

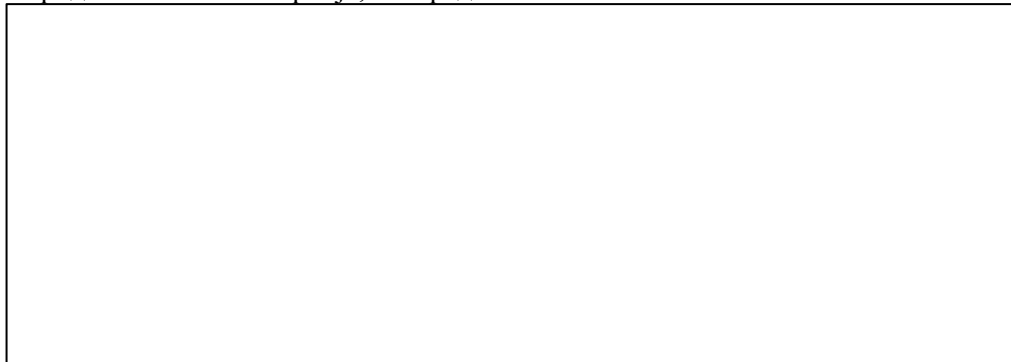
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Book of Abstracts

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Magnetic properties of *periodo-bicyclic hydrocarbons*

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The concept of double aromaticity was introduced by Schleyer [1]. Compounds that possess two circularly delocalized electron systems can be considered as double aromatic. A well-known example is the hexaiodobenzene dication, $[C_6I_6]^{2+}$. [2] In this molecule, both π and σ electrons generate diatropic currents: the π electrons induce diatropic currents within the benzene ring, while the σ electrons induce diatropic currents in the outer ring formed by the iodine atoms. In this study, the double aromatic character of *periodo-bicyclic hydrocarbons* was examined based on their magnetic properties and electronic aromaticity indices. Current densities, computed using the diamagnetic-zero variant of the continuous transformation of the origin of the current density (CTOCD-DZ) method, proved to be a powerful tool for both qualitative and quantitative assessments of double aromaticity. The magnetic aspects of double aromaticity were further compared with electronic aromaticity indices.

References

1. J. Chandrasekhar, E. D. Jemmis. P. v. R. Schleyer, *Tetrahedron Lett.* **1979**, 20 (39), 3707.
2. I. Ciofini, P. P. Lainé and C. Adamo, *Chem Phys Lett.* **2007**, 435, 171.

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