INFRARED SPECTRA OF SIZE-SELECTED METHANOL CLUSTERS USING IR-VUV PHTOTIONIZATION

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We investigated the CH and OH stretching modes of size-selected methanol clusters, $(CH_3OH)_n$ with $n \le 5$, in a pulsed supersonic jet with the IR-VUV ionization technique. Emission at 118 nm, frequency tripled in a mixture of Xe and Ar from the 355 nm nm output of a Nd: YAG laser, serves as the ionization source of a time-of-flight mass spectrometer. The tunable IR laser emission from an OPA/OPO system pumped with a second Nd: YAG laser serves as a source of predissociation or excitation before ionization. The variation of intensity of each ion signal was monitored as the IR laser light was tuned across the range 2700-3750 cm⁻¹. Careful processing of raw data based on photoionization efficiencies and the production and loss of each cluster due to predissociation yields identical IR spectra for the size-selected cluster even under diverse experimental conditions. The OH region of methanol clusters has been investigated a, but the spectra in the CH region are new. In the region 2800-3050 cm⁻¹, each absorption band of the methanol monomer splits into two components for the methanol dimer that correspond to proton donor and proton acceptor, indicating that methanol dimer has a preferred open-chain structure. In contrast, for the methanol trimer, the splitting diminishes and the band widths become narrower, indicating a preferred cyclic structure. For tetramer and pentamer, spectral patterns similar to those of the trimer but with greater widths are observed, supporting theoretical computations that predict the most stable structure to be cyclic.

^aU. Buck, and F. Huisken, *Chem. Rev.* **100**, 3863 (2000).