Journal Name

ARTICLE

Dynamics in Bi(III)-containing Apatite-Type Oxide Ion Conductors: A Combined Computational and Experimental Study

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Supplementary Information

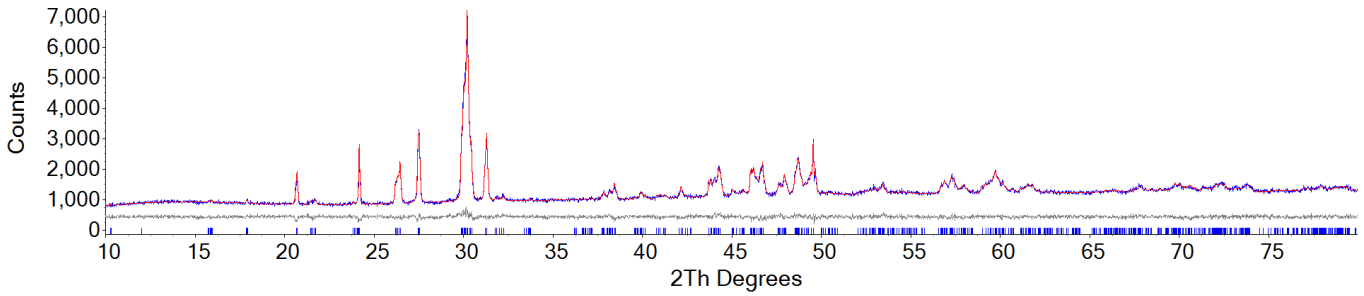

Fig. S1: Rietveld refinement of $Bi_2La_8Ge_6O_{27}$ carried out using the structural model of Tate et al.[1] and laboratory X-ray diffraction data, confirming the purity of the sample used for the neutron scattering experiment. The observed pattern is shown in blue, calculated in red and the difference curve in grey.

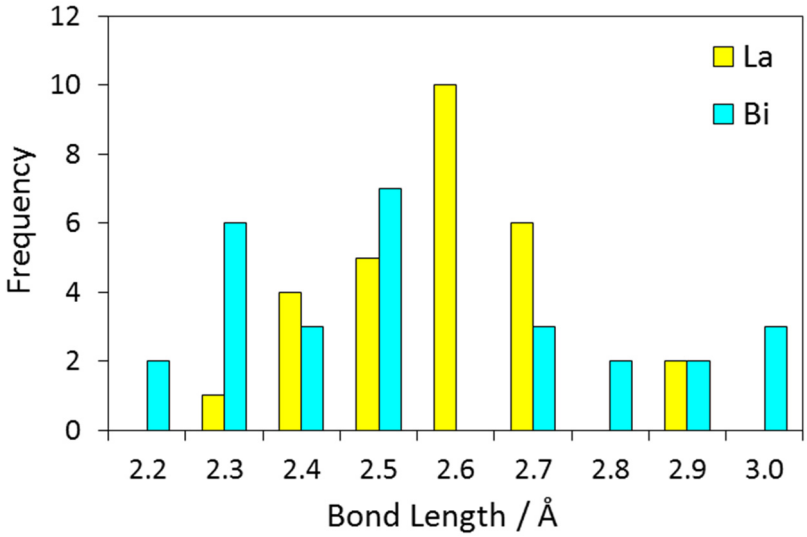

Fig. S2: Distribution of bond lengths to oxygen for the Bi atoms in $Bi_2La_8Ge_6O_{27}$ (blue) and the La atoms on the equivalent sites in $La_{10}Ge_6O_{27}$ (yellow). On doping with Bi the coordination environment becomes less symmetric, with some of the bonds to oxygens becoming shorter than those in the parent material and some longer.

Table S1: The Mulliken bond populations and M-O bond lengths for four A2 sites containing La in $La_{10}Ge_6O_{27}$ and Bi in $Bi_2La_8Ge_6O_{27}$

Bonded Oxygen	Bi Site 1		Bi Site 2		Bi Site 3		Bi Site 4	
	La-O Bond Population	Bi-O Bond Population	La-O Bond Population	Bi-O Bond Population	La-O Bond Population	Bi-O Bond Population	La-O Bond Population	Bi-O Bond Population
O1	0.14	0.02	0.13	0.01	0.12	0.03	0.16	0.03
O2	0.17	0.11	0.14	0.04	0.15	0.05	0.19	0.11
O3a	0.15	0.07	0.22	0.09	0.23	0.06	0.15	0.08
O3b	0.15	0.14	0.21	0.19	0.20	0.16	0.21	0.14
O3c	0.19	0.22	0.30	0.23	0.29	0.28	0.19	0.21
O3d	0.27	0.13	0.21	0.13	0.22	0.17	0.26	0.14
O4	0.33	0.24	0.36	0.24	0.33	0.24	0.38	0.22

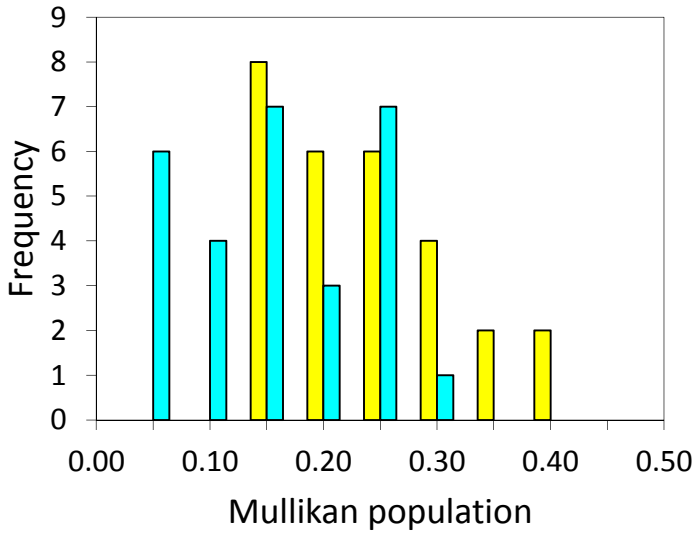

Fig. S3: Distribution of Mullikan populations for the Bi atoms in $Bi_2La_8Ge_6O_{27}$ (blue) and the La atoms on the equivalent sites in $La_{10}Ge_6O_{27}$ (yellow).

References

1. M. Tate, D. Blom, M. Avdeev, H. Brand, G. McIntyre, T. Vogt and I. Evans, *Advanced Functional Materials*, 2017, **27**.