III-D Spectroscopy and Dynamics of Vibrationally Excited Molecules and Clusters

This research group, which started in April 1997, is planning to study spectroscopy and dynamics of molecules and clusters in higher vibrational state by two-color double resonance spectroscopy. New spectroscopic methods will also be developed to observe the higher vibrational state under collision-free condition.

III-D-1 Overtone Spectroscopy of Jet-Cooled Phenol Studied by Nonresonant Ionization Detected IR Spectroscopy

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Vibrational transitions of jet-cooled phenol have been detected by nonresonant two-photon ionization due to UV laser from 3400 cm^{-1} to 14000 cm^{-1}. The UV frequency dependence of IR-UV double resonance signals is used for discussion on the mechanism of ionization. The spectrum shows a well-resolved structure due to the first to the fourth quantum of OH stretching vibrations, CH overtones and various combination vibrations. The vibrational frequency, anharmonisity and the dissociation energy of the OH stretching mode has been measured. The bandwidth of the OH overtone is found to decrease with increase in the vibrational quantum number.

III-C-2 Structure of 1-Naphthol-Water Clusters Studied by IR Dip Spectroscopy and Ab Initio Molecular Orbital Calculation

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IR spectrum of *cis*-1-naphthol, *trans*-1-naphthol, and 1-naphthol·$(H_2O)_n$ (n = 1–3) clusters has been measured by the IR dip spectroscopy in a supersonic jet. The spectra show clear vibrational structures of the monomers and the clusters in the energy region from 3000 cm^{-1} to 3800 cm^{-1}. Observed vibrational transitions are assigned to the OH stretching vibrations of 1-naphthol and waters in the clusters. The size dependence of the IR bands and the cluster geometries are analyzed by using the ab initio MO method at MP2/6-31G level. From the comparison between the observed and calculated IR spectra, we have concluded that the 1-naphthol acts as the proton donor and a cyclic hydrogen-bond network is formed in the n = 2 and 3 clusters.