

Supporting Information

Elucidating the structure and binding nature of thianaphthene dimers using gas-phase infrared spectroscopy

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1. Full mass spectrum of thianaphthene clusters
2. π -stacked conformations and relative energies
3. Computed vibrational spectra of the π -stacked conformations
4. Comparison of IR spectra of monomer and dimer

1. Full mass spectrum of thianaphthene clusters

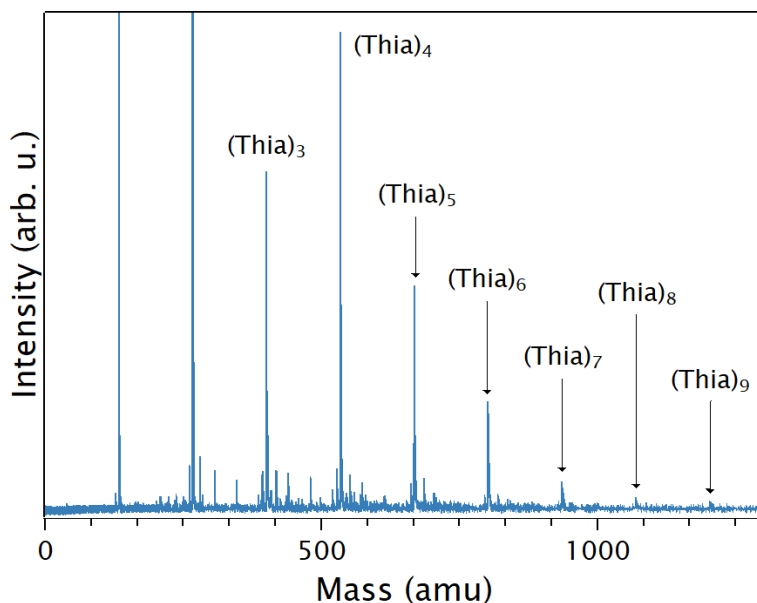


Figure S1. Mass spectrum of neutral thianaphthene clusters in the molecular beam, constructed as the average over all scanned REMPI resonances. The first two peaks correspond to (Thia)1 and (Thia)2, out of scale in the figure.

2. π -stacked conformations and relative energies

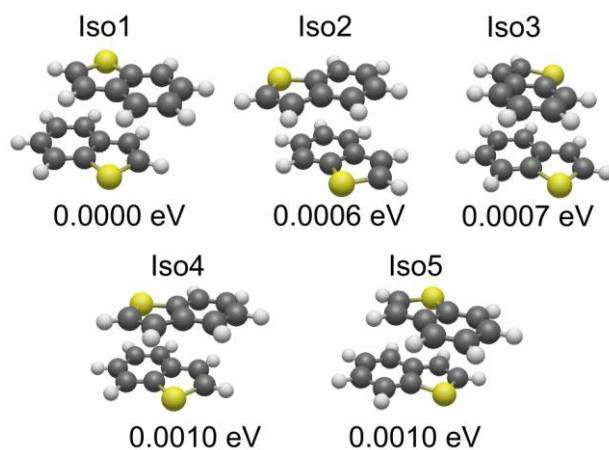


Figure S2. π -stacked conformations and relative energies of the thianaphthene dimer.

3. Computed vibrational spectra of the π -stacked conformations

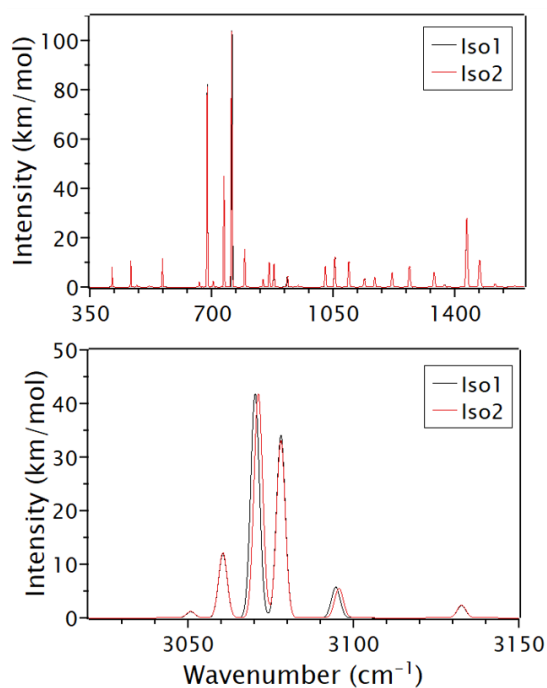


Figure S3. Vibrational spectra of Iso1 and Iso2 of the π -stacked conformations for the thianaphthene dimer.

4. Comparison of IR spectra of monomer and dimer

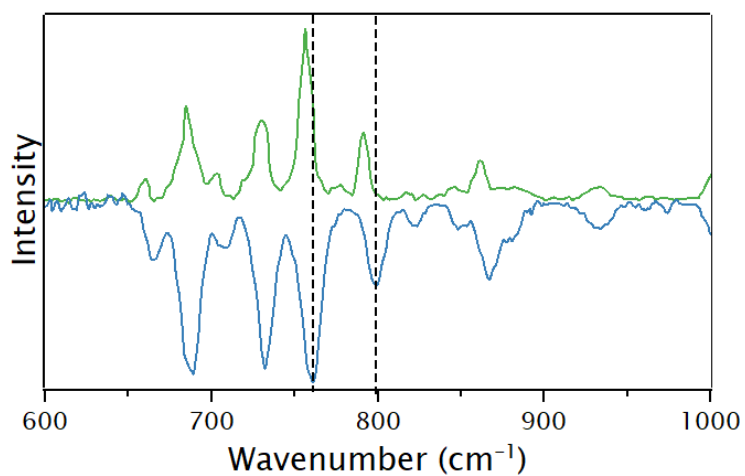


Figure S4. Comparison of the IR spectra of thianaphthene dimer and monomer in the region between 600 and 1000 cm^{-1} . For visualization purposes, the spectrum of the monomer is multiplied by -1. Vertical dashed lines are included to help visualize small differences in the spectra.