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Lithium-ion conductivity in $\text{Li}_6\text{Y}(\text{BO}_3)_3$: a thermally and electrochemically robust solid electrolyte[†]

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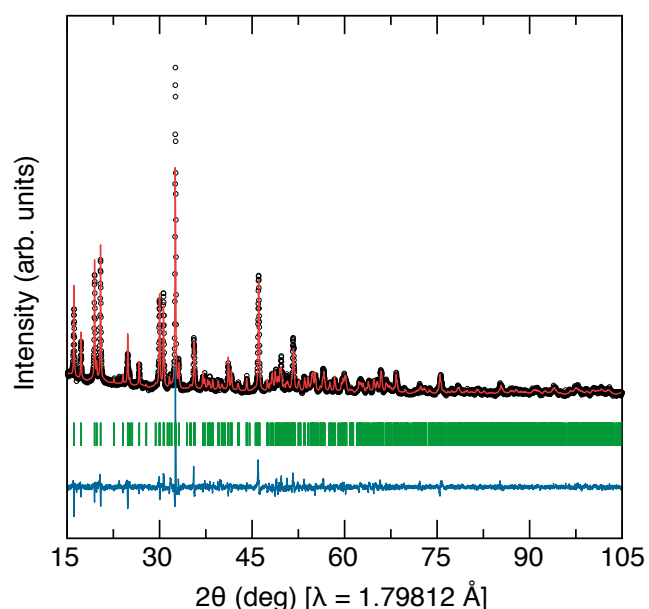


Figure S 1 Results of the Rietveld refinement of laboratory X-ray diffraction data on $\text{Li}_6\text{Y}(\text{BO}_3)_3$. $R_{\text{Bragg}}=9.5\%$. The reflection markers (green) show no secondary reflections of any possible secondary phases.

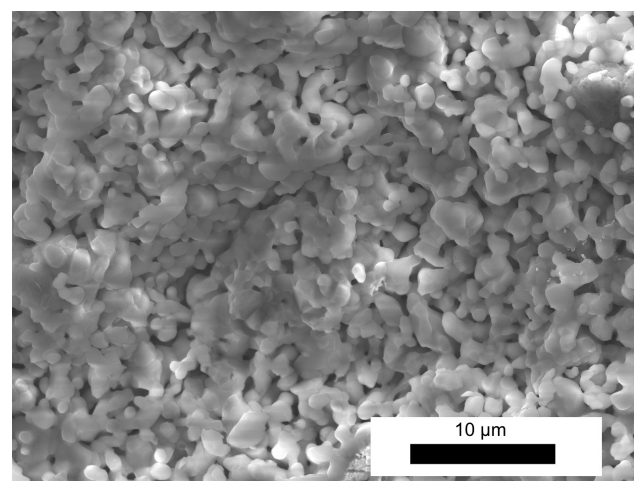


Figure S 2 Scanning electron microscopy micrographs of a fractured surface of $\text{Li}_6\text{Y}(\text{BO}_3)_3$ in secondary electron mode, showing a $\sim 70\%$ dense materials with grain sizes between $1 \mu\text{m}$ to $5 \mu\text{m}$ and good connectivity between the grains. The random orientation of the grains corroborates a negligible degree of preferred orientation.

Table S 1 Temperature dependent lithium ion conductivity of $\text{Li}_6\text{Y}(\text{BO}_3)_3$, obtained using AC impedance measurements

T (K)	σ ($\text{S}\cdot\text{cm}^{-1}$)
323	$1.93\cdot 10^{-8}$
373	$3.23\cdot 10^{-7}$
423	$2.64\cdot 10^{-6}$
473	$1.57\cdot 10^{-5}$
523	$4.71\cdot 10^{-5}$
573	$1.74\cdot 10^{-4}$
623	$7.04\cdot 10^{-4}$
673	$2.27\cdot 10^{-3}$
723	$6.59\cdot 10^{-3}$
773	$1.75\cdot 10^{-2}$

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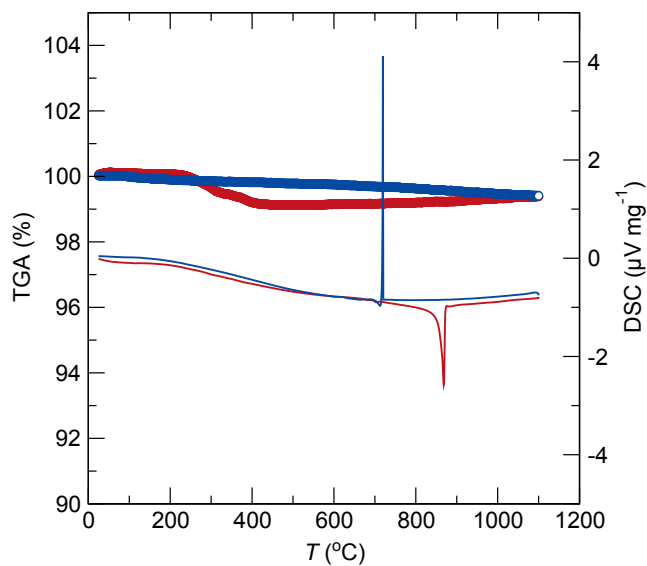


Figure S 3 Thermal analysis of $\text{Li}_6\text{Y}(\text{BO}_3)_3$ exhibits no changes in weight or reactions up to the melting point of 870° . The very minor change in weight, on the order of 1%, can be attributed to small errors associated with changes in buoyancy or potentially the evaporation of a small amount of surface moisture.

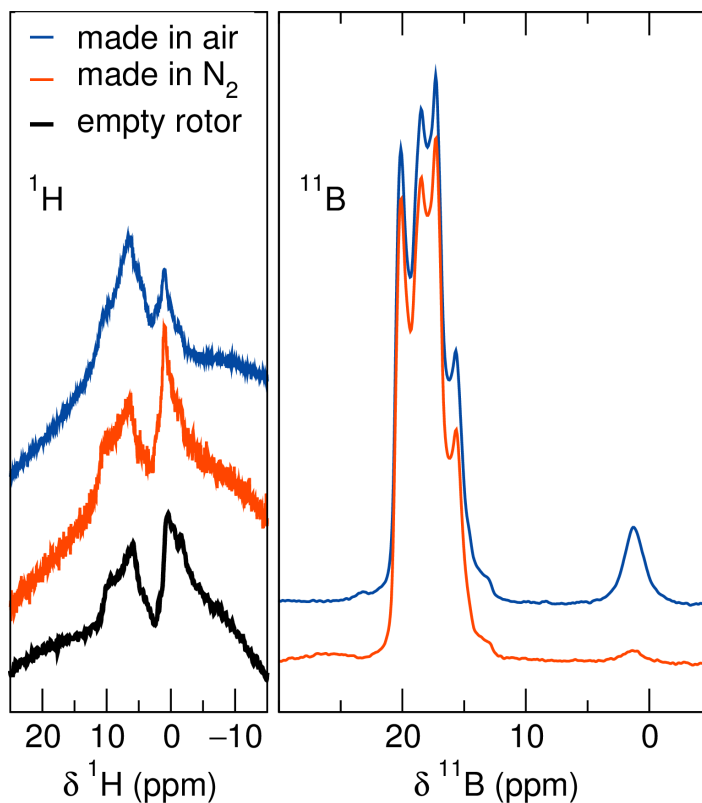


Figure S 4 ^1H and ^{11}B MAS NMR spectra of $\text{Li}_6\text{Y}(\text{BO}_3)_3$ samples prepared by heating in air or N_2 .

Table S 2 Energy of formation for vacancies at various Li positions, ΔE_f and energies relative to the most stable vacancy position, ΔE_{vac} .

Li site	ΔE_f (eV)	ΔE_{vac} (eV)
A	4.094	0.000
B	4.267	0.174
C	4.401	0.307
D	4.512	0.418
E	4.715	0.621
F	4.794	0.701