SPECTROSCOPIC AND THEORETICAL DETERMINATION OF ACCURATE CH/π INTERACTION ENERGIES IN BENZENE-HYDROCARBON CLUSTERS.

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Accurate interaction energies in benzene-X clusters (X=ethane, propane, n-butane, and cyclohexane) were determined by two-color two-photon ionization spectroscopy. The experimental interaction energies agree well with those evaluated by high precision ab initio calculations at the CCSD(T)(basis set limit) level. The magnitude of the interaction energy is proportional to the averaged polarizability of the hydrocarbon moiety, indicating that the CH/π interaction is dominated by the dispersion force.