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Spectral properties and aromaticity of pyrazinannelated hemihexapyrazine

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To date, research on the chemistry of macrocyclic compounds is one of the most important and promising areas of science. Special attention is paid to hemihexaphyrins (Hhp) [1], which are six-membered macrocycles with thiadiazole and pyrrole rings are linked together through nitrogen atoms. These compounds have a promising potential for the discovery of substances with valuable properties, such as biological activity. Modification of hemihexaphyrins with different substituents and metal atoms in their coordination backbones opens up new possibilities for obtaining compounds with desired properties. Replacing benzene rings with electron-deficient groups such as pyrazines leads to a reduction in the electron density and total aromaticity of the compound, affecting its spectral properties. To confirm the non-aromatic character of the macrocycles, AICD method was used. According to the macrocyclic conjugation system, diamagnetic currents are observed in some parts of the molecule, but they do not cover the entire conjugation circuit. At the same time, paramagnetic currents occur on the thiadiazole subunits.

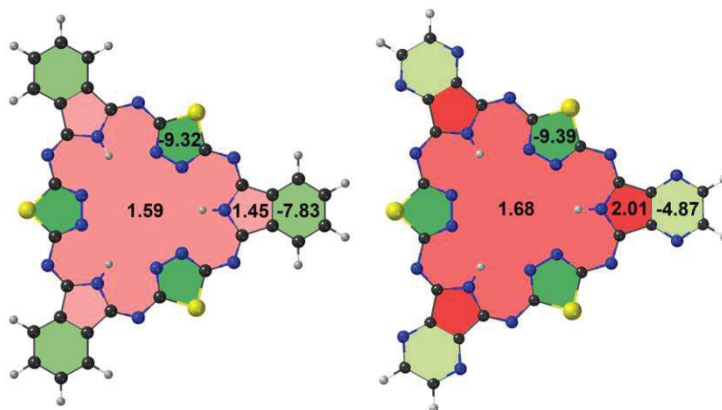


Fig.1 Calculated NICS criteria of benzoannelated (left), pyrazinannelated (right) hemihexapyrazines at the CAM-B3LYP/6-31G(d,p)/GIAO theory level.

ЛИТЕРАТУРА

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