Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Structure, Stoichiometry and Transport Properties of Lithium Copper Nitride Battery Materials: Combined NMR and Powder Neutron Diffraction Studies

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Electronic Supplementary Information

Linewidth of the ^{7}Li Central Transition

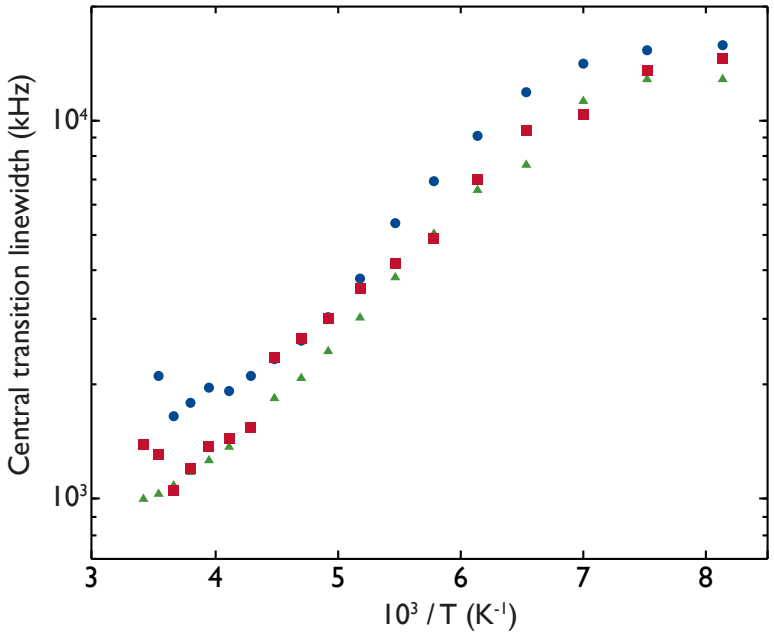

Figure S1. Linewidth of the ^{7}Li central transition as a function of temperature for **1** (blue circles), **2** (green triangles) and **3** (red squares).

Calculation of Diffusion Coefficients

Diffusion coefficients for intra- and inter-layer processes are obtained from the corresponding mean Li^{+} jump rate by the Einstein-Smoluchowski relation

$$D = \frac{d^2 f\nu}{g}$$

where d is the distance between Li sites and g is a dimensionality factor. Ion hopping was assumed to be uncorrelated in both cases. so that f was set to 1. For intra-layer diffusion the dimensionality factor g is 4 and d is the distance between adjacent Li(2) sites measured by neutron diffraction (Table 2). For inter-layer diffusion g is 2 and d is the distance between the exchanging Li(1) and Li(2) sites obtained by neutron diffraction (Table 2).

Calculation of High-temperature ^{7}Li C_Q Values

Low-temperature ^{7}Li C_Q values for the Li(1) site which vary with Li environment were obtained by spectral simulation as described in the main text. Table S1 shows an average low-temperature C_Q for the Li(1) site in each material obtained from Table 3 and low-temperature ^{7}Li C_Q values for the Li(2) site which are obtained directly from the spectra recorded at 193 K in Figure 3. Weighting by the occupancies of the Li(1) and Li(2) sites results in the average high-temperature $\langle C_Q \rangle$.

Table S1. Experimental low-temperature and calculated high-temperature Li(1) and Li(2) C_Q values

Sample (x)	**1** (0.17)	**2** (0.29)	**3** (0.35)
Li(1) Occupancy	0.83	0.71	0.65
Li(2) Occupancy	2	2	2
C_Q Li(1) / kHz	575	568	562
C_Q Li(2) / kHz	-266	-259	-253
HT $\langle C_Q \rangle$	-19	-42	-53