

Integrated experimental and computational spectroscopy study on π -stacking interaction: the anisole dimer

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Integrated experimental and computational results help to clarify the nature of the intermolecular interactions in a simple, isolated π -stacked dimer prepared in a molecular beam. The properties of bimolecular anisole complexes are examined and discussed in terms of the local/supramolecular nature of the electronic wavefunctions. Experimental resonance-enhanced multi-photon ionization spectra of clusters with different isotopic compositions confirmed the fundamentally localized nature of the $S_1 \leftarrow S_0$ electronic transition. A detail analysis of the experimental results however shows the existence of non-negligible excitonic coupling for the excited-state wavefunctions leading to the doubling of the single-molecule vibronic levels in the S_1 state, with a splitting of about 30 cm^{-1} . Theoretical simulation of the vibrationally resolved electronic spectra and computations of the excitonic coupling convincingly support the experimental findings. The overall combined experimental/theoretical study allows a detailed description of the stacking interaction in the anisole dimer.

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