DOUBLE RESONANCE VIBRATIONAL SPECTROSCOPY FOR THE INVESTIGATION OF STRUCTURES AND DYNAMICS OF MOLECULAR CLUSTERS

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Double resonance vibrational spectroscopy is becoming a powerful spectroscopic method for the determination of molecular clusters formed in supersonic free jets. By using an advantage of high sensitivity and selectivity of electronic spectroscopy, we can measure IR and Raman spectra of the size- and isomer-selected cluster. Several spectroscopic methods will be introduced[a]; IR-UV and stimulated Raman-UV double resonance spectroscopies for the clusters the electronic ground state, and UV-IR double resonance spectroscopy for the electronically excited clusters. We first demonstrate their application to the clusters in the electronically ground state, such as van der Waals clusters of benzonitrile[b] and hydrogen-bonded clusters of 7-hydroxyquinoline[c]. The observed spectra are compared with those obtained by ab initio calculations, and their structures, dynamics and reactivities are discussed. We then change the subject to the OH and/or NH stretching vibrations of electronic excited molecules and their hydrogen-bonded clusters to see how the electronic excitation affects the strength of the hydrogen-bonding.

[a] T. Ebata, A. Fujii and N. Mikami, Int. Rev. Phys. Chem. 17, 331 (1998)
[b] R. Yamamoto, S. Ishikawa, T. Ebata, and N. Mikami, J. Raman Spectrosc. 31,295(2000)
[c] Y. Matsumoto, T. Ebata, and N. Mikami, Chem. Phys. Lett. In press