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π-Delocalization in Strongly Conjugated Systems – A Source of Controllable Properties

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Strongly conjugated carbon-based systems are extensively explored in several aspects focusing on optimisation of synthetic paths and followed by understanding the properties hidden within the skeletons of different size and shape. An extended conjugation based on sp^2 hybridization of carbon allows tuning of the behaviour extracted from the number of available π-electrons eventually controlling optical and magnetic properties including a biradical character. An incorporation of a heteroatom into π-extended system is a separate possibility of modification that can be treated as a source of modulation of the optical properties. A boron involvement into those systems is a vibrant field deeply modifying the recorded properties [1], and based on the properties of boron itself and an electron deficiency of this element that deeply disturbs the electron distribution in defected π-conjugated systems [2,3], but also stabilizes derivatives with a paratropic character typical for antiaromatic derivatives [4,5].

The precisely planned strategy for formation of hybrid structures linking in one skeleton acene(s) or heteroacenes modulated by a presence of a specific defect predefined for binding small cation creates strictly designed systems. It results in, depending on the complexity of the final molecule, the observation of local effects of conjugation efficiently influencing properties of each subunit. A specific construction opens a possibility for observation of the reactivity characteristic for isolated unsaturated units [6] in addition creating an opportunity for switching on the global diatropic currents [2-5] or stabilization of a biradical character [7]. All those effects will be presented and discussed focusing on the delocalization paths within precisely designed structural motifs introducing triangular defect(s) open for a post-synthetic modifications [8] or opening potential for a dynamic equilibrium and stabilization of open-shell character by showing the synthetic approach followed by the spectroscopic behaviour extended by XRD analysis and theoretical support.

Keywords: Biradicals; optical properties; aromaticity; antiaromaticity; helicity

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