Supplementary Information for:

Dual Ionic Conductivity in $Ba_3InGa_2O_{7.5}$: Correlating Structure and Electrochemical Properties

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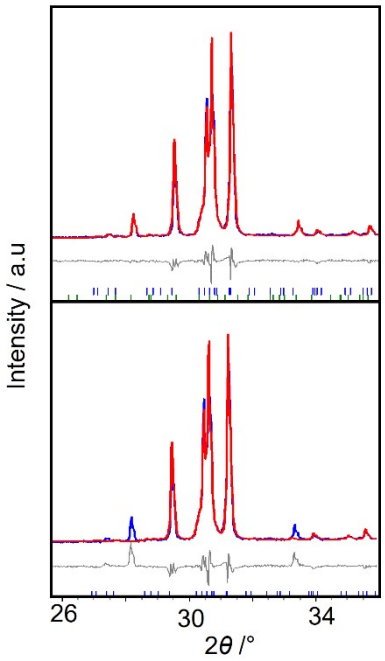

Fig. S1 Partial XRD pattern collected on $Ba_3InGa_2O_{7.5}$ after initial 20-hour synthesis fitted with *P*2/*c* model and both with and without $BaGa_2O_4$ included as a secondary phase. The peaks at ~28.0 and 33.2° are also present in the work of Kochetova *et al*.[1]

Table S1. Crystallographic data for room temperature $Ba_3InGa_2O_{7.5}$ with unit-cell parameters *a* = 7.9557(13) Å, *b* = 5.8762(9) Å, *c* = 18.2237(3) Å and β = 91.570(1) ° in space group *P*2/*c*.

Atom	Site	*x*	*y*	*z*	Occ.	B_{iso} /Å^2
Ba1	2*e*	0	0.267(3)	0.25	1	1.51(3)
Ba2	2*f*	0.5	0.295(2)	0.25	1	1.51(3)
Ba3	4*g*	0.0267(6)	0.754(2)	0.0871(3)	1	1.51(3)
Ba4	4*g*	0.5007(7)	0.246(2)	0.5802(4)	1	1.51(3)
In1	4*g*	0.2443(7)	0.250(2)	0.4109(4)	0.86(2)	0.67(4)
Ga1	4*g*	0.2443(7)	0.250(2)	0.4109(4)	0.14(2)	0.67(4)
Ga2	4*g*	0.244(2)	0.254(3)	0.0595(6)	1	0.67(4)
Ga3	4*g*	0.223(1)	0.767(3)	0.2699(5)	0.86(2)	0.67(4)
In2	4*g*	0.223(1)	0.767(3)	0.2699(5)	0.14(2)	0.67(4)
O1	2*e*	0	0.78(1)	0.25	1	0.2(2)
O2	4*g*	0.046(4)	0.74(1)	0.604(2)	1	0.2(2)
O3	4*g*	0.470(4)	0.25(2)	0.092(2)	1	0.2(2)
O4	4*g*	0.268(4)	0.169(6)	0.293(2)	1	0.2(2)
O5	4*g*	0.233(6)	0.536(7)	0.337(3)	1	0.2(2)
O6	4*g*	0.254(6)	0.543(7)	0.491(3)	1	0.2(2)
O7	4*g*	0.233(5)	0.983(8)	0.004(3)	1	0.2(2)
O8	4*g*	0.363(4)	0.296(7)	0.691(2)	1	0.2(2)

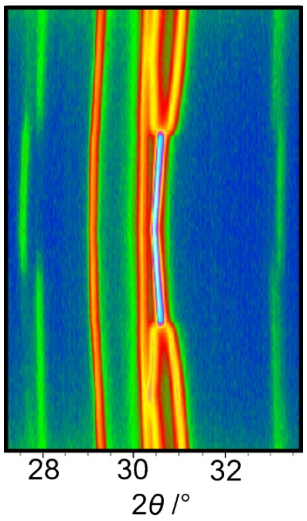

Fig. S2 Expanded view of 30-1000-30 °C VT-PXRD patterns in the 2θ region of ~27-34° showing the evolution of the 2 wt% $BaGa_2O_4$ impurity phase with temperature through the peaks at ~28.0 and 33.2°.

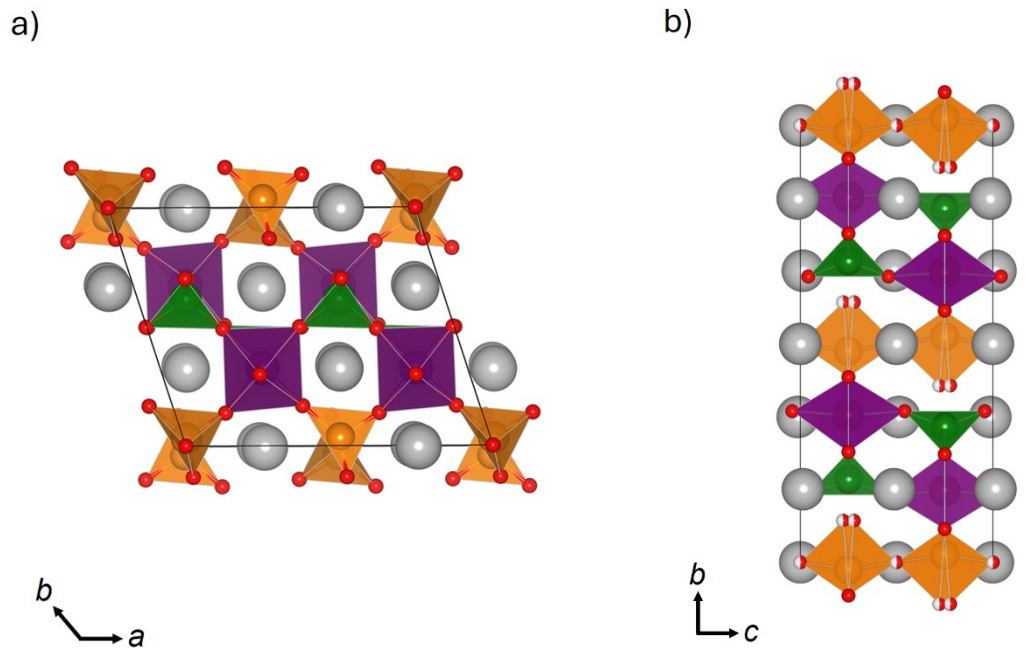

Fig. S3 The potential high temperature structural models. a) The $P2_1/a$ model. b) The final *Cmcm* model. (A^{2+} in grey, Oh^{3+} in purple, Td^{3+} in green/orange and O^{2-} in red).

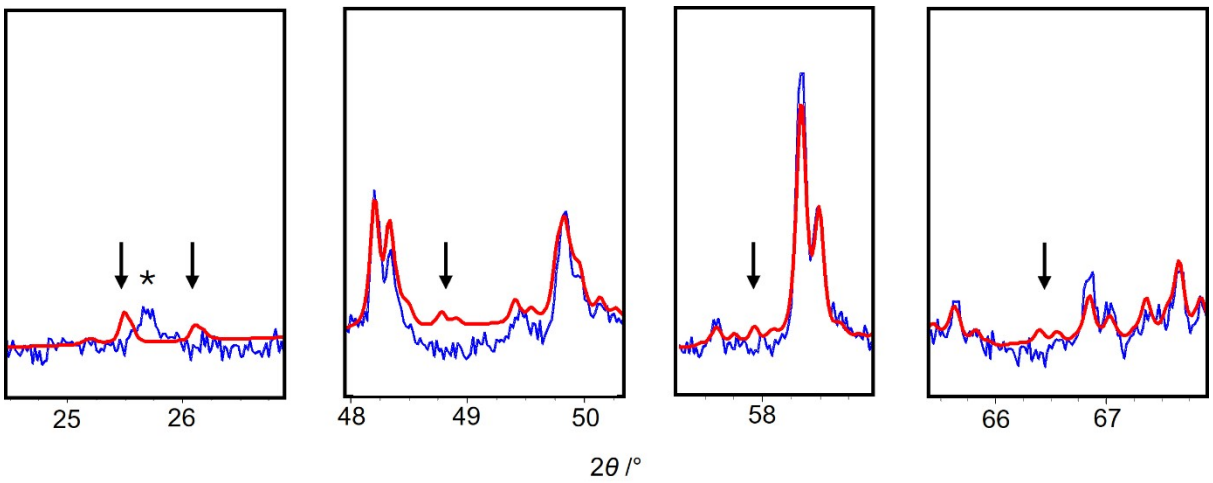

Fig. S4 Example 2θ regions from the Rietveld fit of the $P2_1/a$ model against the high temperature PXRD pattern for $Ba_3InGa_2O_{7.5}$. The peak marked with an ‘ ’ is a minor impurity peak.

Table S2. Crystallographic data for $Ba_3InGa_2O_{7.5}$ at 1000 °C with unit-cell parameters *a* = 5.9251(3) Å, *b* = 18.4230(7) Å, *c* = 8.0957(3) Å in space group *Cmcm*.

Atom	Site	*x*	*y*	*z*	Occ.	B_{iso} /Å^2
Ba1	4*b*	0	0.5	0	1	2.75(7)
Ba2	8*f*	0	0.1674(4)	0.0133(5)	1	2.75(7)
In1	4*c*	0	0.3364(6)	0.25	0.88(3)	1.2(2)
Ga1	4*c*	0	0.3364(6)	0.25	0.12(3)	1.2(2)
Ga2	4*c*	0	0.6896(7)	0.25	1	1.0(2)
Ga3	4*c*	0	0.9834(7)	0.25	0.88(3)	1.0(2)
In2	4*c*	0	0.9834(7)	0.25	0.12(3)	1.0(2)
O1	4*a*	0	0	0	0.5	1.5(3)
O2	8*f*	0	0.654(2)	0.042(2)	1	1.5(3)
O3	8*g*	0.256(7)	0.924(3)	0.25	1	1.5(3)
O4	8*g*	0.753(6)	0.753(3)	0.25	1	1.5(3)
O5	8*f*	0	0.095(3)	0.278(8)	0.5	1.5(3)

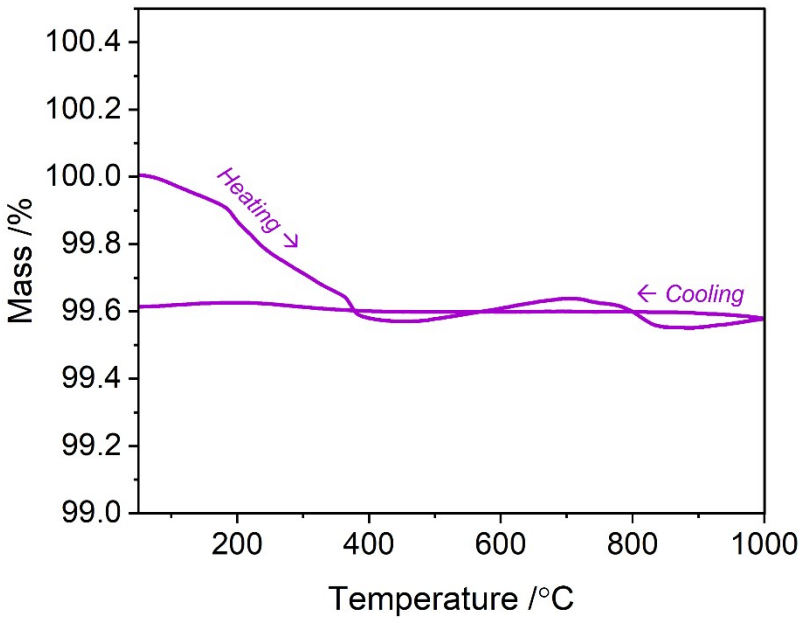

Fig. S5 TGA trace on heating and cooling for $Ba_3InGa_2O_{7.5}$.

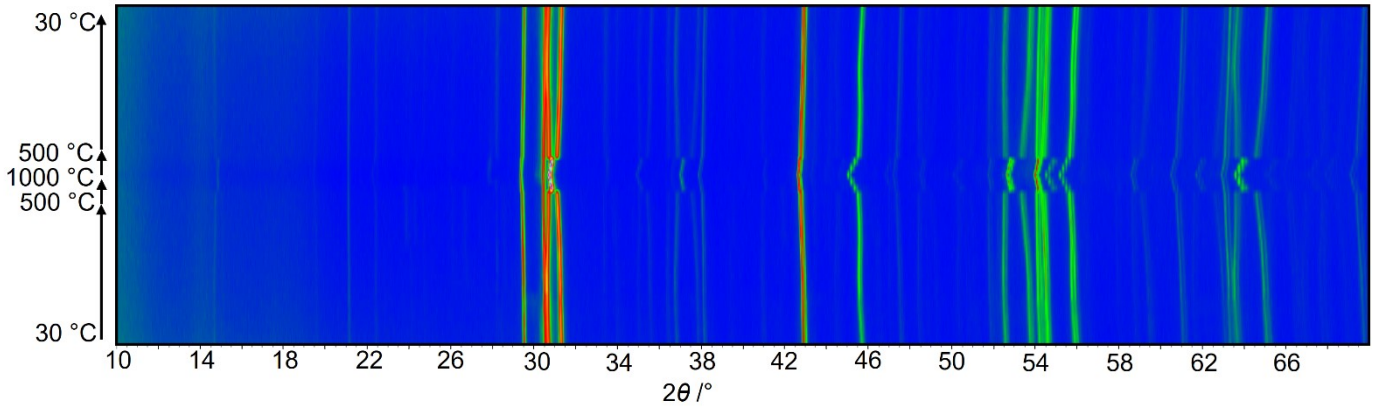

Fig. S6 Powder X-ray diffraction patterns of $Ba_3InGa_2O_{7.5}$, viewed as a colour map where blue and red correspond to regions of low and high intensity, as a function of temperature between 30 and 1000 °C. The limited number of data points above 500 °C is due to larger temperature intervals.

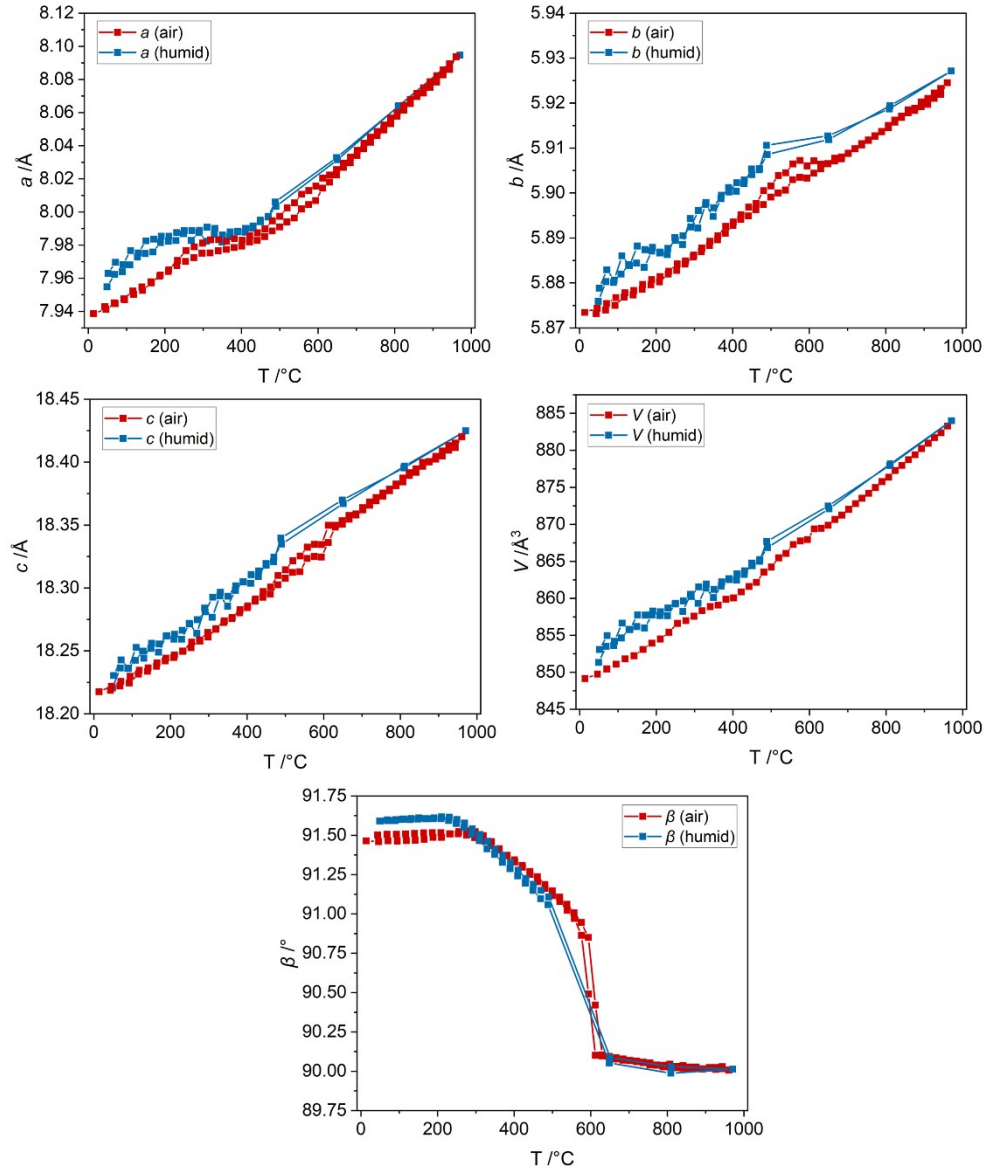

Fig. S7 Extracted unit-cell parameters as a function of temperature under humidified and normal atmospheres.

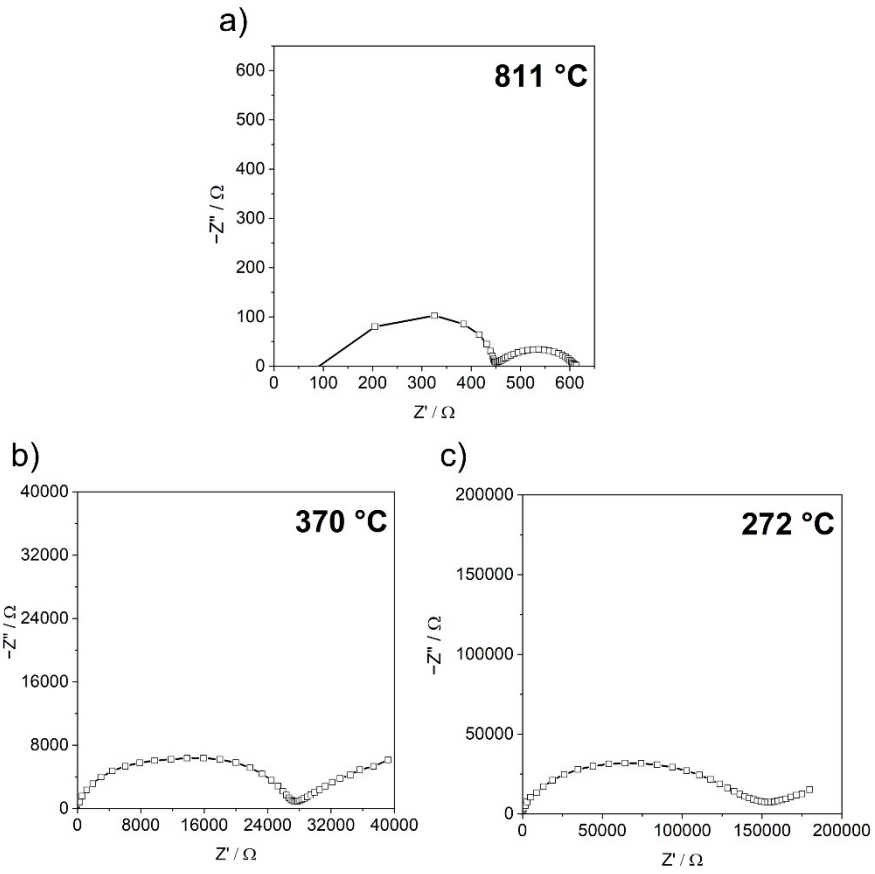

Fig. S8 Complex plane plots at a) 811 °C b) 370 °C and c) 272 °C for $Ba_3InGa_2O_{7.5}$ measured in air.

References

[1] N. Kochetova, V. Cherepanova, A. Pikalova and A. Gilev, *Chim. Techno Acta*, 2024, **11**, 202411102.