

Influence of the substituents on the structure and properties of benzoxaboroles.

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Streszczenie

Benzoxaboroles possessing aryl substituents in the oxaborole ring were synthesized, and their structures were determined by single-crystal X-ray diffraction. Structures in the solid state are centrosymmetric dimers with two intermolecular hydrogen bonds. These compounds were investigated using a combination of the spectroscopic and the computational approach, comparing their properties with the unsubstituted compound. Investigated compounds were characterized by ^1H , ^{13}C , and ^{11}B NMR spectroscopy in solution. Assignment of ^1H and ^{13}C signals was made on the basis of HSQC and HMBC spectra. The molecular structure of 1,3-dihydro-1-hydroxy-3-phenyl-2,1-benzoxaborole was calculated by the density functional (B3LYP) method with the extended 6-311++G(d,p) basis set. The calculated geometrical parameters were compared with experimental X-ray data, and the differences between experimental and calculated values were found to be of the order of experiment standard deviation, confirming a good description by this level of theory. The harmonic frequencies, potential energy distribution (PED), and IR intensities of this compound and its deuterated analogue were calculated with the B3LYP method. The assignment of the experimental spectra was made on the basis of the calculated PED. The consequence of dimer formation is the splitting of the vibrational modes into symmetric and antisymmetric vibrations. The structure modification resulting from the hydrogen bonded dimers formation is presented.

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