

Multiresponsive Chromic Soft Materials: Formation of Strongly Coupled σ -Dimers from IndoloCarbazole-based Biradicaloids

Irene Badía-Domínguez,^a Franktišek Hartl,^b Hongxiang Li,^c J. Carlos Sancho García^d, Andrés Pérez Guardiola^d, Sandra Rodríguez-González,^a Juan T. López Navarrete,^a V. Hernández,^a M. Carmen Ruiz Delgado^a

^a Department of Physical Chemistry, University of Málaga, Campus de Teatinos s/n, 229071, Málaga, Spain.

^b Department of Chemistry, University of Reading, Whiteknights, Reading RG6 6AD, United Kingdom.

^c Key Laboratory of Synthetic and Self-assembly Chemistry for Organic Functional Materials, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, China.

^d Department of Physical Chemistry, University of Alicante, E-03080 Alicante, Spain

E-mail: badia@uma.es

Dynamic covalent chemistry is focused on the creation of structural scaffolds based on chemical components that interact through strong but reversible bonds. In fact, dynamic covalent bonds receive lot of attention because of their unique feature to become reversible under mild conditions.¹ π -conjugated biradical compounds has emerged as essential building blocks in DCC (dynamic covalent chemistry).² We have recently demonstrated the potential of a para-substituted carbazole with terminal dicyanomethylene groups to act as building blocks in DCC.³ In fact, this quinoid carbazole monomer transform to a macrocycle cyclophane upon soft external stimuli (temperature, pressure, light), showing strong chromic features. Here, we explore the effect of the elongation of the carbazole backbone on the formation of stimuli-responsive cyclophanes by self-assembly. To this end, we use a join experimental and theoretical approach that links vibrational spectroscopy (Raman and IR) with DFT calculations.

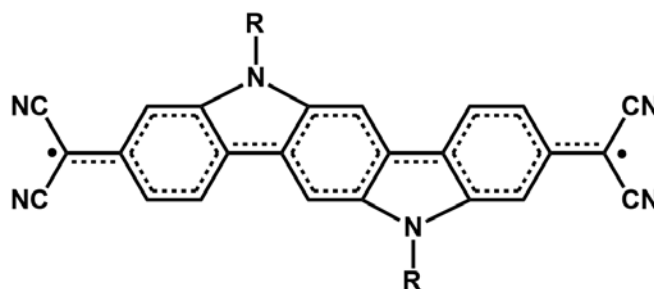


Figure 1. Indolocarbazole-based Biradicaloid under study.

¹ Lehn, J.-M., *Chemical Society Reviews* **2007**, *36*, 151.

² Kohei, O.; Shota, H.; Yuki, I.; Daisuke, S.; Shu, S., *Angewandte Chemie International Edition* **2017**, *56*, 16597.

³ D. Wang, C. C. Ferrón, J. Li, S. G. Valenzuela, R. P. Ortiz, J. T. L. Navarrete, V. H. Jolin, X. Yang, M. P. Álvarez, V. G. Baonza, F. Hartl, M. C. R. Delgado, H. Li, *Chem. Eur. J.* **2017**, *23*, 1.