

## ISOMER-SPECIFIC SPECTROSCOPY OF ETHYL NAPHTHALENE DERIVATIVES: SPECTROSCOPIC FOUNDATION FOR UNDERSTANDING ETHYL-BRIDGED DINAPHTHLYLS

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The incomplete combustion of gasoline under fuel-rich conditions leads to soot formation, an unwanted pollutant and energetically wasteful product. While it is known that soot is composed of  $\pi$ -stacked graphitic-like structures, the incipient stages of soot formation are still something of a mystery, with conflicting evidence as to whether  $\pi$ -stacked polycyclic aromatic hydrocarbon (PAH) aggregates can form and survive at combustion temperatures still unresolved. The mechanism by which the initial aggregation of PAH precursors occurs is still under active investigation. This talk will describe studies of two isomeric naphthalene derivatives containing short alkyl chains: 1-ethyl naphthalene and 2-ethyl naphthalene. The structural isomers differ in the position of substitution of the ethyl side-chain on the naphthalene framework. These molecules are not only components of diesel fuel and of early stages of PAH formation in flames, but are also close analogs of a series of ethyl-bridge dinaphthyl compounds studied by our group. We will present the jet-cooled LIF excitation, dispersed fluorescence, and fluorescence-dip infrared spectra of these molecules, cooled in a supersonic free jet. The vibronic spectroscopy of these molecules is similar to that in naphthalene, modified only subtly by the ethyl side chain. Vibronic coupling between  $S_1$  and  $S_2$  states is pervasive, leading to textbook evidence of Herzberg-Teller coupling. We have also observed the onset of the  $S_0$ - $S_2$  transition near 288 nm. These results will be compared with calculations of the excited states, setting a foundation for understanding the fascinating vibronic spectroscopy of the ethyl-bridged dinaphthyl compounds.