

Charge-transfer supported supramolecular host–guest interactions in a tailored hexabenzocoronene host

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The vast majority of supramolecular host–guest systems based on π -conjugated molecules are governed by dispersion interactions between adjacent π -surfaces,^[1] which most recently even allowed us to derive a correlation between the area of interacting π -surface and the Gibbs binding energy.^[2] Herein, contrary to this common observation, we present our recent results from a detailed host–guest study on a hexabenzocoronene-based host (Figure 1) that illustrates the significance of charge-transfer interactions in supramolecular binding. In our study, polycyclic aromatic hydrocarbons (PAHs) showed poor binding and revealed no correlation between the size of the π -surface and the binding strength. However, electron deficient guests exhibited a substantial binding, and the binding strength was increased in relation to increased electron deficiency of the guest with the binding constant reaching up to 10^7 M⁻¹ for the most electron deficient guest.

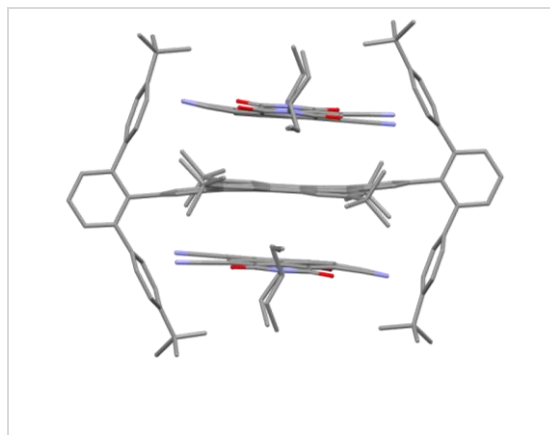


Figure 1: Hexabenzocoronene-based host with two encapsulated guests.

References:

- [1] E. M. Perez, N. Martin, *Chem. Soc. Rev.* **2015**, *44*, 6425-6433.
- [2] J. R uhe, M. Rajeevan, K. Shoyama, R. S. Swathi, F. W rthner, *Angew. Chem. Int. Ed.* **2024**, e202318451