Canonical orbital contributions to the magnetic fields induced by global and local diatropic and paratropic ring currents

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The induced magnetic field (IMF) of naphthalene, biphenyl, biphenylene, benzocyclobutadiene, and pentalene is dissected to contributions from the total ? system, canonical ?-molecular orbitals (CMO), and HOMO??* excitations, to evaluate and interpret relative global and local diatropicity and paratropicity. Maps of the IMF of the total ? system reveal its relative strength and topology that corresponds to global and local diatropic and paratropic ring currents. The total ? magnetic response is determined by this of canonical HOMOs and particularly by paratropic contributions of rotational excitations from HOMOs to unoccupied ?* orbitals. Low energy excitations and similar nodal structure of HOMO and ?* induce strong paratropic fields that dominate on antiaromatic rings. High energy excitations and different nodal structures lead to weak paratropic contributions of canonical HOMOs, which are overwhelmed by diatropic response of lower energy canonical orbitals in aromatic rings. CMO-IMF analysis is found in agreement with ring current analysis. © 2017 Wiley Periodicals, Inc.

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local aromaticity

orbital excitations

polycyclic aromatic hydrocarbons

Aromatic compounds

Aromatic hydrocarbons

Aromatization

Magnetic fields

Molecular orbitals

Naphthalene

Polycyclic aromatic hydrocarbons

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Low-energy excitations

Magnetic response

Orbital contribution

Orbital excitations

Relative strength

Rotational excitation

Magnetism