Division of Mathematical and Physical Sciences	Research field	Molecular Physics	Lab. ID MP10
Laboratory web site	http://www.s.kanazawa-u.ac.jp/phys/bunshi/molphys/index.html		

Research subjects

Our purpose at this laboratory is to elucidate the physicochemical properties and behavior of a molecule in the aqueous solution from a microscopic viewpoint. For that purpose, we are investigating experimentally how the structure and the property of an organic molecule change when a hydrogen bond molecular complex is formed. When a solute molecule and a small number of water molecules form a hydrogen bond complex, it is called the "micro-solvation cluster" and it is the most fundamental model of a hydration or a solvation. Since the hydrogen bond is weak compared with chemical bonds, such as a covalent bond, it will break immediately by collision not only in a solution but in a gas phase. Therefore, the lifetime of a complex is extremely short, and even now, it is very difficult to observe the detailed structure and behavior of the individual molecules in the aqueous solution exactly.

We generate a very-low-temperature molecular flow of about 1K translational-temperature in a high vacuum by the supersonic pulse-jet technology which realizes a quasi-isolated state. Because the hydrogen-bond complex is stable in the supersonic-jet, it makes possible the detailed and precise measurement of the pure rotational spectrum. This method is called "the supersonic pulse nozzle jet Fourier-transform microwave-spectroscopy". The pure rotational spectrum is a spectrum caused by the transition between the energy levels corresponding to an overall rotation of the molecule, and is usually observed in a microwave frequency range. Because the geometric structure of a molecule is strongly reflected in the rotational energy levels, the exact molecular structure can be determined by the measurement of the pure rotation spectrum. Due to the extremely high spectral resolution of our spectrometer, it is possible to make observation of completely separated spectra of various complexes in which numbers of H2O, hydrogen bonding site and orientation are different. Moreover, we can also obtain the accurate information about dynamical behaviors, such as a molecular vibration and intramolecular tunneling motion.

Until now, we have investigated the N-methyl-acetamide water complex system, and the methyl-lactate/methyl-glycolate water complex system. N-methyl-acetamide is a model molecule of the peptide chain which is a main chain of proteins and we are working for clear understanding of the effect of hydrogen bond formation on the flexibility of a peptide chain. Methyl lactate and a methyl glycolate are the molecules which have an intramolecular hydrogen bond. We are investigating the competition and cooperation effects between the intermolecular hydrogen bond and the intramolecular hydrogen bond in the aqueous solution. We will further develop the studies and try to elucidate the nature and the behavior of a molecule in the aqueous solution from a microscopic viewpoint.

Master/Doctor course: Education policy, curriculum, typical activity in the laboratory

All members should participate in a seminar, an exercise and a research-activities debrief session which are held about once per week, respectively. In the seminar, a textbook in conjunction with both molecular physics and molecular spectroscopy is used. Arbitrarily, lectures on selected themes about the experiment or theory relating to each research subject to all the members or individual are given. In most experiments, the spectrometer can be operated by one student alone, but it is the shared equipment in our laboratory. In order to complete the spectrum measurement of one molecule, it takes usually the period of two to three months. Therefore, the period when each student can use the spectrometer for own work will be limited considerably. During one's own measurement period, the student must concentrate on the experiment and be careful not to waste time.

According to each research subject and interest, learning support of program languages (Fortran, LabVIEW, MATLAB etc.) or CAD software, and instruction of the usage of quantum chemical calculation software package (Gaussian) is carried out.

The theme of the research is decided during the first semester of the first grade, after consultation with the teacher. Methods of the research include "measurement and analysis of the spectrum", "improvement or development of equipment", "new development of spectral-analysis method and programming", "utilization of quantum chemical calculation to consider the experimental result", and "further understanding of the nature of molecules based on it", etc. Ideally, it is desirable to experience all the methods mentioned above.

The students are encouraged to participate in research conferences or meetings and perform presentations as much as possible

Daily life in the laboratory, etc.

Since it is a small-scale laboratory, the student can take favorable communication with the teacher, and therefore can receive careful instruction. All persons of the members are gentle. The students of other laboratories visit my room to enjoy a lighthearted conversation. I am living the peaceful research life. The research subject of each student is related strongly with each other (it is not group project), and thus I can discuss each subject with not only teacher but students and can deepen the understanding mutually. Since the experiment is usually carried at daytime, I can lead a regular life, without straining oneself. The student room is located near the experiment room and is completely isolated and therefore comfortable research environment and study time is secured. (M2)

The risk of most experiments is low. However, in order to ensure safety, the experiment is basically performed in the daytime because the confirmation of the security by plural members is possible. Usually, students have free time on weekend, unless there are the special reasons such as the preparation for presentation at an academic meeting.

Message or comments by the laboratory faculty staffs	
Students will be able to have much free time at this laboratory. However self-management is required, in order to carry out the research steadily and to achieve success. Please utilize time effectively. We actively participate in publicity works such as the Open-campus for general visitors and in community support activities such as a scientific classroom for kids. For such events, we study hard the physical phenomenon which is not related to research, and may expend much time and effort on production of an experimental apparatus and a presentation. I hope that the students can acquire the ability to explain "importance" and "fun" of science or physics for ordinary persons other than a specialist, by carrying out those activities.	
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