

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 $\text{Na}_2\text{B}_{12}\text{H}_{12}$ or $\text{Li}_2\text{B}_{12}\text{H}_{12}$ 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 *closo* anion ($\text{B}_{12}\text{H}_{12}^{2-}$) 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 $\text{B}_{12}\text{H}_{12}$ 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.

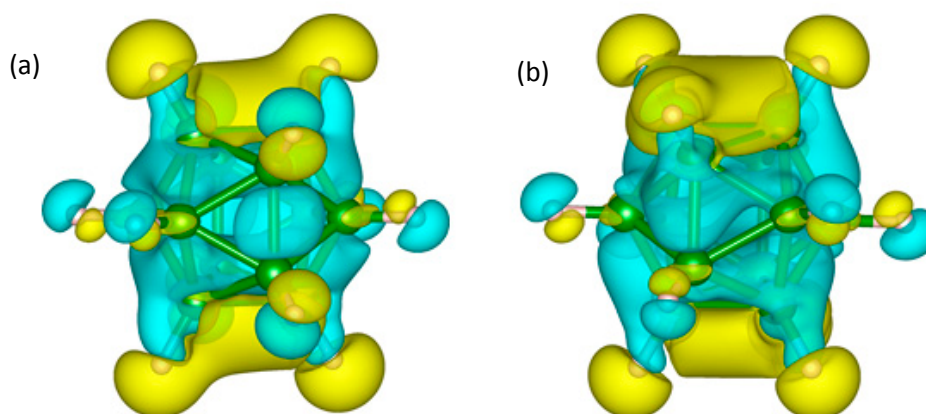


Figure 1. The charge density difference of $\text{B}_{12}\text{H}_{12}$ *closo* anion deformed along C_3 symmetry axis (a) and C_2 axis (b). Yellow colour is for charge accumulations, cyan—charge depletion. Yellow balls are for boron, grey—hydrogen.

Reference

- 1 Sadikin, Y.; Schouwink, P.; Brighi, M.; Łodziana, Z.; Černý, R. Modified Anion Packing of Na₂B₁₂H₁₂ in Close to Room Temperature Superionic Conductors *Inorg. Chem.* **2017**, *56*, 5006.



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