A report of stay in Photon Science Institute of the Manchester University in U.K through the JSPS Core to Core Program

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I had an opportunity to visit The Photon Science Institute of Manchester University as a part of the JSPS Core to Core Program. I studied in Professor Klaus Muller-Dethlefs research group for 12 days. From 25th April to 8th May. This is report of my stay.

Introduction

A) Purpose

1, I am a beginner of spectroscopy. Through Core-to-Core program, I can study how to do experiment and measurement, consideration of the result. In addition, I can study the role of each device, because I have to optimize each device. So, this stay is very useful for me.

2, Experience of debating by English is very important. My English skill will be improved, because I have to communicate by English.

B) Subject of this research

This joint research focuses on molecule that has both van der Waals site at the π electron cloud of aromatic ring and hydrogen bond site such as the OH group. The aim is clarify which site is coordinated with any solvent or ligand in different condition. And, what changes generate the switching of the bonding site. Such kind of molecule that has van der Waals site and hydrogen bond site are related many biological molecule. For this reason, this research is important not only for physical chemistry, but also for biologically.

Interpretation of Photoionisation-induced switching reaction of phenol (PhOH)-Argon (Ar) 1:1 cluster is different between our laboratory and prof, Klaus Muller-Dethlefs laboratory. Our laboratory suggests that ionized PhOH-Ar (1:1) cluster changes the

bonding site from π site to OH site. But, despite of Mass Analyzed Threshold Ionization (MATI) spectrum indicates structure after ionization, the MATI spectrum had reported that the reaction does not occurred. Thus, experiment that resolves the conflict is planed. This stay intends to prepare the experiment.

C) The University of Manchester and Prof, Klaus Muller-Dethlefs laboratory

The University of Manchester was founded in 2004 by merging the University of Manchester Institute of Science and Technology and the Victoria University of Manchester. The University of Manchester is the biggest university in Middle-England and is a center of excellence.

The Photon Science Institute where I went was established in 2005 to foster wide range of science experts and to provide great research environment in photon science. The Figure, 1 shows Prof, Klaus Muller-Dethlefs laboratory with us.

Fig, 1 Prof, Klaus Muller-Dethlefs laboratory with us

<u>What I studied</u>

A) MATI (Fig.2)

MATI spectroscopy is a high resolution spectroscopic technique used to observe vibrational states of cation. High Rydberg state is regarded as cation, because high n Rydberg electron is bound very weakly but this molecule is electrically neutral. By detecting cation generated by high Rydberg, estimation of vibrational modes of cation state can be achieved. The schematic is indicated next.

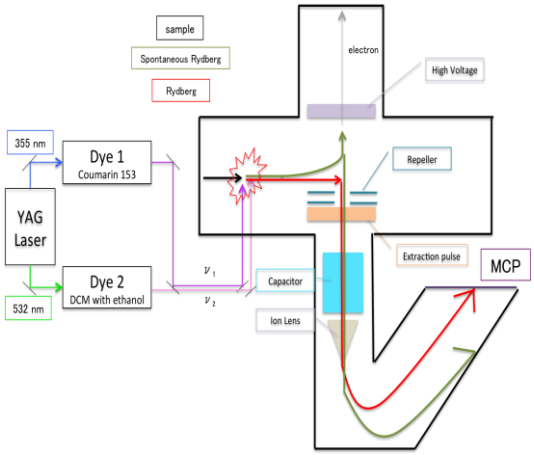


Fig.2 Schematic of MATI

1, At top of the valve, solid of phenol is heated and the phenol becomes gas. Then phenol gas pulse is injected by Ar gas.

2, The gas pulse through skimmer be molecular beams.

3, Spontaneous Rydberg (cation) and Rydberg (neutral) are generated by ν_1, ν_2 where 5 mm left side from center of chamber.

4, Spontaneous Rydberg that has charge is shifted to upper side by extraction pulse (1-2 V). Then Spontaneous Rydberg and Rydberg are spatially divided.

5, Rydberg is ionized by High Voltage (1 kV).

6, Two types of cation are sent to down side by repeller.

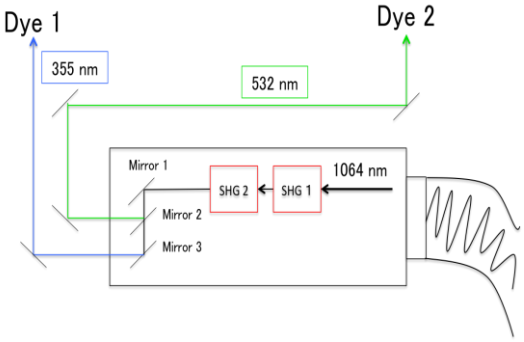
7, Capacitor suppresses horizontal speed according to potential difference between left side (minus) and right side (plus).

8, Ion Lens collects cation. After that Rydberg is led to micro channel plate (MCP) by reflector (REF).

Spontaneous Rydberg has larger potential energy than Rydberg, because Spontaneous Rydberg starts to go down from higher position than Rydberg position. Reflector can not lead Spontaneous Rydberg to MCP due to the larger energy of Spontaneous Rydberg. Thus, MCP detects only cation generated by Rydberg.

B) YAG Laser (Fig, 3)

YAG laser oscillates the 532 nm light and the 355 nm light with using SHG (1064 nm → 532 nm), SFG (1064 nm + 532 nm → 355 nm) and two type of mirrors that different wavelength are transmitted and reflected. The 355 nm light is weaker than the 532 nm lights, because the 532 nm light is generated by passing both SHG and SFG crystal.



	Reflect	Transmit
Mirror 1	532,355 nm	1064 nm
Mirror 2	532 nm	355 nm
Mirror 3	355 nm	

Fig,3 Schematic of YAG laser

C) Dye Laser (Fig, 4)

1, Oscillator that is including dye converts the lights from YAG.

2, Reflection type grating separates

the light in each wavelength.

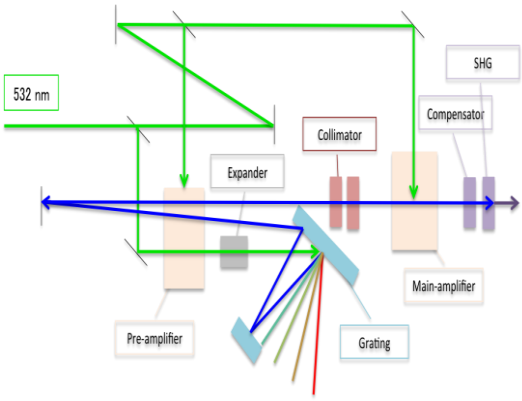
3, Pre-amplifier amplifies the light.

4, the light is expanded and paralleled by Collimator.

5, Main-amplifier more amplifies the light.

6, SHG crystal converts the light into second order harmonic wave.

Compensator prevents to displacement of the optical axis, because optical axis of different wavelength light is different.



Fig,4 Schematic of Dye Laser

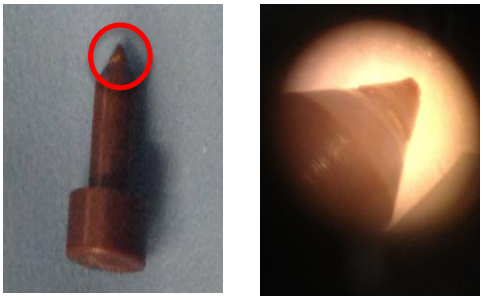
Oscillator of Dye 1 is including coumarin 153 (peak 535 nm, range 517-574 nm) UV light from Dye 1 is abstracted by several separation mirrors that reflects UV light at rate of 99 % and 1 % others.

Oscillator of Dye 2 is including DCM with ethanol (peak 627 nm, range 602-660 nm) UV light from Dye 2 is abstracted by 4-prisum-pellin-broca -separations. Only UV light can out of the box, due to the difference of refractive index between the UV light and others.

Improvement and Optimization

A) Valve

Sample gas pulse is injected by poppet opening and closing the hole of sample holder. But, because the cone head poppet was shaved by cylindrical hole of sample holder, the damaged poppet generated the leaking. (Fig,5) Improvement is indicated next.



Fig,5 damaged poppet

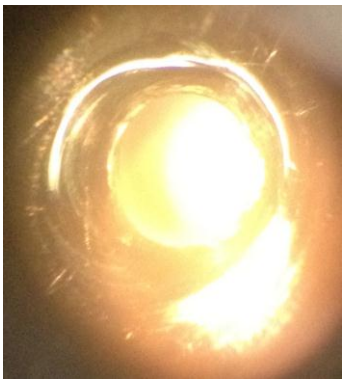
1, Sample holder hole was improved from cylindrical to conical.

2, Entrance of the hole was shaved as smooth. (Fig,6)

3, New Teflon poppet was used. But, the Teflon poppet also generated the leaking problem, because new one was shaved immediately.

3, The Leaking problem was

almost solved by shaving tip of the poppet little and little.



Fig,6 improved hole of sample holder

There were many failure points to shave the poppet. For example, the poppet could not close the hole, because tip of the hole was shaved too much and the poppet had continued closing the hole, because tip of the hole is longer.

B) Devices and Optimization (Fig,7)

I could operate almost devices to optimize experiment condition. And I confirmed the effectiveness of each device. Function of each device and configuration of the MATI system is indicated next.

1, Pressure Meter shows pressure of top of chamber.

2, Pressure Meter shows pressure of center of chamber.

3, Function Generator is not used.

4, Hi-Res MATI pulse Generator operates voltage of extraction pulse.

5, Oscilloscope

6, DG 535 role is connection of other device.

7, Auto-Tracker operator sends information of the timing to auto-tracker.

8, DUAL RAMP Generator operates voltage of capacitor.

9, Amplifier is not used.

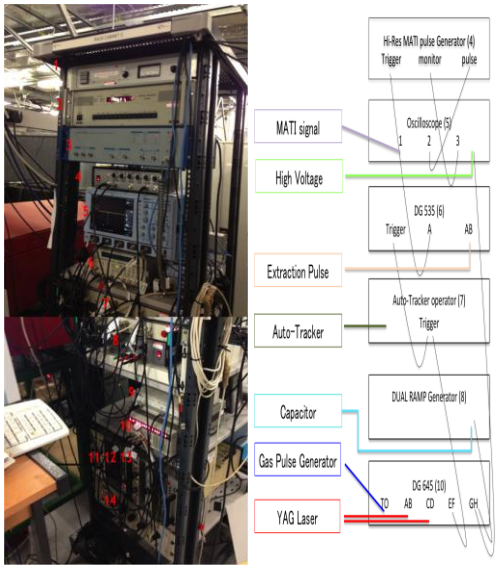
10, DG 645 decides the timing between gas pulse and laser irradiation.

11, Repeller operator operates voltage of repeller.

12, Ion Lens operator operates voltage of ion lens.

13, MCP operator operates voltage of MCP.

14, Reflector operator operates voltage of reflector



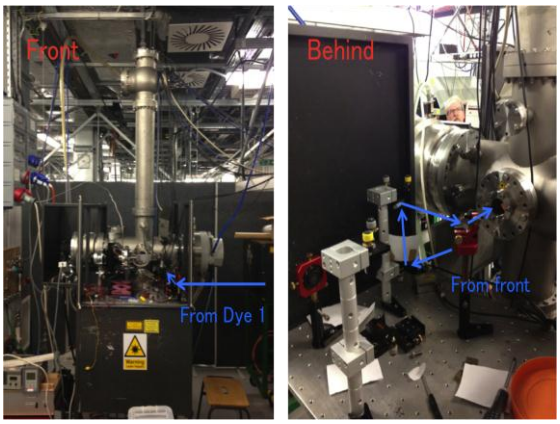
Fig,7 Photo of devices and configuration of MATI system

C) Alignment

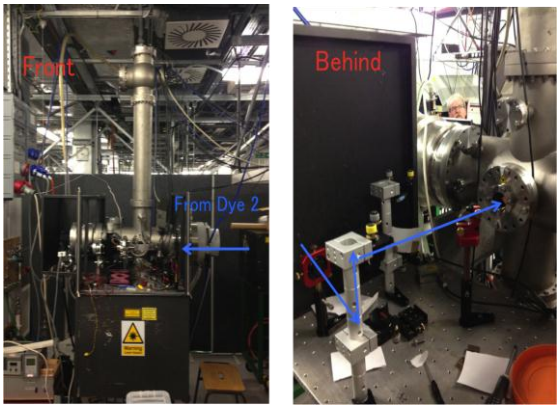
1, Mirror that reflects only the 266 ± 10 nm light is selected.

2, Laser route is expanded gradually, while cutting the travel direction light with using paper.

3, The light is aligned by adjusting the mirror with screws. (Fig.8,9)



Fig,8 Alignment of ν_1



Fig,9 Alignment of ν_2

My stay in England and Appreciation

I was surprised that many students from other country are studying in Manchester University. For this reason the cafeteria in the university provides many types of food, thus I had enjoyed eating lunch everyday. And I really enjoyed barbecue and drinking in the Prof, Klaus Muller-Dethlefs home. Thanks for the inviting.

Finally, I would like to express my deep appreciation to Prof, Klaus Muller-Dethlefs in Manchester University and Prof. M, Fujii in Tokyo institute of Technology and all the staff who assisted with this program.

Summery

1, I could study mechanism of laser, how to alignment and optimization by operating almost devices.

2, In England, often I could not understand what was a person saying. I felt that I need to study English harder.