Abstract

Vibrational Properties of Closo–Borane Anions in Superionic Conductors †

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Metal closo-borate compounds have attracted recent attention as superionic lithium or sodium conductors. In Na₂B₁₂H₁₂ or Li₂B₁₂H₁₂ the superionic phases are related to the temperature induced phase transitions [1]. Modification of the crystal structure or ion substitution provide the means of tuning their cation conductivity. Spectroscopic fingerprint of internal \textit{closo} anion (B₁₂H₁₂²⁻) vibrations provides unique opportunity to study influence of such modification in the crystal properties. Dynamical fingerprint of anion vibrations is related to the nature of cation–anion interactions.

We report on theoretical calculations of the change of IR and Raman modes of B₁₂H₁₂ structure upon deformation along the high symmetry axes as well as interaction of such anion with model configuration of cations. These anions are aromatic structures and even smallest deformations are related to changes in B–H stretching frequencies of entire structure. Deformation is related to change of the electronic structure that extends over entire anion, Figure 1. Our systematic studies of anion dynamical properties are confronted with experimental evidence of Raman modes and cation conductivity.

![Figure 1](https://example.com/figure1.png)

\textbf{Figure 1.} The charge density difference of B₁₂H₁₂ \textit{closo} anion deformed along C₃ symmetry axis (a) and C₁ axis (b). Yellow colour is for charge accumulations, cyan–charge depletion. Yellow balls are for colour, grey–hydrogen.
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