Interpreting Aromaticity and Antiaromaticity through Bifurcation Analysis of the Induced Magnetic Field

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In all molecules, a current density is induced when the molecule is subjected to an external magnetic field. In turn, this current density creates a particular magnetic field. In this work, the bifurcation value of the induced magnetic field is analyzed in a representative set of aromatic, non-aromatic and antiaromatic monocycles, as well as a set of polycyclic hydrocarbons. The results show that the bifurcation value of the ring-shaped domain adequately classifies the studied molecules according to their aromatic character. For aromatic and nonaromatic molecules, it is possible to analyze two ring-shaped domains, one diatropic (inside the molecular ring) and one paratropic (outside the molecular ring). Meanwhile, for antiaromatic rings, only a diatropic ring-shaped domain (outside the molecular ring) is possible to analyze, since the paratropic domain (inside the molecular ring) is irreducible with the maximum value (attractor) at the center of the molecular ring. In some of the studied cases, i. e., in heteroatomic species, bifurcation values do not follow aromaticity trends and present some inconsistencies in comparison to ring currents strengths, showing that this approximation provides only a qualitative estimation about (anti)aromaticity.

aromaticity

bifurcation analysis

induced magnetic field

magnetic criteria

topological analysis