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Investigating the Self-assembled Structure of Polycyclic Aromatic Hydrocarbons Using Two Dimensional Infrared Spectroscopy JENEE D. CYRAN, Max Planck Institute of Polymer Research, AMBER T. KRUMMEL, Colorado State University

— Self-assembly mechanisms are required for many biological and material processes, such as chlorophyll in photosynthesis, the tobacco mosaic virus and in the formation of molecular crystals. The self-assembly process can be favorable in the case of formation of nanoparticles for electronic devices. However, self-assembly processes, such as asphaltene nanoaggregation, can be unwarranted. Studying the structure of self-assembled supramolecules is important to understand how to mimic or inhibit the formation of the nanoaggregates. In this research, we studied the monomer and self-assembled structure of two polycyclic aromatic hydrocarbons (PAHs), lumogen orange and violanthrone-79, using two-dimensional infrared spectroscopy (2D IR). The carbonyl stretching and the ring breathing vibrational modes were used as vibrational probes. For violanthrone-79, a local mode basis and an electrostatic coupling model were applied to three nanoaggregate structures; parallel, antiparallel, and 28 degrees rotation. The experimental and simulated 2D IR spectra are best represented by majority of the antiparallel configuration with some angular distribution. For lumogen orange, vibrational cross peaks appear as the concentration is increased from a monomer to a nanoaggregate. The 2D IR cross peaks indicate vibrational coupling, which relates directly to the nanoaggregate structure. Comparison between the self-assembled structure of lumogen orange and violanthrone-79 can determine the role of side chains in the nanoaggregate structure.

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