TABLE 5 for deposit

TABLE 5. Interatomic distances (Å) and T-O-T angles (°) of cavansite under ambient conditions and after partial dehydration at 75, 175, and 350 °C

Ca coordination	RT	75 °C	175 °C	350 °C
Ca-O1 (2×)	2.3941(11)	2.3726(14)	2.3356(15)	2.292(11)
Ca-O2 (2×)	2.4418(12)	2.4081(14)	2.3291(16)	2.271(11)
Ca-O7 (2×)	2.3894(16)	2.407(9)	2.402(15)	2.31(5)
Ca-O7a (2×)		2.47(1)	2.453(11)	
Ca-O7b (2×)		2.409(4)	2.41(2)	2.42(6)
Ca-O8	2.501(2)	2.473(4)	2.402(5)	2.07(8)
Ca-O9	2.834(4)	2.82(3)		
Mean	2.473	2.469*	2.359*	2.260*

*The mean value of the split positions is given.

V coordination	RT	75 °C	175 °C	350 °C
V-O1 (2×)	2.0026(11)	2.0032(14)	2.0017(15)	2.01(1)
V-O2 (2×)	1.9843(11)	1.9843(14)	1.9718(15)	1.980(9)
V-O6	1.5956(18)	1.590(2)	1.590(3)	1.559(13)
Mean	1.914	1.913	1.907	1.908

Si1 coordination	RT	75 °C	175 °C	350 °C
Si1-O1	1.6027(12)	1.6030(15)	1.6090(16)	1.60(1)
Si1-O3	1.6231(12)	1.6239(15)	1.6220(16)	1.60(1)
Si1-O4	1.6406(11)	1.6357(14)	1.6343(15)	1.620(8)
Si1-O5	1.6298(11)	1.6279(13)	1.6269(15)	1.617(9)
Mean	1.624	1.623	1.623	1.609

Si2 coordination	RT	75 °C	175 °C	350 °C
Si2-O2	1.5922(12)	1.5908(14)	1.5947(16)	1.59(1)
Si2-O3	1.6231(12)	1.6202(14)	1.6233(16)	1.612(9)
Si2-O4	1.6248(11)	1.6283(14)	1.6265(16)	1.625(9)
Si2-O5	1.6234(11)	1.6230(13)	1.6251(15)	1.625(9)
Mean	1.616	1.616	1.617	1.613

T-O-T angles	RT	75 °C	175 °C	350 °C
Si2 O3 Si1	136.36(8)	136.92(9)	135.18(10)	137.3(4)
Si2 O4 Si1	127.78(7)	127.77(9)	127.32(10)	127.0(5)
Si2 O5 Si1	131.42(7)	131.46(9)	128.24(10)	126.2(4)
Mean T-O-T	131.85	132.05	130.25	130.17

TABLE 6 for deposit

TABLE 6. Results of bond valence calculations for cavansite RT, parameters from Brown and Altermatt (1985)

Site	O1	O2	O3	O4	O5	O6	O7	O8	O9	Bvs[#]
V	0.56	0.59				1.67				3.97
	2 × →	2 × →								
Ca	0.28	0.26					0.29	0.23	0.11	2.00
	2 × →	2 × →					2 × →			
Si1	1.06		0.97	0.93	0.95					3.91
Si2		1.04	0.97	0.96	0.97					3.93
H7a							0.8		0.2	1
									2 × ↓	
H7b					0.2		0.8			1
H8			0.2					0.8		1
								2 × ↓		
H9a						0.2			0.8	1
H9b									1*	1
Bvs[#] without H					1.92	1.67	0.29	0.23	0.11	
Bvs[#] with H	1.90	1.89	2.14	1.89	2.12	1.87	1.89	1.83	2.31	

[#] bond valence sum.

*No acceptor was found for H9b.