

Supplementary information

Superionic Conduction in β -eucryptite: Inelastic Neutron Scattering and Computational Studies

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The phase purity of the LiAlSiO_4 sample is ascertained from the Rietveld refinement of the XRD data and compared with the reported structural parameters for β -eucryptite [25-29]. The crystalline nature of the sample is reflected as the sharp diffraction lines in the XRD pattern. Also the observed peaks in the diffraction pattern do not show any anomalous broadening attributable to size and strain induced effects and hence indicate the microcrystalline nature of the sample. The broadening is similar to the instrumental broadening as seen from the Si standard reference powder. The refined structural parameters (Table 1S) and the Rietveld refinement plot (Fig. 1S) for LiAlSiO_4 are given in the supplementary information. The refined unit cell parameters as observed from the powder XRD data are: $a = 10.4959(5) \text{ \AA}$, $c = 11.1625(8) \text{ \AA}$ and $V = 1064.9(1) \text{ \AA}^3$, which are in very good agreement with the previously reported unit cell parameters [26,28,29].

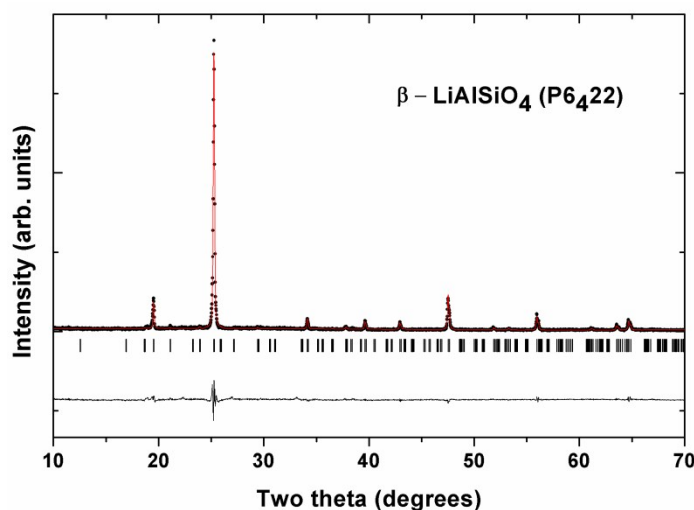


Figure-1S Rietveld refinement plot of powder XRD data of LiAlSiO_4 at ambient temperature. (Rp: 14.0 %, Rwp: 18.3 %, χ^2 : 2.25), Space Group: $P6_422$)

Table-1S: Refined position coordinates of LiAlSiO₄ at ambient temperature.

Atoms	Wyc.	x	y	z
Al1	<i>6h</i>	0.2513(5)	0	0.5
Al2	<i>6j</i>	0.2505(3)	0.5008(7)	0.5
Si1	<i>6g</i>	0.2481(5)	0	0
Si2	<i>6i</i>	0.2469(3)	0.4938(7)	0
O1	<i>12k</i>	0.0891(10)	0.1912(8)	0.2502(14)
O2	<i>12k</i>	0.6033(20)	0.7010(11)	0.2657(18)
O3	<i>12k</i>	0.1096(21)	0.7104(12)	0.2597(21)
O4	<i>12k</i>	0.5921(14)	0.2032(10)	0.2510(13)
Li1	<i>3b</i>	0	0	0.5
Li2	<i>3c</i>	0.5	0	0
Li3	<i>6f</i>	0.5	0	0.3229(8)

Hexagonal, Space Group: P6₄22, No. 181)

a = 10.4959(5)Å, c = 11.1625(8) Å, V = 1064.9(1) Å³, Z = 12.

B_{ov} = 3.5(1) Å²

Rp: 14.0 %, Rwp: 18.3 %, χ^2 : 2.25, R_B : 9.50 %