

Supplemental Table OM1. Experimental details for bennesherite

Crystal Data	
Bennesherite	
Crystal system	tetragonal
Unit cell dimensions	$a = 8.2334(14) \text{ \AA}$ $c = 5.2854(8) \text{ \AA}$ $\alpha = 90^\circ, \beta = 90^\circ, \gamma = 90^\circ$
Space group	$P\bar{4}2_1m$, no.113
Volume	$358.29(13) \text{ \AA}^3$
Z	2
Density (calculated)	4.27 g/cm^3
Chemical formula sum	$(\text{Ba}_{1.70}\text{Ca}_{0.30})(\text{Fe}_{1.62}\text{Mg}_{0.38})\text{Si}_2\text{O}_7$
Crystal size (μm)	$30 \times 30 \times 20 \text{ \mu m}$
Data collection	
Diffractometer	STOE IPDS II
Exposure time / step size	$1800\text{s} / 1^\circ$
Number of frames	180
Max. θ -range for data collection	29.16
Index ranges	$-11 \leq h \leq 11$ $-11 \leq k \leq 11$ $-6 \leq l \leq 7$
No. of measured reflections	2758
No. of unique reflections	533
No. of observed reflections ($I > 2\sigma(I)$)	463
Refinement of the structure	
no. of parameters	36
R_{int}	0.0401
$R\sigma$	0.0229
$R1, I > 2\sigma(I)$	0.0469
$R1$ all data	0.0595
$wR2$ on (F2)	0.1110
GooF	1.129
$\Delta\rho$ min (-e. \AA^{-3})	$2.59 (0.91 \text{ \AA from Mg1/Fe1})$
$\Delta\rho$ max (e. \AA^{-3})	$-1.33 (0.84 \text{ \AA from Ca1})$