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Probing Intermolecular Interactions in Polycyclic Aromatic Hydrocarbons with 2D IR Spectroscopy¹

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Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous in the environment and impact geochemical processes that are critical to sustainable energy resources. For example, asphaltenes exist naturally in geologic formations and their aggregates heavily impact the petroleum economy. Unfortunately, the chemical dynamics that drive asphaltene nanoaggregation processes are still poorly understood. Solvent dynamics and intermolecular interactions such as π -stacking interactions play integral roles in asphaltene nanoaggregation. Linear and nonlinear vibrational spectroscopy including two-dimensional infrared spectroscopy (2DIR), are well suited to explore these fundamental interactions. Teasing apart the vibrational characteristics in PAHs that model asphaltenic compounds represents an important step towards utilizing 2D IR spectroscopy to understand the intermolecular interactions that are prevalent in asphaltene nanoaggregation. A solar dye, N,N'-Diocetyl-3,4,9,10-perylenedicarboximide, is used in this work to model asphaltenes. Carbonyl and ring vibrations are used to probe the nanoaggregates of the model compounds. However, the characteristics of these normal modes change as a function of the size of the conjugated ring system. Thus, in order to fully understand the nature of these normal modes, we include a systematic study of a series of quinones. Our investigation employs a combination of 2DIR spectroscopy and electronic structure calculations to explore vibrational coupling in quinones and PAHs. We compare the calculated vibrational characteristics to those extracted from 2DIR spectra.

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