Nature of cucurbituril-halogen encapsulation. Structural and interaction energy consideration in the X2@CB[: N] (X = Cl, Br, I, n = 6, 7, 8) from relativistic DFT calculations

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The formation of host-guest species is a relevant issue in the obtaining of supramolecular arrays. In this work, the encapsulation of dihalogen molecules into different cucurbituril hosts allows further evaluation of the role of size and interaction energy for the stabilization of host-guest species. Our results for the X2@CB[n] (X = Cl, Br, I, n = 6, 7, 8) series, allow exploration of the hosts providing increasing cavity sizes, resulting in different host-guest scenarios. It is found that the interaction is mostly given by London type interactions (59% to 65%), followed by the electrostatic character of the interaction (31-27%). For species with a packing coefficient (PC) within the suggested favorable range (PC = 55-68%), and lower, the strength of the stabilizing electrostatic interaction and covalent character, and the repulsive Pauli term, remain similar. Moreover, the dispersion term varies to a large extent, owing to its relation to the available interacting internal face of CB[n], which is less in n = 7 and 8 counterparts. Hence, greater host flexibility is able to maximize the host-guest interactions, where this feature can be viewed as an interesting characteristic towards molecular recognition capabilities, which can be further studied in other related species such as cyclodextrins, pillararenes and other supramolecular hosts.