TOPOLOGY, AROMATICITY, AND GROUND-STATE STABILITY IN INDENOFLUORENE FRAMEWORKS

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Conjugated polycyclic hydrocarbons (CPHs) have gained considerable interest due to their versatile applications in optoelectronic devices, organic spintronics, and semiconductors, as well as energy storage devices. Among such CPHs, conjugated indenofluorenes (IFs) possess one of the most interesting topologies of delocalized π-electrons with different types of behavior (aromatic/antiaromatic) and ground state electronic structure (biradical/quinoidal). They exhibit a 6-5-6-5-6 ring architecture, which is obtained by a fusion of the indene unit to various positions of the fluorene unit to generate five possible isomers. In this work, the Ground State Stability (GSS) rule is introduced. It allows predicting the nature of the ground state of indenofluorene (IF)-type systems from the simple counting of the Clar π-sextets in the closed- and open-shell configurations.[1] Then, the molecular and electronic structure of the non-alternant indeno[2,1-b]fluorene system is examined using density functional theory and high-level *ab initio* calculations. Our results reveal the existence of a flat potential energy surface (PES) with a bond-localized C_s structure and a more delocalized, mirror-symmetric C_{2v} structure.[2] Depending on the level of calculation, the latter is a minimum on a single-well PES or a transition state connecting two C_s structures in a double-well PES. The change of the PES can also be modulated with substituents.[3]

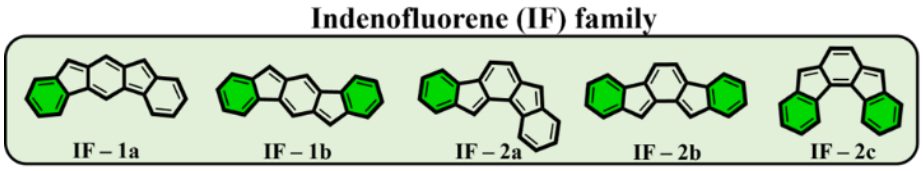

Figure 1. The five members of the indenofluorene family

REFERENCES

[1] G. George, A. J. Stasyuk, M. Solà. *Chem. Sci.* **2024**, 15, 13676-13687.

[2] S. Mishra, G. George, A. J. Stasyuk, F. Albrecht, M. Vilas, D. Peña, I. Rončević, A. Baiardi, M. Solà, L. Gross, in preparation.

[3] G. George, F. Maseras, A. J. Stasyuk, M. Solà, to be submitted.