Supplementary material (ESI) for Journal of Materials Chemistry

Results from Rietveld Refinement[+] of XRD Data for Samples 47, 51 and 73[*]

Sample 47

Atom	Wyckoff	x	y/z	Occupancy	Uiso
Zn(1)	16d	0.500	0.500	0.262	0.0497(5)
Bi		0.500	0.500	0.738	0.0497(5)
Zn(2)	16c	0.000	0.000	0.188	0.0330(6)
Nb		0.000	0.000	0.812	0.0330(6)
O(1)	48f	0.3183(7)	0.125	1.0	0.025
O(2)	8b	0.375	0.375	1.0	0.025
wRp = 14.21 Rp = 10.82 Chi^2 = 1.64					

a = 10.5531(2) Å, Space Group: Fd-3m

Sample 51

Atom	Wyckoff	x	y/z	Occupancy	Uiso
Zn(1)	16d	0.500	0.500	0.193	0.0432(6)
Bi		0.500	0.500	0.807	0.0432(6)
Zn(2)	16c	0.000	0.000	0.286	0.0308(8)
Nb		0.000	0.000	0.714	0.0308(8)
O(1)	48f	0.3157(8)	0.125	1.0000	0.025
O(2)	8b	0.375	0.375	1.0000	0.025
wRp = 16.97 Rp = 14.07 Chi^2 = 2.83					

a = 10.5702(4) Å, Space Group: Fd-3m

Sample 73

Atom	Wyckoff	x	y/z	Occupancy	Uiso
Zn(1)	16d	0.500	0.500	0.266	0.0689(9)
Bi		0.500	0.500	0.733	0.0689(9)
Zn(2)	16c	0.000	0.000	0.254	0.0260(8)
Nb		0.000	0.000	0.754	0.0260(8)
O(1)	48f	0.3188(8)	0.125	1.0000	0.025
O(2)	8b	0.375	0.375	1.0000	0.025
wRp = 18.69 Rp = 15.85 Chi^2 = 2.49					

a = 10.5574(1) Å, Space Group: Fd-3m

[+] See Figure 6 in the paper for graphical comparison of starting experimental compositions and those calculated from Rietveld refinement

[*] Thermal and occupancy parameters for oxygen sites O(1) and O(2) are fixed in these cases as the XRD data are insensitive to oxygen atoms dominated by heavier cations. Results given for sample 37 (in the paper) show a fixed oxygen occupancy according to the speculative oxygen content from experimental phase diagram studies