002(4)
O2	0.0189(6)	0.0110(6)	0.0207(6)	0.0016(5)	0.0079(5)	0.0029(5)
O3	0.0132(6)	0.0262(7)	0.0127(6)	0.0049(5)	–0.0020(5)	–0.0008(5)
O4	0.0098(5)	0.0142(6)	0.0199(6)	–0.0018(5)	0.0039(5)	–0.0005(5)
O5	0.0121(6)	0.0154(6)	0.0138(6)	0.0030(5)	–0.0049(4)	–0.0021(4)
O6	0.0289(12)	0.0370(13)	0.0222(10)	0	–0.0080(9)	0
O8	0.0215(15)	0.099(3)	0.106(4)	0	–0.0007(18)	0

Table 3c. Anisotropic displacement parameters ( $\text{\AA}^2$ ) for cavansite at 175 °C

Site	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
V	0.0140(2)	0.0168(2)	0.0185(2)	0	0.00103(17)	0
Ca	0.0163(3)	0.0197(3)	0.0194(3)	0	–0.0001(2)	0

Si1	0.0108(2)	0.0170(3)	0.0146(3)	0.00178(17)	−0.00055(18)	0.00016(17)
Si2	0.0124(2)	0.0155(2)	0.0131(2)	0.00137(17)	0.00162(17)	0.00114(18)
O1	0.0153(6)	0.0172(7)	0.0272(8)	−0.0011(6)	0.0017(5)	−0.0002(5)
O2	0.0248(7)	0.0168(7)	0.0237(7)	0.0027(5)	0.0087(6)	0.0043(6)
O3	0.0180(7)	0.0328(9)	0.0169(7)	0.0063(6)	−0.0025(5)	−0.0008(6)
O4	0.0144(7)	0.0194(7)	0.0250(7)	0.0001(5)	0.0050(6)	−0.0003(5)
O5	0.0158(7)	0.0220(7)	0.0190(7)	0.0037(5)	−0.0051(5)	−0.0018(5)
O6	0.0326(13)	0.0404(14)	0.0282(13)	0	−0.0086(11)	0
O8	0.035(2)	0.172(6)	0.157(6)	0	0.029(3)	0

Table 3d. Anisotropic displacement parameters ( $\text{\AA}^2$ ) for cavansite at 350 °C

Site	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
V	0.0308(12)	0.0317(11)	0.0343(13)	0	0.0063(10)	0
Ca	0.0358(14)	0.0357(14)	0.0405(17)	0	−0.0030(12)	0
Si1	0.0211(12)	0.0300(12)	0.0255(14)	0.0024(9)	−0.0021(9)	0.0000(8)
Si2	0.0241(11)	0.0293(11)	0.0195(13)	0.0015(9)	0.0041(9)	0.0008(9)
O1	0.030(3)	0.033(3)	0.049(4)	0.001(3)	0.002(3)	0.000(2)
O2	0.048(4)	0.032(3)	0.033(4)	0.004(3)	0.016(3)	0.006(3)
O3	0.034(3)	0.054(4)	0.022(3)	0.007(3)	−0.003(3)	−0.002(3)
O4	0.023(3)	0.035(3)	0.035(3)	0.003(2)	0.003(3)	0.000(2)
O5	0.031(3)	0.038(3)	0.024(3)	0.008(2)	−0.004(3)	−0.001(2)
O6	0.067(7)	0.068(7)	0.048(7)	0	−0.010(6)	0