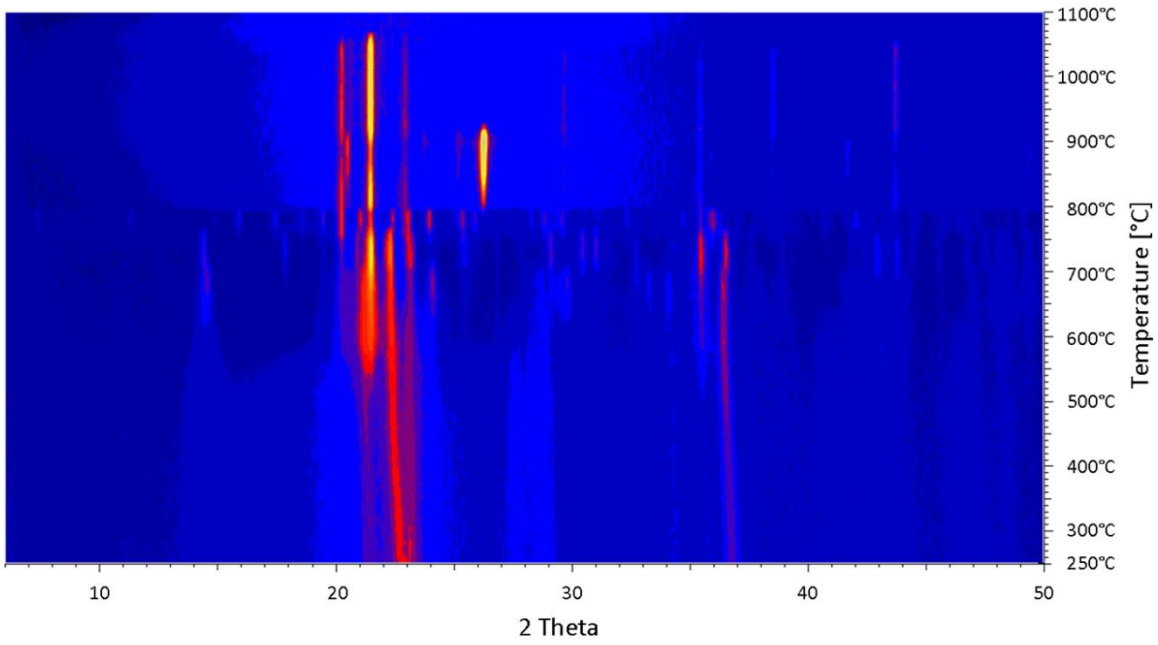
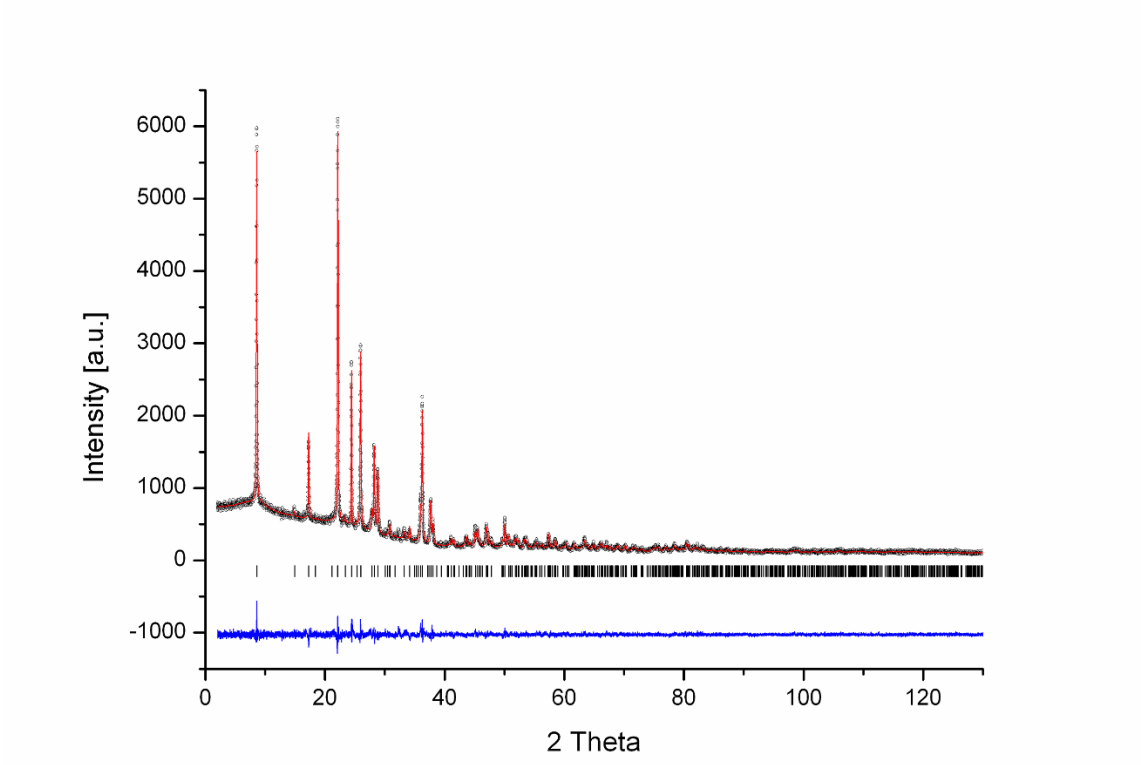
Supplemental information for "Temperature- and moisture-dependent powder X-ray diffraction studies of kanemite ($NaSi_2O_4(OH)\cdot 3H_2O$)" by Daniela Schmidmair, Volker Kahlenberg, Daniel M. Többens, Herwig Schottenberger, Jochem de Wit and Ulrich J. Griesser.



Supplemental Figure A. Waterfall plot of the sequence of temperature dependent powder X-ray diffraction patterns of kanemite collected in situ in the range between 25 and 1100°C in steps of ΔT=10°C.



Supplemental Figure B. Observed (circles) and calculated (solid line) step intensities and their difference (line at bottom of figure) for the synthetic kanemite starting material ($NaSi_2O_4(OH)\cdot 3H_2O$). Peak positions permitted by unit-cell metric are indicated by tick marks (middle portion). Residuals of the Rietveld refinement are R_{wp} = 18.2%, R_{Bragg} = 5.97%, χ^2 = 1.22.

Supplemental Table. Wyckoff positions, atomic coordinates, isotropic displacement parameters (Å^2) and bond-valence sums for kanemite ($NaSi_2O_4(OH)\cdot 3H_2O$). Hydrogen atoms have been refined using a riding model with a d_{O-H} target value of 0.90 Å. The position H2A is only half occupied.

Atom	Wyckoff positions	x	y	z	U(iso)	Bond-valence sum
Si	8*d*	0.0498(3)	0.29320(6)	0.0377(2)	0.0189(8)	4.19
Na	4*c*	0.5	0.5125(2)	0.75	0.0371(18)	1.13
O1	4*c*	0	0.3135(3)	0.25	0.040(3)	2.02
O2	8*d*	0.0016(10)	0.35623(11)	–0.08074(17)	0.0061(16)	1.15
O3	8*d*	0.8587(5)	0.23313(18)	–0.0202(10)	0.059(3)	2.03
O4	8*d*	0.4868(4)	0.57346(13)	0.0127(6)	0.0228(17)	0.43
O5	4*c*	0	0.54216(13)	0.75	0.067(3)	0.26
H2A	8*d*	0.0167(10)	0.37863(11)	0.79936(17)	0.0061(16)	
H4A	8*d*	0.6442(4)	0.40007(13)	–0.0650(6)	0.0228(17)	
H4B	8*d*	0.3632(4)	0.40407(13)	–0.0570(6)	0.0228(17)	
H5A	8*d*	0.0067	0.50816(13)	0.6653	0.067(3)	