

Investigation of the Charge-transport and Optoelectronic Properties of Carbazole-based Macrocycles

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Molecular systems have proven to be efficient active materials in electronics, being possible alternatives to the inorganic semiconductors used nowadays in electronic devices. In this project, an experimental and theoretical study of two carbazole-based macrocycles is presented (Figure 1). Specifically, we investigated the impact of the inclusion of acetylene groups on the electronic and molecular structures of these macrocycles, as well as their potential as charge transporting materials. The first studied compound (**Cz**) is composed by four carbazole groups linked at their para position with respect to the nitrogen atom¹. In the second compound (**ACz**), the carbazole units are connected through ethynylene groups². For this study, Raman and UV-Vis absorption spectroscopies have been used in combination with theoretical calculations based on the density functional theory (DFT). In addition, the two studied compounds have been implemented in organic field-effect transistors (OFETs), to assess their potential as active materials in organic electronics. Overall, the inclusion of ethynylene groups as π -conjugated spacers is found to be a good strategy to improve the electronic delocalization in macrocycles.

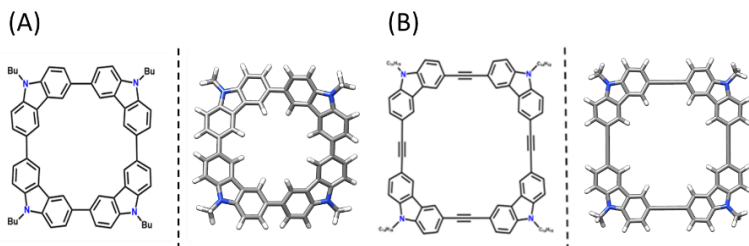


Figure 1. Chemical structures (left) and DFT-optimized geometries (right) of the studied macrocyclic carbazoles: (A) **Cz** and (B) **ACz**

References

1. Zhu, H. et al. Cyclo[4]carbazole, an Iodide Anion Macrocyclic Receptor. *Org. Lett.* 18, 5054–5057 (2016).
2. Wei Zhang, Hyeon Mo Cho and Jeffrey S. Moore. Publication, A. Preparation of a Carbazole-Based Macrocycle Via Precipitation-Driven Alkyne Metathesis. *Org. Synth.* 84, 177 (2007).