Dicyanomethylene-substituted Indolocarbazole Diradicals: Investigating their challenging chemical reactivity and physical properties.

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π-Conjugated diradical compounds, with unpaired electrons in the ground state, are fundamentally important for understanding the nature of chemical bonds and have potential applications in material science[1]. It has been demonstrated that these diradicals systems are essential building blocks in dynamic covalent chemistry (DCC) since they form structural scaffolds based on chemical components that interact through reversible covalent bonds constructing macrocyclic, staircase oligomers or polymers by self-assembly processes[2,3]. In this sense, we have recently reported an experimental and theoretical study of a family of indolocarbazole-based (ICz-based) diradicaloids with dicyanomethylene (DCM) groups incorporated via para or meta positions aiming to investigate the tunability of the diradical character for different structural motifs such as the substitution pattern of lateral groups or the molecular isomerism[4]. Herein, it will be necessary to broaden and deepen the analysis with the experimental comparison of ICz-based systems substituted with para- or meta-DCM groups (p-ICz and m-ICz) to identify new potential design strategies for stimuli-responsive materials. To this end, we use a joint experimental and theoretical approach that links electronic absorption and vibrational spectroscopy with DFT calculations to disclose how their chemical reactivity and physical properties are affected by structural changes.

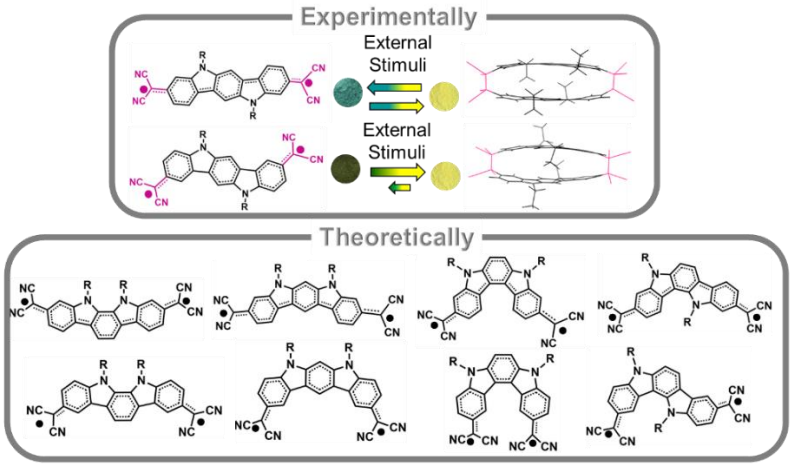

Figure 1. Chemical structures of the studied positional ICz isomers substituted with DCM groups.

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[1] M. Abe, Chem. Rev., 113, 7011 – 7088 (2013)
[2] I. Badía-Domínguez, et al. ACS Omega, 4, 4761−4769 (2019)
[3] I. Badía-Domínguez, et al. Chem. Eur. J., 27, 1 – 13. (2021)
[4] I. Badía-Domínguez, et al. J. Phys. Chem. Lett., 13, 6003-6010 (2022)