

A combined experimental and theoretical study of benzoxaborole derivatives by Raman and IR spectroscopy, static DFT, and first-principle molecular dynamics.

Autorzy

Aneta Jezierska

Jarosław J. Panek

G. Z. Żukowska

A. Sporzyński

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Physicochemical properties of 1,3-dihydro-1-hydroxy-3-morpholin-4-yl-2,1-benzoxaborole (**IIa**) and 1,3-dihydro-1-hydroxy-2,1-benzoxaborole (**IIb**) were investigated using a combination of spectroscopic and computational approaches. The compound **IIa** belongs to the group represented by the prototypical benzoxaborole **IIb**, which exhibits receptor activity toward sugars in aqueous solution. Additionally, the **IIb** can serve as a pattern structure for physicochemical description of benzoxaborole derivatives. The infrared and Raman spectroscopy measurements were performed in solvents and in the solid state. Furthermore, experimental findings served as a reference data source for further computational investigations. DFT calculations *in vacuo* were used to estimate the binding energy of the dimeric forms, indicating the strength of the intermolecular hydrogen bonds. AIM and ELF theories were applied to give an insight into the electronic structure of the studied compounds. The last part of this study contains Car–Parrinello molecular dynamics investigations in the solid state. Computational results indicated that the key intermolecular feature, the pair of hydrogen bonds, is rather harmonic and the extent of the anharmonicity is temperature dependent as shown by the O–H stretching envelope calculations performed for **IIa**. Inclusion of the quantum effects in the proton motion does not significantly change the qualitative description of the intermolecular H-bond dynamics of the investigated compound.

Słowa kluczowe

AIM, benzoxaborole, ELF, IR, Raman, Solid state CPMD

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