

## Multiresponsive Chromic Soft Materials: Formation of Macrocycles from Carbazole-based Biradicaloids

M. Carmen Ruiz Delgado,<sup>a</sup>

<sup>a</sup>Department of Physical Chemistry, University of Malaga, Campus de Teatinos s/n, 229071, Malaga, Spain

E-mail: carmenrd@uma.es

$\pi$ -conjugated biradical compounds become essential building blocks in DCC (dynamic covalent chemistry).<sup>1</sup> This field is based on the creation of structural scaffolds based on chemical components which interact through strong but reversible bonds. Importantly, dynamic covalent bonds will be at the center of attention because of their unique feature to become reversible under mild conditions.<sup>2</sup> Recently, we have demonstrated the reversible interconversion between a stable quinoid precursor based on a para-substituted carbazole with terminal dicyanomethylene groups and a macrocycle cyclophane upon soft external stimuli (temperature, pressure, light), which results on strong chromic features.<sup>3</sup> In this work, we investigate the interconversion of the monomer/cyclophane transformation in carbazole-based systems, both in solution and solid state, upon external stimuli. To this end, we use a combined experimental and theoretical study that links vibrational spectroscopy (Raman and IR) with DFT calculations.



**Figure 1.** Interconversion between 2,7-Dicyanomethylenecarbazole-based Biradicaloid (right) and Corresponding Cyclophane Tetramer (left).

<sup>1</sup> Kohei, O.; Shota, H.; Yuki, I.; Daisuke, S.; Shu, S., *Angewandte Chemie International Edition* **2017**, 56, 16597.

<sup>2</sup> Lehn, J.-M., *Chemical Society Reviews* **2007**, 36, 151.

<sup>3</sup> 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.