

A theoretical investigation of the diradical character and cyclophane formation in π -conjugated diradicals

Juan Sánchez Rincón,^a Irene Badía-Domínguez,^a M. Carmen Ruiz Delgado^{*a}

a) Department of Physical Chemistry, University of Malaga, Campus de Teatinos s/n, 29071, Malaga Spain.

*carmenrd@uma.es

π -Conjugated diradical compounds which feature unpaired electrons in the ground state are essential for understanding the nature of chemical bonds and have potential applications in material science¹. In fact, an important research effort by our group has been directed towards carbazole-based diradicaloids², aiming to explore how external stimuli impacts on supramolecular organization, and thus on the resulting optical and electronic properties. Thanks to this research, we have demonstrated that these materials are potential building blocks for dynamic covalent chemistry (DCC)³. In our present work, we wanted to explore beyond carbazole-based diradicals and analyse what would be the diradical character after modification of the chemical structure of the carbazole skeleton. For this purpose, we will analyse the structural and electronic properties of carbazole-based diradicals after the following chemical modifications: (i) heteroatom substitution, (ii) core elongation and (iii) insertion of donor/acceptor groups. In addition, the effect of the heteroatom substitution on the dynamic interconversion between the monomer and cyclophane aggregates will be also investigated.

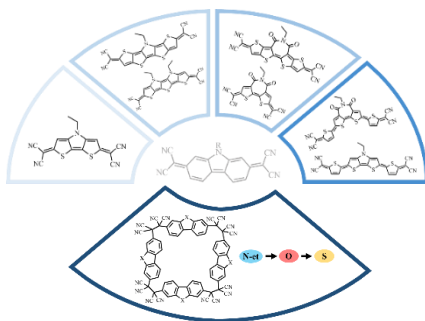


Figure 1. Chemical structures of π -conjugated diradical systems under study.

References

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