

Magnetically induced current density using London atomic orbitals of dihydroindeno-[1,2-b]-fluorenes

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We present a study of the magnetically induced current density, calculated using London atomic orbitals, for the cis and trans isomers of dihydroindeno-[1,2-b]-fluorene (IF) and a set of 12 substituted macrocycles (where R = H, NH₂, O-tBu, CH₃, Si(CH₃)₃, OH, OCH₃, F, Cl, Br, CN and NO₂). Qualitative and quantitative analyses were done at Hartree-Fock and density functional theory (DFT) levels. The DFT results are not very sensitive to the choice of the density functional (BLYP and B3LYP). We found a linear correlation between the integrated magnetic susceptibilities values (χ_{total}) and Hammett parameters (ρ_p) of the substituent group bonded directly to the outer six-member rings of the macrocycle structure. Our results suggest that the aromaticity of IF is not extensively modified by the presence of acceptor and donor substituent groups. The effect is rather local, and only strong π donor ligands lead to an aromaticity decrease of the outer six-member rings of the macrocycle directly attached to the substituent. Therefore, this series of indenofluorene derivatives correspond to a set of alternant aromatic and antiaromatic ring moieties, rather than a completely delocalized system. The effect of IF derivatives on the local aromaticity could not be reproduced using the nucleus independent chemical shift (NICS) calculations, which seem insensitive to the change of ligands. © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique.