

Shedding Light on the Nature of Host-Guest Interactions in PAHs-ExBox4+ Complexes

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Host-guest (HG) systems formed by polycyclic aromatic hydrocarbons and ExBox4+ are suitable models to gain a deeper understanding of π - π interactions, which are fundamental in supramolecular chemistry. The physical nature of HG interactions between ExBox4+ (1) and polycyclic aromatic hydrocarbons (PAHs) (2-12) is investigated at the light of the energy decomposition (EDA-NOCV), noncovalent interactions (NCI), and magnetic response analyses. The EDA-NOCV results show that the dispersion forces play a crucial role in the HG interactions in PAHs-ExBox4+ complexes. The HG interaction energies are dependent on both the size of the PAH employed and the number of π -electrons in the guest molecules. The parallel face-to-face arrangement between HG aromatic moieties is also fundamental to maximize the dispersion interaction and consequently for the attractive energy which leads to the inclusion complex formation. © 2016 American Chemical Society.