Probing Asphaltene Nanoaggregation Using Two-Dimensional Infrared Spectroscopy Amber T. Krummel, Department of Chemistry, Colorado State University

During year 1 (2011-2012) our attention has focused on completing our 2D IR spectrometer, identifying compounds that are suitable models of asphaltenes, and generating protocols to produce nanoaggregates in a reproducible manner. The model compounds we have identified are violanthrone-79 and N,N'-dioctyl-3,4,9,10perylenedicarboxide, shown at right. Also shown at right are representative linear IR spectra of the respective nanoaggregates of these molecules in deuterated toluene and carbon tetrachloride. A suite of electronic structure calculations have been performed on these model compounds and provide a basis for a local mode description of the vibrational modes of the carbonyls directly bound to the macrocyclic ring structures.

In addition, we have completed our 2D IR spectrometer and have improved pulse-shaping technology for mid-infrared light.





During year 2 (2012-2013) we will focus on developing a detailed molecular picture of the nanoaggregates and the process by which they are formed in solution. At the left two hypothetical stacking configurations of violanthrone-79 are shown. We will use 2D IR spectroscopy to discriminate between these hypothetical stacking configurations.

