In situ and ex situ Raman studies on $LiBH_4$ and related compounds

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Abstract

We have obtained in situ temperature dependent Raman and synchrotron X-ray diffraction data for $LiBH_4$ between 300 and 393K. We have obtained separately further temperature dependent Raman data beween 7 and 450 K as well as synchrotron powder diffraction data at low temperatures.
The in situ experiment reveals directly from the X-ray data that at the phase transition, both phases coexist, while this does not appear so clearly in the Raman data. The first order nature is seen in a heating and cooling run for the Raman spectra alone and reveals clearly a hysteresis loop.
The temperature dependent Raman data show significant spectral shifts in the lattice mode region. Using the available thermal expansion data obtained at SNBL, we can model the quasi-harmonic contribution (related to the lattice expansion) to the Raman band shift for two well defined lattice modes. It appears that above ca 80 K, a further anharmonic contribution must be considered.
It is also interesting to note that above ca 80K, the splitting of the E –symmetry deformation band of the BH_4^- ions starts to decrease significantly from ca 47 cm^{-1} at 10 K to 20 cm^{-1} at the phase transition.
Preliminary results on other systems will be presented.