

TABLE 1: CCD Data collection and refinement of $P2_1/c$ kanoite.

Diffractionmeter	Siemens SMART CCD system
X-ray radiation	sealed tube MoK α
X-ray power	50 kV, 40 mA
Temperature	293 K
Detector to sample distance	5.21 cm
Detector 2 Θ angle	27°
Resolution	0.77 Å
Rotation axis and width	ω / 0.3°
Total number of frames	1271
Frame size	512 x 512 pixels
Data collection time per frame	10 s
Collection mode	automated hemisphere
Reflections measured	2391
Max 2 Θ	54.3; -8 \leq h \leq 7, -10 \leq k \leq 10, -8 \leq l \leq 4
Unique reflections	913
Reflections > 2 σ (I)	781
Space group, cell dimensions (Å)	$P2_1/c$, $a = 9.722(2)$, $b = 8.920(2)$, $c = 5.2478(10)$, $\beta = 108.52(3)^\circ$
Volume (Å ³)	431.54
R(int)	4.04% after empirical abs. correction
R(σ)	3.54%
Number of l.s. parameters	94
Goof	1.082
R1, Fo > 4 σ (Fo)	2.92%
R1, all data	3.66%
wR2 (on F ²)	7.99%

$R_{\text{int}} = [\sum |F_o^2 - (F_o^2)_{\text{mean}}|] / (\sum F_o^2)$, $R_\sigma = (\sum \sigma_{F_o^2}) / \sum F_o^2$, $R1 = (\sum ||F_o| - |F_c||) / (\sum |F_o|)$
 $wR2 = [(\sum (F_o^2 - F_c^2)^2) / (\sum (w(F_o^2)^2))]^{1/2}$, $Goof = [(\sum w(F_o^2 - F_c^2)^2) / (n-p)]^{1/2}$
