High-Pressure Synthesis and Local Structure of Corundum-Type $In_{2-2x}Zn_xSn_xO_3$ ($x \leq 0.7$)

Supporting Information

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X-ray diffraction (XRD) patterns of *cor*-$In_{0.8}Zn_{0.6}Sn_{0.6}O_3$ ($x = 0.6$) were calculated based on the space groups *R3c* (average $LiNbO_3$-type arrangement, Table S1) and *R-3c* (average corundum-type arrangement, Table S2). The fractional coordinates of the In, Sn and Zn cations were the same for each Wyckoff position. The program PowderCell[S1] was used to calculate the diffraction pattern with a selected wavelength of 0.412 Å and a 0.002° step in 2θ. The peaks were computed using a pseudo-Voigt profile and a constant FWHM = 0.012° in 2θ to simulate the experimental high-resolution XRD data.

The calculated XRD pattern of *cor*-$In_{0.8}Zn_{0.6}Sn_{0.6}O_3$ ($x = 0.6$), based on the *R3c* space group, used the fractional coordinates that were determined for the $LiNbO_3$-type $ZnSnO_3$ unit cell reported by Inaguma, *et al*. (reference 13 in the main text). Half of the In were substituted on the Zn site and half of the In were substituted on the Sn site.

	Wyckoff	*x/a*	*y/b*	*z/c*	SOF	B (temp)
Zn	6a	0	0	0.2859	0.6	0.5
In	6a	0	0	0.2859	0.4	0.5
Sn	6a	0	0	0.0000	0.6	0.5
In	6a	0	0	0.0000	0.4	0.5
O	18b	0.0405	0.350	0.0709	1.0	0.5

Table S1. Unit cell used to calculate expected XRD pattern of $LiNbO_3$-type *cor*-$In_{0.8}Zn_{0.6}Sn_{0.6}O_3$ ($x = 0.6$). Space group *R3c*, $a = 5.365$, $c = 14.322$ Å.

The calculated XRD pattern of *cor*-$In_{0.8}Zn_{0.6}Sn_{0.6}O_3$ ($x = 0.6$), based on the *R-3c* space group, used the fractional coordinates that were determined for the corundum In_2O_3 unit cell reported by Prewitt, *et al*. (reference 11 in the paper). Zn and Sn were substituted onto the In site. Although short-range ordering may be present, the average structure would appear corundum-like.

	Wyckoff	*x/a*	*y/b*	*z/c*	SOF	B (temp)
In	12c	0	0	0.3573	0.4	0.5
Zn	12c	0	0	0.3573	0.3	0.5
Sn	12c	0	0	0.3573	0.3	0.5
O	18e	0.298	0	0.25	1.0	0.5

Table S2. Unit cell used to calculated expected XRD pattern of corundum-type *cor*-$In_{0.8}Zn_{0.6}Sn_{0.6}O_3$ ($x = 0.6$). Space group *R-3c*, $a = 5.365$, $c = 14.322$ Å.

The simulated diffraction patterns show a small difference in relative intensities, which are listed in Table S3 for the first ten reflections. The relative intensities of the experimental high-resolution XRD data ($x = 0.6$) are also listed in Table S3 for comparison. The calculated

and experimental diffraction patterns are plotted in Figure S1 and it is apparent that the expected diffraction patterns of *cor*-$In_{0.8}Zn_{0.6}Sn_{0.6}O_3$ ($x = 0.6$) based on the space groups *R3c* and *R-3c* are very similar to each other. The relative intensities of the first three peaks suggests $LiNbO_3$-type ordering is present. The origin of the differences of the experimental and calculated relative peak intensities for the (113) and (116) reflections remains unknown.

hkl	d (Å)	I_{rel} (*R3c*)	I_{rel} (*R-3c*)	I_{rel} (*x = 0.6*)
012	3.8977	24.78	19.13	23
104	2.8361	100.00	100.00	100
110	2.6825	88.84	89.58	89
006	2.3870	4.70	4.09	5
113	2.3386	5.86	5.92	8
202	2.2097	2.84	1.98	3
024	1.9489	42.69	42.52	45
116	1.7832	38.52	37.21	53
211	1.7431	0.27	0.32	0

Table S3. Relative intensities of the calculated diffraction peaks for *cor*-$In_{0.8}Zn_{0.6}Sn_{0.6}O_3$ ($x = 0.6$) based on the *R3c* and *R-3c* space groups and the high-resolution XRD data.

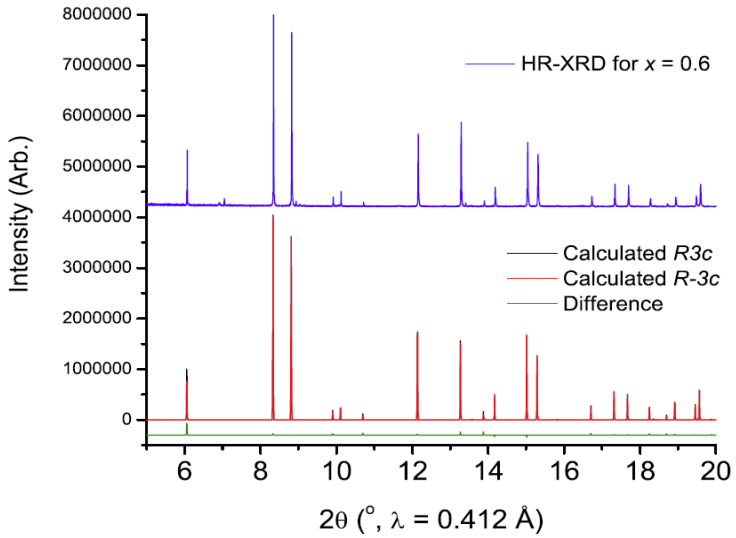

Figure S1. The experimental high-resolution XRD pattern of *cor*-$In_{0.8}Zn_{0.6}Sn_{0.6}O_3$ ($x = 0.6$, top blue line) and the calculated XRD patterns of *cor*-$In_{0.8}Zn_{0.6}Sn_{0.6}O_3$ based on the *R3c* space group (black line) and the *R-3c* space group (red line). The difference pattern of the calculated XRD patterns based on the space groups *R3c* and *R-3c* is plotted on the bottom (green line). The peaks observed in the experimental pattern (top) at $2\theta \sim 7°$ are due to trace amounts of SnO_2 and an unknown phase.

References

S1. Kraus, W. and Nolze, G., *J. Appl. Cryst.* **1996**, *29*, 301-303.