Supplementary Information

Stannaborates: Tuning the Ion Conductivity of Dodecaborate Salts with Tin Substitution

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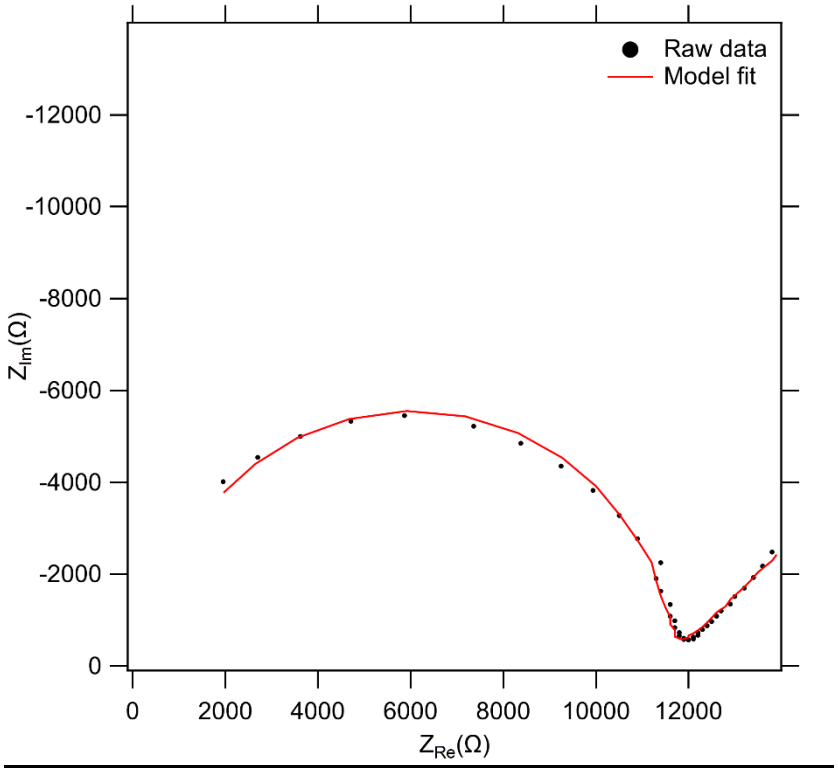

Figure S1: Example of a Nyquist plot of $Na_2B_{11}H_{11}Sn{\bullet}xH_2O$ at 90 °C, using an R_s-$R_1|C_1$-W circuit model.

Table S1 – Atomic Coordinates of $B_{11}H_{11}Sn^{2-}$ ion

Atom No.	x	y	z
B1	0.255802	0.755762	0.881357
B2	0.205457	0.894609	0.780497
B3	0.372747	0.838548	0.775072
B4	0.371572	0.661241	0.785832
B5	0.201589	0.607139	0.794924
B6	0.100840	0.752155	0.796693
B7	0.110495	0.651556	0.650069
B8	0.112575	0.840286	0.642544
B9	0.294824	0.895553	0.627062
B10	0.403098	0.739727	0.631714
B11	0.289579	0.589437	0.644272
H1	0.262282	0.770772	0.998774
H2	0.172624	1.000000	0.823749
H3	0.459391	0.898628	0.829284
H4	0.459451	0.596902	0.832650
H5	0.175126	0.513352	0.862449
H6	0.000000	0.747252	0.858852
H7	0.019250	0.590763	0.604969
H8	0.018325	0.903601	0.608425
H9	0.336478	0.993048	0.574005
H10	0.508037	0.741887	0.576607
H11	0.313340	0.478982	0.608365
Sn1	0.233488	0.735628	0.482036

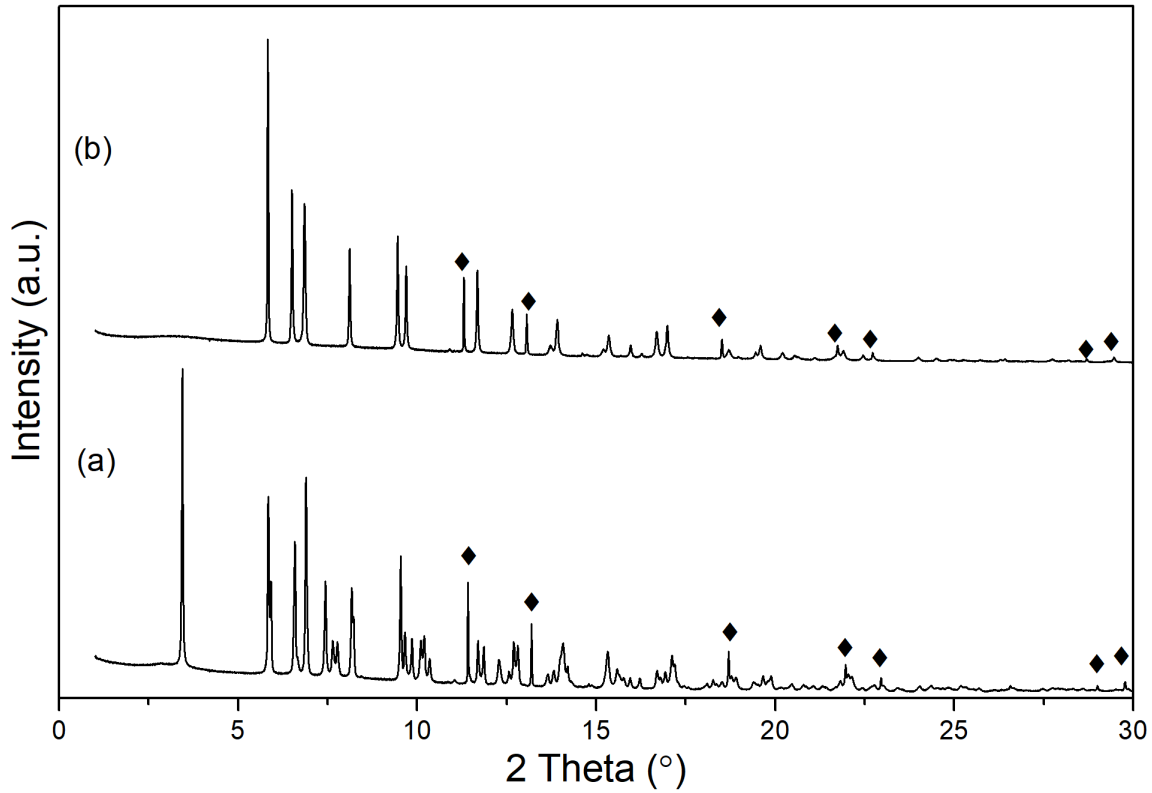

Figure S2. Synchrotron XRD pattern of $Li_2B_{11}H_{11}Sn$ at (a) room temperature and (b) 230 °C. Diamonds represent the peaks for LiCl. λ = 0.59096(1)Å.

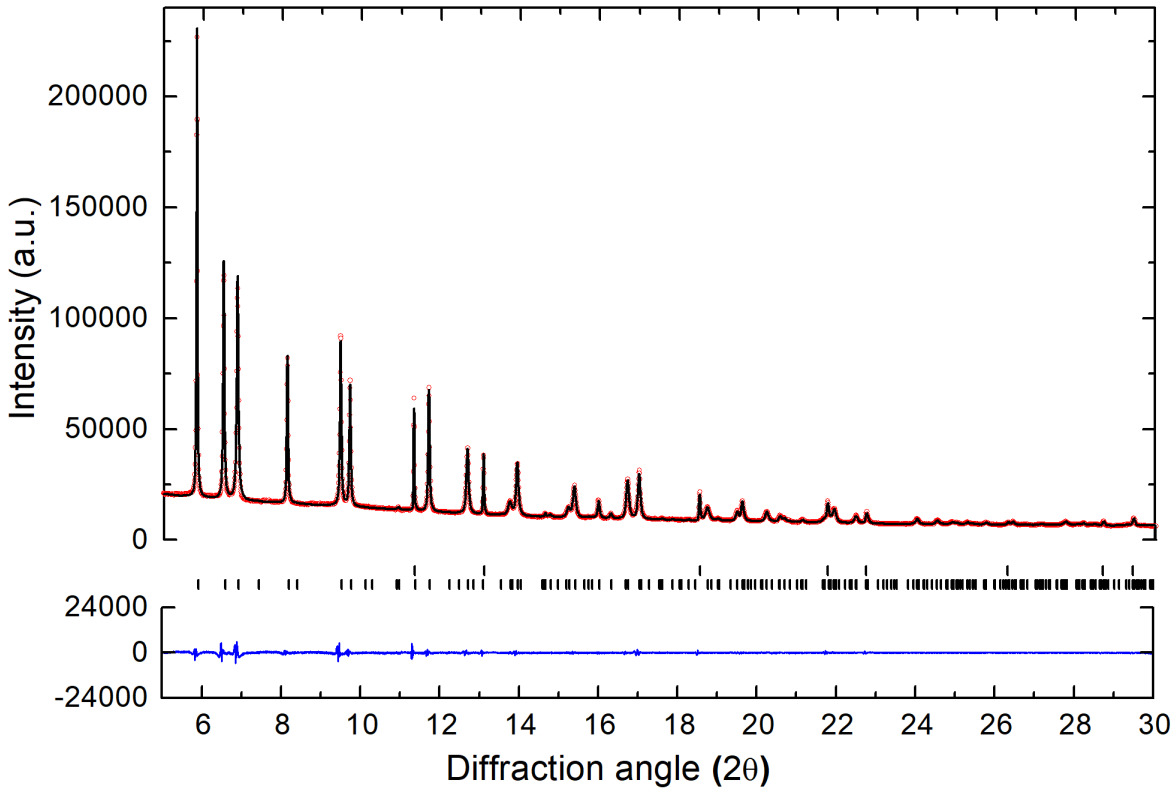

Figure S3. Synchrotron XRD pattern and Le Bail fit of $Li_2B_{11}H_{11}Sn$ at 230 °C. Experimental data as red circles, calculated diffraction pattern as black line and the difference plot in blue. Tick marks show positions for LiCl and $Li_2B_{11}H_{11}Sn$, top to bottom respectively. λ = 0.59096(1)Å. Le Bail plot for employed *hkl*'s for $Li_2B_{11}H_{11}Sn$ generated using space group *P*42/*ncm* with unit cell parameters $a = b = 9.8923(4)$, $c = 10.4149(3)$ giving an $R_{wp} = 2.141$.

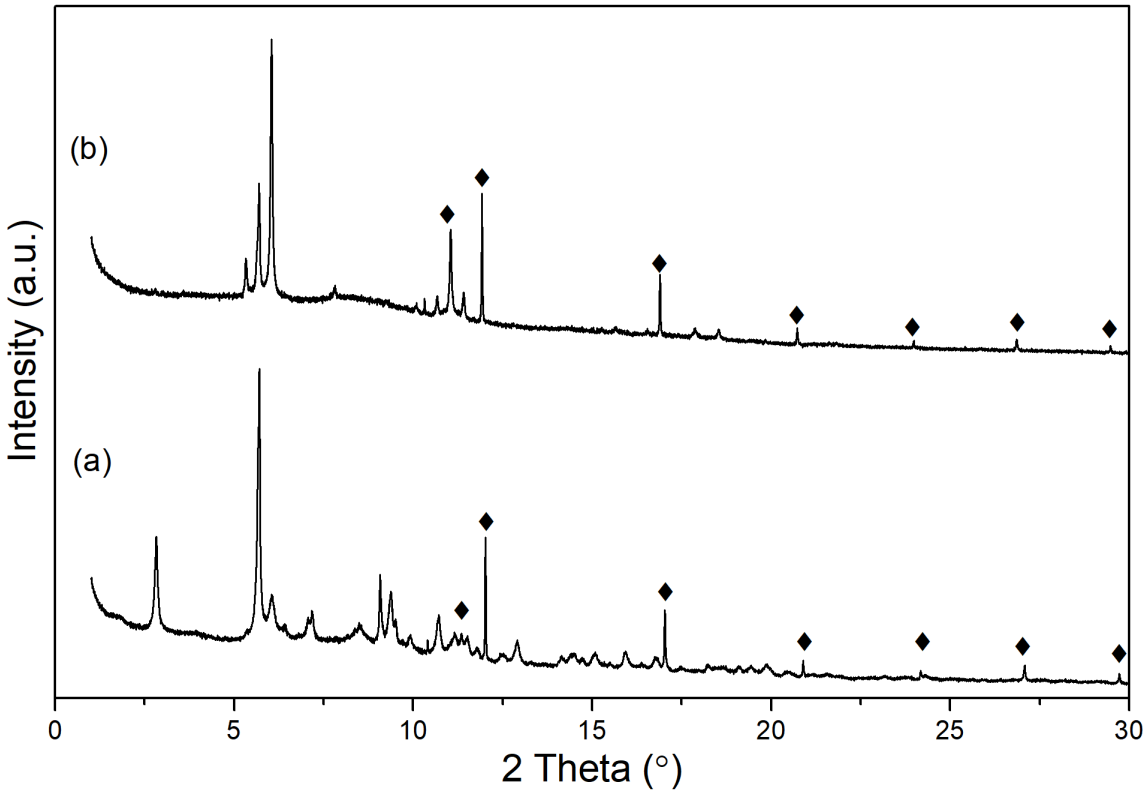

Figure S4. Synchrotron XRD pattern of $Na_2B_{11}H_{11}Sn$ at (a) room temperature and (b) 217 °C. Diamonds represent the peaks for NaCl. λ = 0.59096(1)Å.

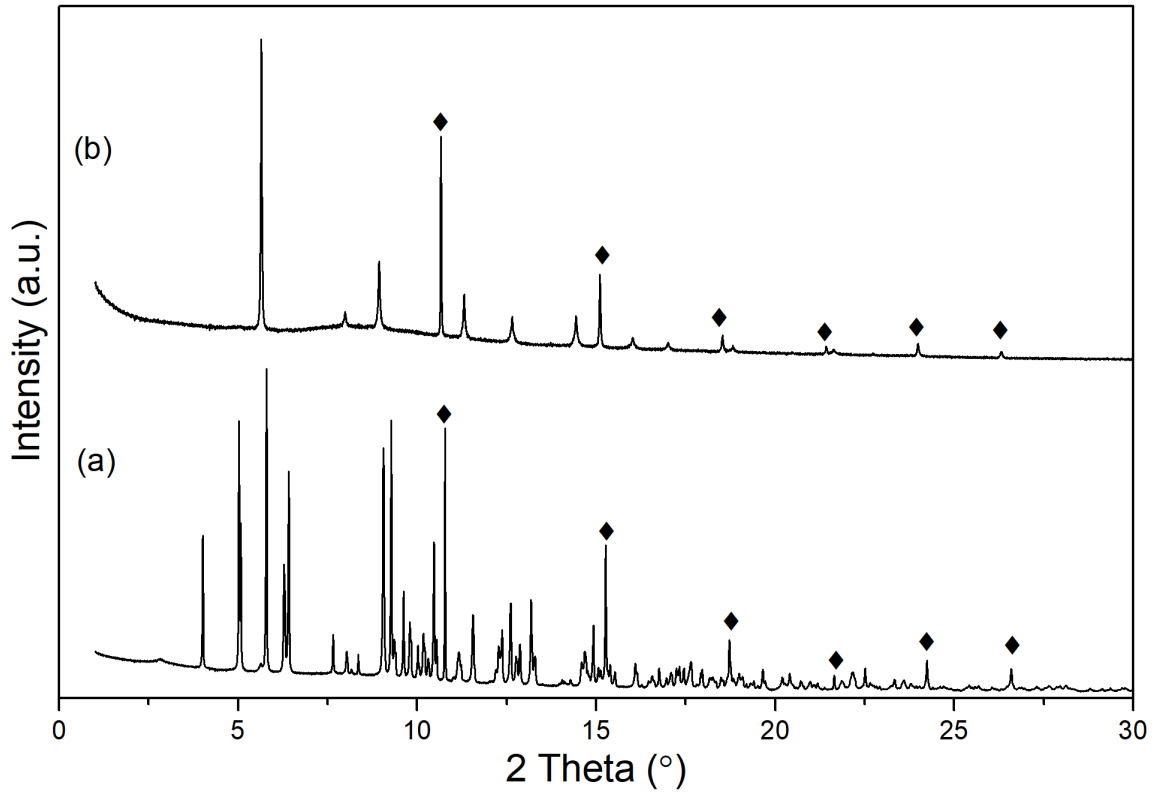

Figure S5. Synchrotron XRD pattern of $K_2B_{11}H_{11}Sn$ at (a) room temperature and (b) 278 °C. Diamonds represent the peaks for KCl. λ = 0.59096(1)Å.

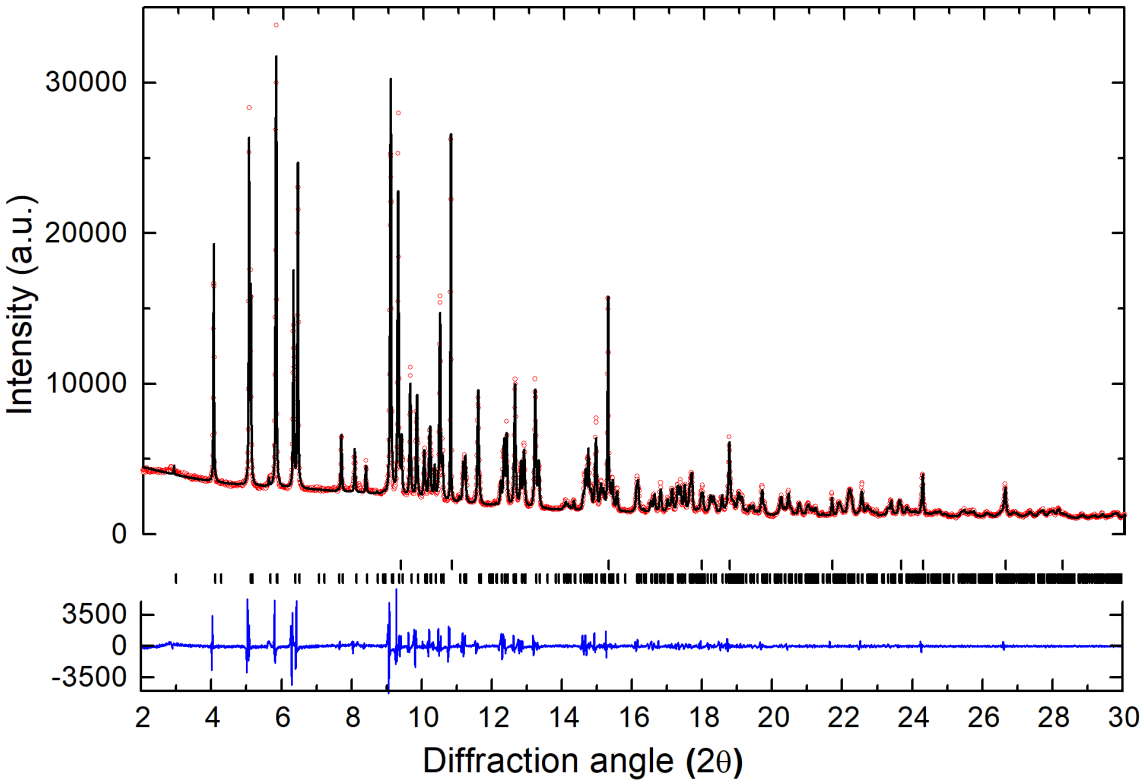

Figure S6. Synchrotron XRD pattern and Le Bail fit of $K_2B_{11}H_{11}Sn$ at room temperature. Experimental data as red circles, calculated diffraction pattern as black line and the difference plot in blue. Tick marks show positions for LiCl and $K_2B_{11}H_{11}Sn$, top to bottom respectively. λ = 0.59096(1)Å. Le Bail plot for employed *hkl*'s for $K_2B_{11}H_{11}Sn$ generated using space group $P2_12_12$ with unit cell parameters a = 11.7216(3), b = 8.1006(1), c = 12.0948(3) giving an R_{wp} = 6.505.