第１８５回　化学コロキウムのお知らせ

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Spectroscopic probes of hydrogen bonds: From aqueous clusters to bulk water

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The *structural-spectral* correspondence describes the relationship between the underlying hydrogen bonding network and the resulting vibrational infrared (IR) spectra in the "fingerprint" OH stretching region (3,000 – 4,000 cm^{-1}). For small aqueous clusters this allows for the assignment of the structures based on the spectra and vice versa. The onset of intracluster reactions can also be probed.　In some instances the harmonic spectra are sufficient, whereas for strong hydrogen bonds accurate anharmonic spectra are required.　In contrast, for liquid water the dynamical nature of the hydrogen bonding network results in a broad OH band. I will present recent results on the accurate calculation of the IR spectra of small aqueous clusters that include the probing of intracluster reactions and use these results to discuss the structure of the broad, structureless OH band in liquid water.

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