Theoretical Study of the Electronic and Charge Transport Properties of Coronoid Carbazole-based Macrocycles

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Carbazole (Cz) units have been recognized as crucial conjugated cores in organic electronics due to their good electro- and photoactive properties compared to other heterocycles.[1] Furthermore, conjugated macrocycles should be useful building blocks for the construction of 2D porous surface networks or 3D inclusion complexes among other supramolecular structures.[2] One of the most interesting features of conjugated cyclic oligomers is that their electronic, structural, and optical properties can be tuned as a function of their interior and exterior domains. Therefore, a systematic study of conjugated macrocycles with well-defined diameters has crucial importance to establish structure-property relationships of these materials. For that purpose, we carried out a purely theoretical study of coronoid molecules based on three different indolocarbazoles (ICz) structural isomers (see Figure 1) as indolo[2,3-a]carbazole **(23a-4MC)**, indolo[2,3-b]carbazole **(23b-4MC)** and indolo[3,2-b]carbazole **(32b-4MC)**. This work aims to identify new macrostructures with interesting electronic properties as well as to display the usefulness of the theoretical tools to advance knowledge in the organic electronics field.

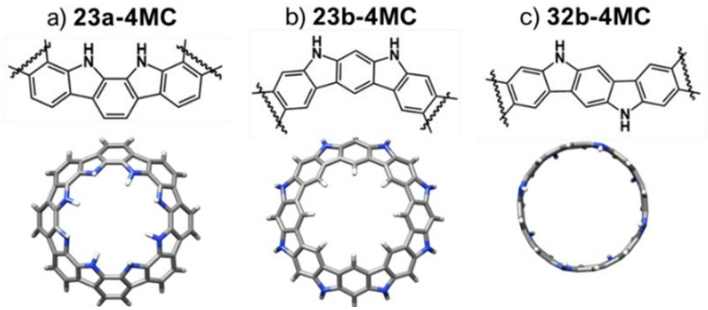

Figure 1. Chemical structures of the three coronoid carbazole-based macrocycles under study: (a) **23a-4MC**, (b) **23b-4MC** and (c) **32b-4MC**.

1. Wex, B.; R. Kaafarani, B.; *J. Mater. Chem. C.* 2017, **5**, 8622.
2. Xu, Z.; Wu, D.; Fang, C.; Li, Y.; *Des Monomers Polym.* 2023, **26**, 90.