

Supplemental Table OM5. Experimental details for fresnoite

Crystal Data	
	Fresnoite
Crystal system	tetragonal
Unit cell dimensions	$a = 8.5262(5) \text{ \AA}$ $c = 5.2199(4) \text{ \AA}$ $\alpha = 90^\circ, \beta = 90^\circ, \gamma = 90^\circ$
Space group	$P4bm$ no. 100
Volume	$379.47(5) \text{ \AA}^3$
Z	2
Density (calculated)	4.383 g/cm^3
Chemical formula sum	$(\text{Ba}_{1.94}\text{Ca}_{0.06})\text{TiO}(\text{Si}_2\text{O}_7)$
Crystal size (μm)	$30 \times 20 \times 20 \text{ \mu m}$
Data collection	
Diffractometer	beamline X06DA, SLS multi-axis goniometer PRiGo PILATUS 2M-F detector $\lambda = 0.70848 \text{ \AA}$
Exposure time / step size	$0.1 \text{ s} / 0.1^\circ$
Number of frames	1800
Max. θ° -range for data collection	34.801
Index ranges	$-12 \leq h \leq 12$ $-13 \leq k \leq 11$ $-8 \leq l \leq 5$
No. of measured reflections	2866
No. of unique reflections	705
No. of observed reflections ($I > 2\sigma(I)$)	689
Refinement of the structure	
no. of parameters	40
R_{int}	0.0383
$R\sigma$	0.0344
$R1, I > 2\sigma(I)$	0.0192
$R1$ all Data	0.0199
$wR2$ on (F2)	0.0454
GooF	1.054
$\Delta\rho$ min (-e. \AA^{-3})	-0.94 (0.61 \AA from CA1)
$\Delta\rho$ max (e. \AA^{-3})	0.79 (0.68 \AA from CA1)