

# The ability of Ex2Box4+ to interact with guests containing $\pi$ -electron-rich and $\pi$ -electron-poor moieties

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The ability of ExBox4+ as a host, able to trap guests containing both  $\pi$ -electron rich (polycyclic aromatic hydrocarbons-PAHs) and  $\pi$ -electron poor (quinoid- and nitro-PAHs) moieties was investigated to shed light on the main factors that control the host-guest (HG) interaction. The nature of the HG interactions was elucidated by energy decomposition (EDA-NOCV), noncovalent interaction (NCI), and magnetic response analyses. EDA-NOCV reveals that dispersion contributions are the most significant to sustain the HG interaction, while electrostatic and orbital contributions are very tiny. In fact, no significant covalent character in the HG interactions was observed. The obtained results point strictly to NCIs, modulated by dispersion contributions. Regardless of whether the guests contain  $\pi$ -electron-rich or  $\pi$ -electron-poor moieties, and no significant charge-transfer was observed. All in all, HG interactions between guests 3-14 and host 2 are predominantly modulated by  $\pi$ - $\pi$  stacking. © 2018 Wiley Periodicals, Inc.

cyclophanes

EDA-NOCV

host-guest

PAHs

$\pi$ - $\pi$  stacking

Charge transfer

Dispersions

Ions

Polycyclic aromatic hydrocarbons

Covalent character

Cyclophanes

Dispersion contribution

EDA-NOCV

Energy decomposition

Host-guests

Non-covalent interaction

Orbital contribution

Electrons