

Supporting information.

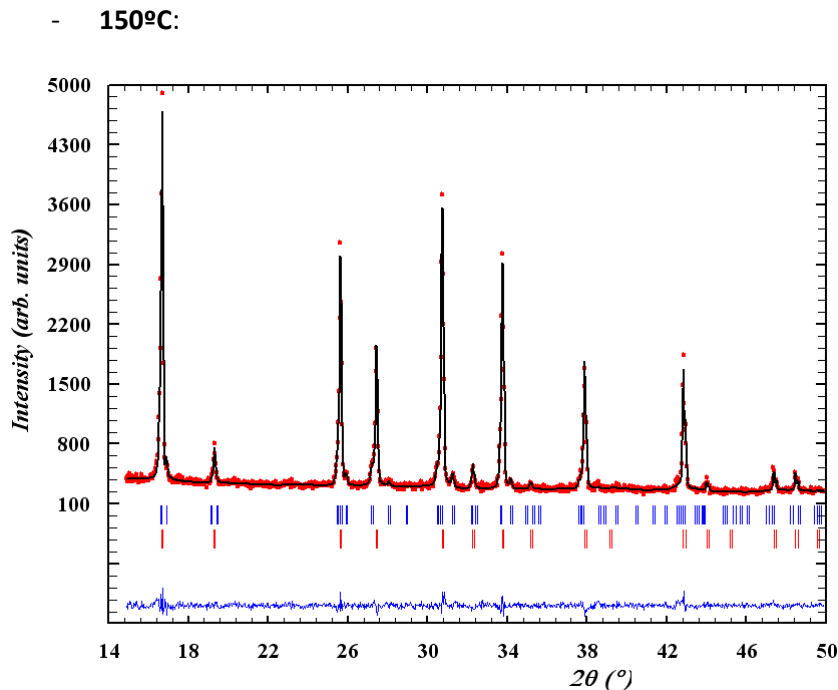
Table 1: FullProf fitting parameters for the thermo-diffractograms shown in Fig. 5 of the main text.

T (°C)	RT	150		250	350		450		525		600	650
	Phase 1	Phase 1	Phase 2	Phase 1	Phase 1	Phase 2	Phase 1	Phase 2	Phase 1	Phase 2	Phase 1	Phase 1
Crystal system	Tetragonal	Tetragonal	Cubic	Cubic	Tetragonal	Cubic	Tetragonal	Cubic	Tetragonal	Cubic	Cubic	Cubic
Space group	I41/acd	I41/acd	Ia3d	Ia3d	I41/acd	Ia3d	I41/acd	Ia3d	I41/acd	Ia3d	Ia3d	Ia3d
a (Å)	13.094(3)	13.110(3)	13.004(2)	13.022 (2)	13.139(3)	13.036(3)	13.163(3)	13.060(4)	13.160(4)	13.069(4)	13.087(2)	13.093(2)
c (Å)	12.680(3)	12.713(4)			12.791(3)		12.820(3)		12.863(3)			
Fract(%)	100 (6)	22 (4)	78 (4)	100 (4)	46 (2)	54 (5)	56 (4)	44 (6)	53 (4)	47 (4)	100 (4)	100 (3)
Rp (%)	7.04	5.07		6.03	5.26		4.96		4.61		4.98	4.68
Rwp (%)	8.97	6.38		7.65	6.7		6.23		5.85		6.32	5.95
Rexp (%)	4.88	4.89		4.96	4.91		4.82		4.71		4.63	4.55
Chi2	3.38	1.7		2.38	1.86		1.67		1.54		1.86	1.71

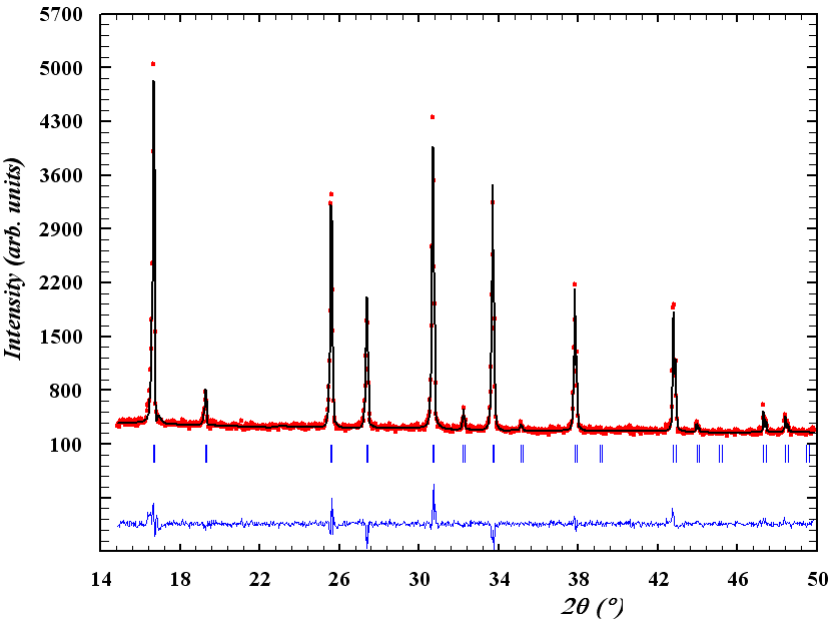
As this table shows, the reliability factors of the RT pattern are worse than those of the other temperatures. They are also worse than those of the just as-grown sample (diffractogram shown in Fig. 1). We attribute this behavior to the incipient hydration effects in this sample. A stoichiometric composition was assumed both for tetragonal and cubic phases. Site occupancy factors were not refined.

Figures:

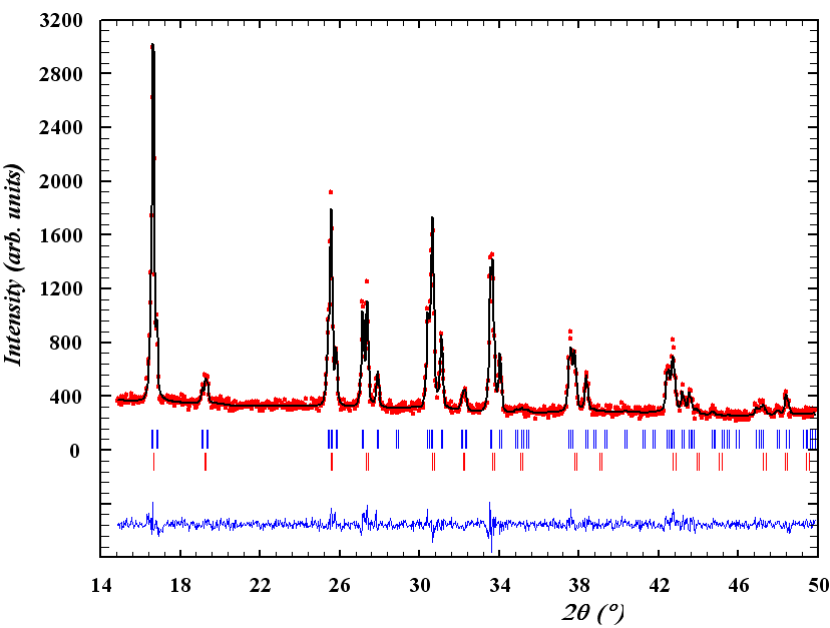
Observed, calculated, and difference powder X-ray diffraction patterns of sample 2 at different temperatures. Vertical bars denote the Bragg reflection positions corresponding to the tetragonal and cubic phases.



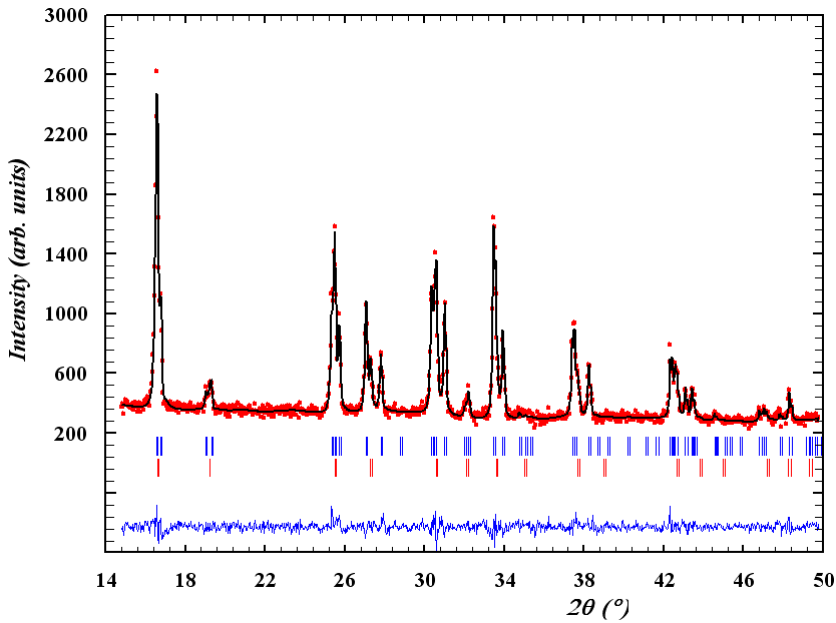
- 250°C:



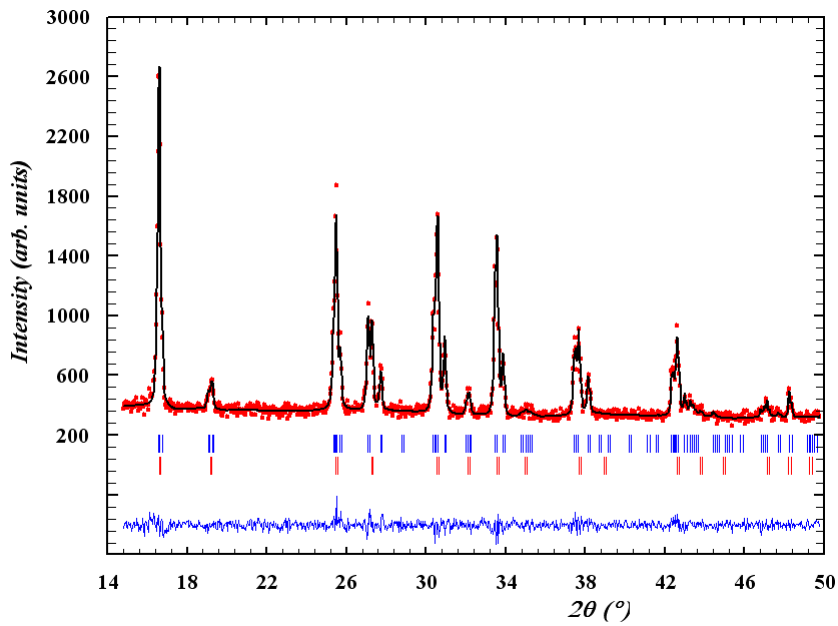
- 350°C:



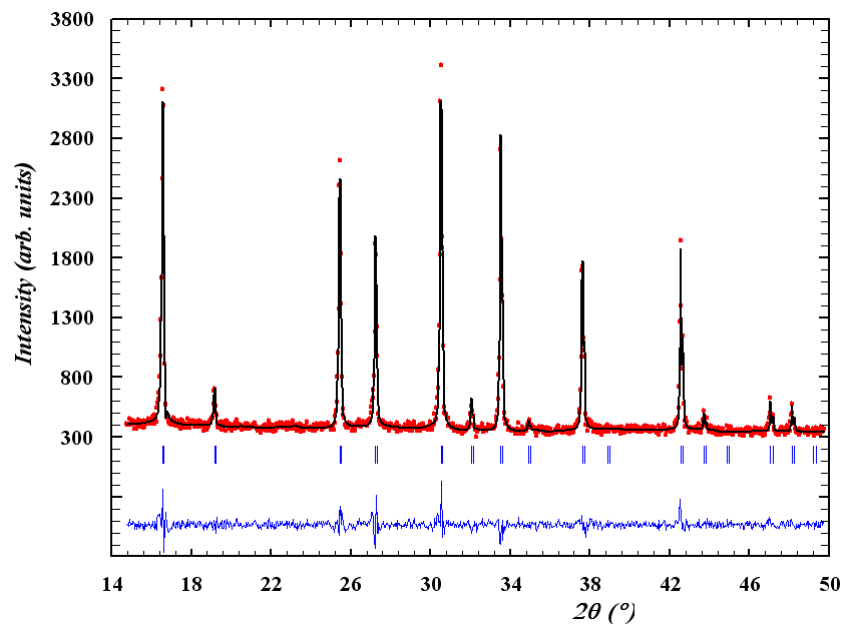
- **450°C:**



- **525°C:**



- 600°C:



- 650°C:

