

This is a postponed Result reached using INDEX.EXE. There was large progress to the indexing algorithms. In every case, a leBail fit gives the final decision about the lattice. New is the solution for sample 4. The final version of INDEX.EXE gives a better triclinic result to sample 7.

sample	ignored peaks/weight allowed reported	cell	lattice constants	R_{wp} (LeBail)	comment
1	— —	monoclinic primitive	$a = 8.5324(13)\text{\AA}$ $b = 10.3279(17)\text{\AA}$ $c = 7.3976(12)\text{\AA}$ $\gamma = 91.3446(27)^\circ$	2.74%	—
2	— —	monoclinic primitive	$a = 11.24370(15)\text{\AA}$ $b = 19.88201(26)\text{\AA}$ $c = 8.19601(11)\text{\AA}$ $\gamma = 106.06325(30)^\circ$	4.31%	—
3	— —	cubic body centered	$a = 18.87851(65)\text{\AA}$	4.53%	—
4	10/10% 10/8%	monoclinic primitive	$a = 30.0148(12)\text{\AA}$ $b = 3.77743(12)\text{\AA}$ $c = 36.6901(13)\text{\AA}$ $\beta = 109.75809(92)^\circ$	9.39%	The pattern shows a strong broad (amorphous) peak near to 3° . Therefore, the angular range $2.75^\circ \dots 3.1^\circ$ was “cutted of” for the LeBail fit.
5	6/10% 6/1%	monoclinic primitive	$a = 6.01140(79)\text{\AA}$ $b = 16.9378(24)\text{\AA}$ $c = 18.2292(26)\text{\AA}$ $\gamma = 92.1877(22)^\circ$	10.57%	—
6	not solved until deadline				
7	5/1% 3/0%	triclinic (better result than that reported at deadline)	$a = 3.99892(86)\text{\AA}$ $b = 11.4820(12)\text{\AA}$ $c = 17.20201(16)\text{\AA}$ $\alpha = 77.6124(96)^\circ$ $\beta = 82.497(16)^\circ$ $\gamma = 82.434(19)^\circ$	9.57%	As a result of the LeBail fit, a tile-like grain shape was observed. The tiles main axis were estimated to: ≈ 80 nm near to the $\{100\}$ direction, ≈ 160 nm near to the $\{010\}$ direction, ≈ 350 nm near to the $\{001\}$ direction.
8	— —	orthorhombic primitive	$a = 3.79612(19)\text{\AA}$ $b = 9.36892(21)\text{\AA}$ $c = 28.91553(69)\text{\AA}$	10.20%	—