Computational Assessment of Macrocyclic Host-Guest Ion-Dipole Interactions With Negative Pores

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Macrocycles are increasingly studied in supramolecular host-guest chemistry due, in part, to their molecular recognition and binding capabilities. Herein, a computational study which employed a revPBE-D3 functional, dispersion-correction, and TZP basis set to analyze the ion-dipole interactions between a negatively charged pore macrocyclic host and a positively charged DABCO derivative guest is presented. The 6-mer oligoamide macrocycle, which commonly forms 2:1 host-guest systems, exists in two distinct enantiomeric forms (M/P) and in two conformations–the bowl and chair. The dimerization of the oligoamide host resulting from p-p stacking interactions ranged from a face-centered to completely parallel-displaced manner. Host-guest interaction strength and specifically ion-dipole forces were evaluated by binding energies and Hirshfeld/Voronoi charges on guest hydrogens and cavity atoms. Guest-locking of host conformation and chirality because of distinct energy minima between the studied 2-host-1-guest systems highlighted the inconsequence of ring-flipping. Future biomedical applications include incorporation in phospholipid bilayers as a molecular shuttle.

Awards Won:
Third Award of $1,000