

Report on 68th Ohio State University International Symposium on Molecular Spectroscopy by JSPS Core-to-Core Program

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As part of the JSPS (Japan Society for the Promotion of Science) Core-to-Core Program, I participated in the international symposium held at the Ohio State University (OSU) to have an oral presentation from 17th to 21st of June, 2013. It was the first time for me to attend an international symposium. I took part in this program with Ms. Hikari Oba and Prof. Haruki Ishikawa. Ms. Oba is also a member of Fujii group while Prof.

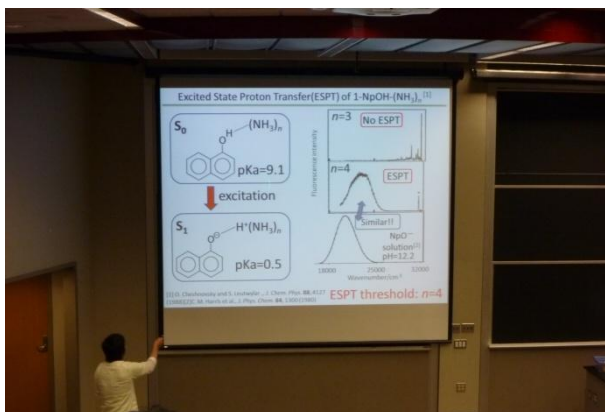


Fig.1 Presentation in the OSU international symposium

Ishikawa is supervisor when I was an undergraduate of kitasato University. In this report, I would like to describe my presentation and impressions of the travel briefly.

Presentation in the symposium

The OSU international symposium is held every year, and it is 68th time this year. This symposium focuses on fundamental molecular spectroscopy. Many researchers and students from across the world make only oral presentations. This symposium will mark the end of an uninterrupted series of annual meetings at the OSU after this time. So this is my first and last chance to attend this symposium.

On 18th June, I gave a talk about progress report of my research work. The presentation entitled "Structure determination and excited state proton transfer reaction of 1-naphthol-ammonia clusters in the S₁ states studied by mid-IR spectroscopy". The purpose of this work is to determine the minimum size at which the ESPT reaction takes place in NpOH-(NH₃)_n system using IR spectroscopy in the mid-IR region. This size was already investigated many researchers in diverse ways. Although they reported $n = 3-5$, it has not established yet. This is because they inferred the ESPT reaction from indirect evidences such as the lifetime of the S₁ states, fragmentation pattern in mass spectra. The most direct way to show occurrence of the ESPT reaction

would be detection of the position of the transferred proton. Therefore, we have tried to record IR spectra to get structural information in the S_1 state that reflects structural change directly. In general, OH and NH stretching vibrations ($3 \mu\text{m}$ region) are expected to most sensitively probe the structure of hydrogen bonding network. When the ESPT reaction occurs, the OH stretching vibration disappears, while the NH stretching vibrations of the ammonium cation appear. Unfortunately, a broad absorption appears even at $n = 1$. It is difficult to determine the cluster structure only from these broad absorption. In order to determine the structure in the S_1 state, we focused on the mid-IR region. These region are expected to provide sharp transitions. One of the typical example is the C-O stretching vibration. In the ground states, this is purely a single bond. However when the ESPT occurs, the C-O bond wears a double bond nature strongly. This change also induces a large blue shift

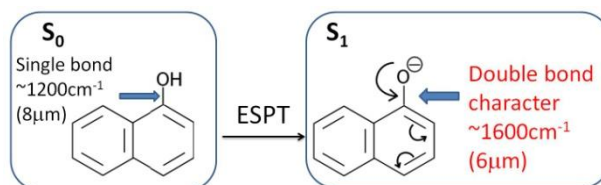


Fig.2 Resonance structure in 1-NpOH after ESPT reaction.

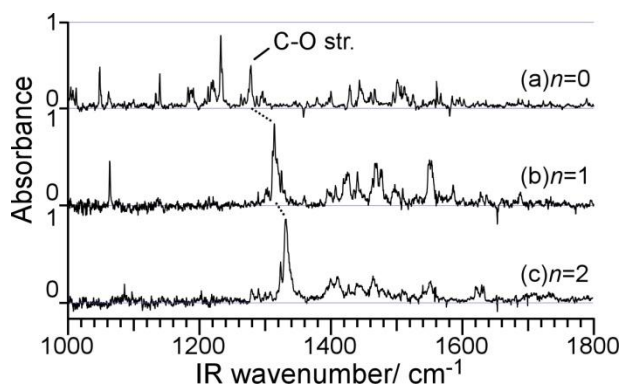


Fig.3 Mid-IR spectra of 1-NpOH-(NH₃)_n in the S_1 states.

of the C-O stretching vibrations from 1200 cm^{-1} to 1600 cm^{-1} . This large blue shift of the C-O stretching vibration is expected to give useful information of the threshold size of the ESPT reaction. In presentation, I introduced mid-IR spectra of 1-NpOH-(NH₃)_n ($n = 0-2$) in the S_0 and S_1 states. From these spectra, I concluded that the C-O stretch shifted toward blue side as the cluster size increases, but the ESPT reaction did not occur in $n = 2$.

After my presentation, I received a number of questions. These questions are informative for me (such as "Why does the number of bands decrease?", "Why does not the number of bands between obs. and calc. match?", "How do lifetimes and quantum yield changes as the cluster size increases?"). Due to my poor listening power of English and tension, I could not adequately answer these questions. But, after end of my presentation, I understood their questions and thought reasonable answers. If I have next chance to visit international symposiums, I would prepare answers of likely questions and study English more hardly.

Impression of the travel

This was the first time for me to go foreign country. In this travel, I underwent many good experiences for the first time. Such as immigration clearance, exploration in the university, shopping at stores, eating local foods in US, etc. Each experience which interacts with native English was fresh and interesting for me. Of course, the preparation for this symposium had so many difficulties for me. However, many people helped me. So, in this time, I feel so happy to join the Ohio symposium.



Fig. 4 In front of the Ohio state university.

Acknowledgement

I would like to express my thanks to Prof. Masaaki Fujii and Prof. Haruki Ishikawa who gave me such a nice opportunity, Dr. Mitsuhiro Miyazaki who gave me helpful advises to prepare my presentation, Ms. Hikari Oba who attended the international symposium together, and all people who are involving in the JSPS Core-to-Core program.