COMPUTATIONAL STUDY OF CORONOID CARBAZOLE BASED MACROCYCLES: INFLUENCE OF ISOMERISM

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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, such as high hole-transporting mobilities, when compared to other heterocycles.[1] On the other hand, 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 is of crucial importance to establish the 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**), which contain four indolecarbazole units (**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. Overall, this investigation contributes to elucidating the electronic properties of coronoid macrocycles, guiding experimental chemists to produce new molecules with desirable properties.

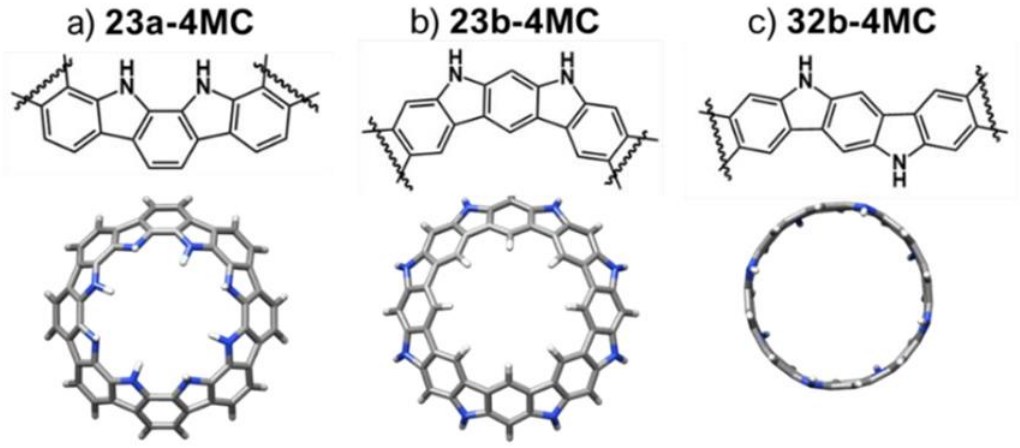

Figure 1. Chemical structures of the three coronoid carbazole-based macrocycles under study: (a) ***23a-4MC****, (b)* ***23b-4MC*** *and (c)* ***32b-4MC****.*

[1] Nayana, V. ; Kandasubramanian. *J Polym Res* **2020** 27, 285.
[2] Iyoda. M. ; Yamakawa. J. ; Rahman. M.J. *Angew* **2011** 50, 10522.