

Carbazole-based Biradicaloids as Potential Building Blocks for Dynamic Covalent Chemistry

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π -conjugated biradical compounds become essential building blocks in DCC (dynamic covalent chemistry).¹ 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.² 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.³ In this work, we investigate the impact of the substitution pattern (*i.e.*, the insertion of dicyanomethylene groups at the 2,7 (*para*) or 3,6 (*meta*) positions or the elongation of the carbazole backbone) on the formation of stimuli-responsive cyclophanes by self-assembly. To this end, we use a combined experimental and theoretical study that links vibrational spectroscopy (Raman and IR) with DFT calculations.

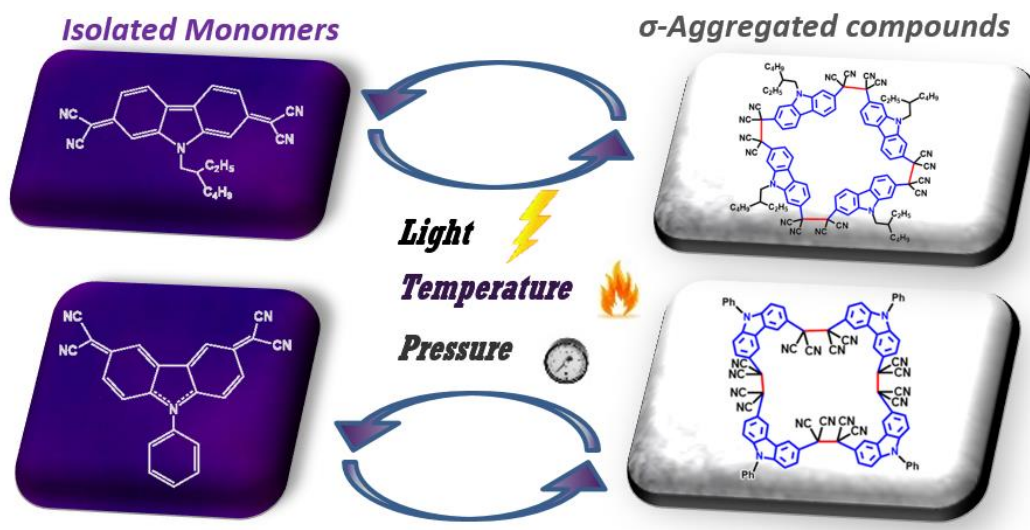


Figure 1. Interconversion between dicyanomethylenecarbazole-based birradicaloids (left) and Corresponding Cyclophane Aggregates (right).

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

² Lehn, J.-M., *Chemical Society Reviews* **2007**, *36*, 151.

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.