

# INTERNATIONAL CONFERENCE ON KEY INTERMEDIATES IN ATMOSPHERIC CHEMISTRY AND ASTROCHEMISTRY

## Keynote Speakers

**David Anderson**

Professor, Department of Chemistry  
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**David W. Chandler**

Sandia Research Fellow  
Combustion Research Facility  
Sandia National Laboratories, USA

**Michael A. Duncan**

Franklin Professor, Department of Chemistry  
The University of Georgia, USA

**Marsha I. Lester**

Christopher H. Browne Distinguished Professor  
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University of Pennsylvania, USA

**Ming-Chang Lin**

Chair Professor, Department of Applied Chemistry  
National Yang Ming Chiao Tung University, Taiwan

**Kopin Liu**

Distinguished Visiting Chair  
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Academia Sinica, Taiwan

**Terry Miller**

Ohio Eminent Scholar Professor Emeritus  
The Ohio State University, USA

**Takamasa Momose**

Professor, Department of Chemistry  
The University of British Columbia, Canada

**Wolfram Sander**

Professor, Faculty of Chemistry and Biochemistry  
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**Richard J. Saykally**

Professor Emeritus, College of Chemistry  
University of California, Berkeley, USA

**Henry F. Schaefer III**

Graham Perdue Professor  
Department of Chemistry  
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**Stephan Schlemmer**

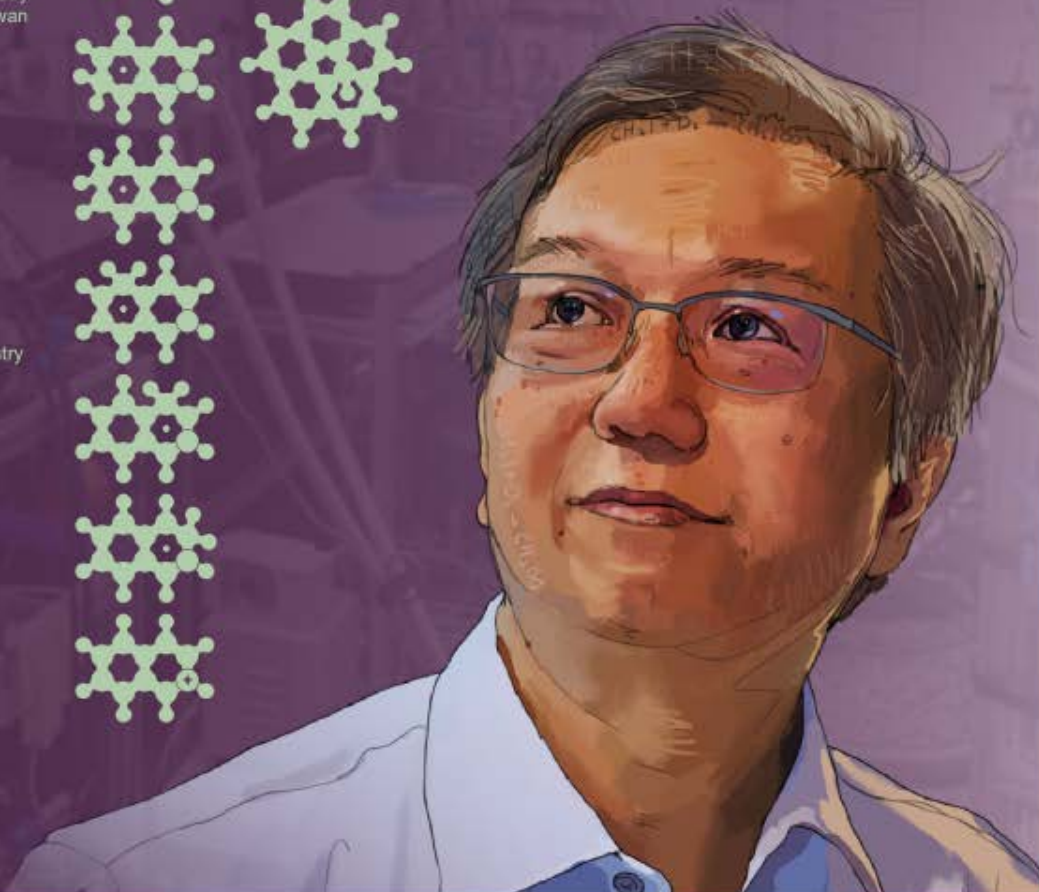
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University of Florida, USA

**Craig A. Taatjes**

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**Honoring Remarkable 42-year Career of Prof. Yuan-Pern Lee in  
Spectroscopy and Chemical Kinetics of Unstable Molecules**

**January 23-25  
2024**

## Venue:

**Department of Applied Chemistry  
National Yang Ming Chiao Tung University**

## Organizer:

Department of Applied Chemistry, National Yang Ming Chiao Tung University  
國立陽明交通大學 應用化學系

## Co-organizers:

Institute of Atomic and Molecular Sciences, Academia Sinica  
中央研究院原子與分子科學研究所  
Department of Chemistry, National Tsing Hua University  
國立清華大學 化學系  
National Synchrotron Radiation Research Center  
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# Welcome Message

Welcome to *International Conference on Key Intermediates in Atmospheric Chemistry and Astrochemistry* to be held in National Yang Ming Chiao Tung University, Hsinchu, Taiwan from January 23 to 25, 2024. This conference aims to offer an opportunity for the exchange of current research results of spectroscopy and chemical kinetics and dynamics of atmospherically and astronomically important molecules, radicals, or ions in gaseous or condensed phases in order to promote higher education in fundamental science and international collaborations in Taiwan. On this occasion, we will also be honoring the remarkable 42-year career of Prof. Yuan-Pern Lee in spectroscopy and chemical kinetics of unstable molecules. Most invited guests have either played an important role or stayed in his group during the career of Prof. Yuan-Pern Lee.

## Organization Committee

Eric Wei-Guang Diau, <i>Chair</i>	National Yang Ming Chiao Tung University
Yu-Jong Wu, <i>Co-Chair</i>	National Synchrotron Radiation Research Center
Jer-Lai Kuo, <i>Co-Chair</i>	Academia Sinica
Yen-Ju Cheng	National Yang Ming Chiao Tung University
Chien-Ming Tseng	National Yang Ming Chiao Tung University
I-Chia Chen	National Tsing Hua University
Jim Jr-Min Lin	Academia Sinica
Kaito Takahashi	Academia Sinica
Li-Kang Chu	National Tsing Hua University
Pei-Ling Luo	Academia Sinica

## Program – Jan. 23 (Tuesday)

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09:00-09:20 Registration

09:20-09:30 Opening & Photo

### Session 1

Chair: Eric Wei-Guang Diau

09:30-10:40 Yuan-Pern Lee  
*Nearly 50 years with unstable species—my enjoyable research life and many thanks*

10:40-11:00 Break

### Session 2

Chair: Yuan-Pern Lee

11:00-11:35 K-1 Henry F. Schaefer III (University of Georgia, USA)  
*Professor Yuan-Pern Lee: A career of scientific distinction*

11:35-12:00 I-1 Hiroshi Masuhara (National Yang Ming Chiao Tung University, Taiwan)  
*Optical binding and swarming of gold nanoparticles at solution interface*

12:00-13:30 Lunch

### Session 3

Chair: Yasuki Endo

13:30-14:05 K-2 Marsha I. Lester (University of Pennsylvania, USA)  
*Reactive intermediates in hydrocarbon oxidation chemistry*

14:05-14:40 K-3 Craig A. Taatjes (Sandia National Laboratories, USA)  
*Directly measuring the kinetics of once-elusive intermediates*

14:40-15:05 I-2 Jim Jr-Min Lin (Academia Sinica, Taiwan)  
*UV spectroscopy and reaction kinetics of Criegee intermediates*

15:05-15:30 I-3 Pei-Ling Luo (Academia Sinica, Taiwan)  
*Absolute line strength measurements of transient free radicals with mid-infrared two-color time-resolved dual-comb spectroscopy*

15:30-15:50 Break

### Session 4

Chair: Keiichi Tanaka

15:50-16:25 K-4 Stephan Schlemmer (University of Cologne, Germany)  
*Missions: Missing ions in laboratory and space*

16:25-16:50 I-4 Yasuki Endo (National Yang Ming Chiao Tung University, Taiwan)  
*Detection of the reaction products between the simplest Criegee intermediate and organic acids*

16:50-17:15 I-5 Li-Kang Chu (National Tsing Hua University, Taiwan)  
*Vibrational characterizations and reactions of geminal diols*

### Poster Session

Chair: Masashi Tsuge

17:15-18:30 Poster flash talks

18:30-19:00 Dinner

19:00-21:00 Poster

## Program – Jan. 24 (Wednesday)

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09:00-09:30 Preparation

### Session 5

Chair: John P. Maier

09:30-10:05 K-5 Takamasa Momose (The University of British Columbia, Canada)

*Asymmetric photolysis of neutral amino acids in solid parahydrogen*

10:05-10:40 K-6 David Anderson (University of Wyoming, USA)

*Adventures in parahydrogen matrix isolation infrared spectroscopy*

10:40-11:00 Break

### Session 6

Chair: György Tarczay

11:00-11:35 K-7 Wolfram Sander (Ruhr-Universität Bochum, Germany)

*Criegee intermediates and carbenes – controlling spin and reactivity of highly reactive molecules*

11:35-12:00 I-6 Yu-Jong Wu (National Synchrotron Radiation Research Center, Taiwan)

*Mass-selected UV/visible absorptions of  $\text{CO}_2^+$  and aniline<sup>+</sup> in solid neon*

12:00-13:30 Lunch

### Session 7

Chair: Yoshiyuki Matsuda

13:30-14:05 K-8 Richard J. Saykally (University of California, USA)

*Reversed fractionation of aqueous carbonate and bicarbonate at the air-water interface*

14:05-14:40 K-9 Michael A. Duncan (The University of Georgia, USA)

*Spectroscopy of iron organometallic ions relevant for astrochemistry*

14:40-15:05 I-7 Asuka Fujii (Tohoku University, Japan)

*Probing acidity of terminal OH sites in hydrogen bond networks by use of weak proton acceptors*

15:05-15:30 I-8 Jer-Lai Kuo (Academia Sinica, Taiwan)

*Fermi resonance in mid- and near-IR & from 1-D to 2D*

15:30-15:50 Break

### Session 8

Chair: Ming-Chang Lin

15:50-16:25 I-9 Hiroyuki Matsui (Toyohashi University of Technology, Japan)

*Thermal decomposition of alkyl radicals and reactions of H atoms with alkanes*

16:25-16:50 I-10 Kaito Takahashi (Academia Sinica, Taiwan)

*Water catalysis in gas phase reactions?*

16:50-17:15 I-11 I-Chia Chen (National Tsing Hua University, Taiwan)

*Study the triplet electronic states using step-scan time-resolved Fourier transform near-infrared spectroscopy*

17:15-17:40 I-12 Nobuhiro Ohta (National Yang Ming Chiao Tung University, Taiwan)

*Electric field effects on structure, dynamics and function in molecules, molecular system and biological system*

17:40-18:30	Break
18:30~	Banquet

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## Program – Jan. 25 (Thursday)

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09:00-09:30	Preparation
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### Session 9

Chair: Chi-Kung Ni

09:30-10:05	K-10 Terry A. Miller (The Ohio State University, USA) <i>Spectroscopy, dynamics, and absorption cross sections of free radical intermediates in the tropospheric oxidation of volatile organic compounds</i>
10:05-10:40	K-11 David W. Chandler (Sandia National Laboratories, USA) <i>Sulfur from SO<sub>2</sub> photochemistry from C state excitation</i>

10:40-11:00	Break
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### Session 10

Chair: Chien-Ming Tseng

11:00-11:35	K-12 Kopin Liu (National Sun Yat-sen University, Taiwan) <i>Quantum-phase control of a polyatomic reaction under ambient conditions</i>
11:35-12:00	Closing Remarks and Poster Awards
12:00-13:30	Lunch
13:30~	Excursion or laboratory visit

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## Poster Presentations

#	Presenter	Title
1	Chen-An Chung	The rate coefficient of <i>syn-trans</i> -MVKO with HCOOH investigated with a quantum-cascade laser system
2	Ching-Hua Chang	Pure rotational spectra and characteristics of triatomic free radicals: CISO and CISS
3	Chun-Yao Hou	<i>In situ</i> and <i>real-time</i> vibrational spectroscopic characterizations of the photodegradation of nitrite in the presence of methanediol
4	Che-Wei Chang	High resolution spectroscopy of HO <sub>2</sub> radical and its self- reaction kinetics
5	I-Yun Chen	Determination of the rate coefficient of the reaction OH + HO <sub>2</sub>
6	Kai-En Zhang	Using spatially differentiated velocity map imaging in the study of large molecule photodissociation
7	Keiichi Tanaka	FTMW spectroscopy of the <sup>13</sup> C/ <sup>18</sup> O-substituted tropolone and the determination of tunneling splitting
8	Liang-Yu Qiu	Studying reaction of aerosol with formaldehyde under different relative humidity via aerosol optical tweezers
9	Tang-Yu Kao	Rate coefficients of CH <sub>3</sub> CHI with O <sub>2</sub> and <i>syn-/anti</i> -CH <sub>3</sub> CHO with HCl investigated with an IR/UV dual probe system
10	Wei Lin	The microwave spectra of ethanesulfonic acid and its monohydrate
11	Yen-Hsiu Lin	Absolute photodissociation cross sections of thermalized methyl vinyl ketone oxide (MVKO) and methacrolein oxide (MACRO) were measured
12	Yu-Lun Hsiao	Spectral studies of the reaction of the Criegee intermediate methyl vinyl ketone oxide (MVKO) with HC(O)OH using a step-scan time-resolved Fourier-transform infrared absorption spectrometer
13	Yoshiyuki Matsuda	Infrared spectroscopic investigation of radical cations of hydrocarbons and its clusters
14	Prasanta Das	Investigation of HBr elimination in the photolysis of bromobenzene at 266 nm using repetitive scan FT-IR spectroscopy and DFT calculations

15	Xiang-He Yang	Investigation of excited state relaxation of hemicyanine dye
16	Qian-Rui Huang	A perturb-then-diagonalize algorithm for high-dimensional anharmonic vibrational analysis
17	Po-Jen Hsu	Infrared spectroscopy and theoretical structure analyses of the protonated 2,2,2-trifluoroethanol and ethanol mixed clusters
18	Yi-Shan Chung	Infrared spectra of isomers of protonated and hydrogenated phenanthridine isolated in solid <i>para</i> -hydrogen
19	Heng Liao	A model for extended red emission: Far-UV-induced photoluminescence in graphene
20	Jun-Ying Feng	Infrared spectra of protonated methane isolated in solid <i>para</i> -hydrogen
21	Chun-Kai Chen	Electronic spectra of protonated and hydrogenated isoquinoline isolated in solid <i>para</i> -hydrogen
22	Chun-Yi Lee	UV-induced photochemical reactions on water-covered carbonaceous grains: Dust thickness and structure effects
23	Kai-Hsi Hung	Infrared spectra of isomers of protonated and hydrogenated phenol isolated in solid <i>para</i> -hydrogen
24	Masashi Tsuge	Experimental investigations on the behavior of free radicals on the surface of icy grain analogues
25	Ni-En Sie	The photodesorption of OH radical triggered by visible light
26	Prasad Ramesh Joshi	Production of HO <sup>•</sup> CHC(O)H, HOCH <sub>2</sub> <sup>•</sup> CO, and HOCH <sub>2</sub> CH <sub>2</sub> O <sup>•</sup> in the reaction H + glycolaldehyde [HOCH <sub>2</sub> C(O)H] in solid <i>p</i> -H <sub>2</sub> and its implication in astrochemistry
27	Reo Sato	In situ electron diffraction analysis of nanoscale ice formed by neon matrix sublimation at cryogenic temperatures
28	Sheng-Lung Chou	Exploring multiphase ion-neutral reactions: The preliminary studies on CO <sub>2</sub> <sup>+</sup> with H <sub>2</sub> in solid H <sub>2</sub>
29	Shun-Lin Tseng	The formation of complex organic molecules via energetic electrons irradiation of astrophysical ices
30	György Tarczay	New insights into H atom reactions of astrophysical significance through <i>para</i> -H <sub>2</sub> matrix isolation
31	Isabella Weber	Electronic spectroscopy of polycyclic aromatic hydrocarbons in solid <i>para</i> -hydrogen
32	Koichiro Yamakawa	Nuclear spin conversion of methane in condensed layers at low

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		temperatures
33	Yen-Yu Hsu	Interstellar ice-dust interactions: UV-induced $^{13}\text{CO}_2$ formation on $^{13}\text{C}$ -Dust with $\text{H}_2\text{O}$ ice deposited at various temperatures
34	Yi-Hsiang Peng	Photochemical reaction of $\text{CH}_4$ in $\text{N}_2$ -rich environment
35	Chih-Hao Chin	Electronic absorption spectra of 4-phenanthridine cations: A theoretical study
36	Brataraj Ghosh	Elucidating structure and properties of charged sugars/glycosaminoglycans using neural network potential
37	Klichchupong Dabsamut	Controlling C-C coupling reactivity through pore shape engineering of B-doped graphyne family
39	Pei-Kang Tsou	A neural network accelerated target search to study the dissociations in Di-saccharides

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# **Plenary Lectures**

## Nearly 50 years with unstable species– my enjoyable research life and many thanks

Y.-P. Lee<sup>1,2</sup>

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After one year of undergraduate research and two years of military service, I went to Department of Chemistry, U. C. Berkeley in 1975 and joined the group of Prof. George C. Pimentel. Later, I also joined the group of Prof. Henry F. Schaefer III to do some computations to verify my experimental results. I received my Ph.D. degree in 1979 and went to Boulder, Colorado to serve as a postdoctoral fellow of Prof. Carleton J. Howard in the Aeronomy Laboratory of National Oceanic and Atmospheric Administration. I became an associate professor in Department of Chemistry, National Tsing Hua University in August, 1981 and was promoted to full professorship in 1985. In 2004, I moved to Department of Applied Chemistry, National Chiao Tung University as a Chair Professor. I served as the Dean of Science from 2005 to 2008 and Director of Center for Interdisciplinary Science and Center for Emergent Functional Matter Science for many years. At age 70, I “officially” retired in January 2022 and was fortunate to have been a contract-based professor since my retirement.

For my research life of nearly 50 years, I have been interested in unstable species, especially those that are important in combustion, atmospheric chemistry, and astrochemistry. I worked mainly on their spectroscopy and reaction kinetics/mechanism. The spectra of more than hundred fifty unstable species have been characterized, including Criegee intermediates and protonated/hydrogenated polycyclic aromatic hydrocarbons (PAH).

In this talk, I will present a brief review of my research route and highlights; I will point out many people who have taught me, assisted me, recognized me, or inspired me. I really appreciate that many of them are participating this memorable event despite their busy schedule and the long travel.

## **Professor Yuan-Pern Lee: A career of scientific distinction**

Henry F. Schaefer III

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Yuan-Pern Lee was a PhD student at the University of California at Berkeley between 1975 and 1979. His PhD advisor was the legendary experimental physical chemist George C. Pimentel. However, to the surprise of some, Yuan-Pern spent a fraction of his time at Berkeley doing theoretical chemistry, with me as his secondary PhD advisor. My gifted PhD student William C. Swope served as mentor to YP during his theoretical studies, which resulted in three important papers. My lecture will recall these early days and then discuss some of YP's subsequent pioneering research.

## Reactive intermediates in hydrocarbon oxidation chemistry

Marsha I. Lester

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Our research is focused on reaction intermediates in atmospheric chemistry that generate hydroxyl radicals (OH), often called the atmosphere's detergent. The OH radical is one of the most powerful oxidizing agents in the troposphere, which is able to react rapidly with other molecules, including most volatile organic compounds emitted in the atmosphere. Our studies have characterized transient carbonyl oxide intermediates, known as Criegee intermediates ( $R_1R_2C=O^+O^-$ ), in the chemical reaction pathways for **alkene ozonolysis** [1-2], an important non-photolytic source of OH radicals. A recent thrust of our research is focused on hydroperoxyalkyl radical ( $\bullet QOOH$ ) intermediates containing a carbon radical ( $\bullet Q$ ) center, which are transient intermediates in **alkane oxidation** [3]. Spectroscopic and time-resolved dynamical studies of these reactive intermediates reveal unconventional unimolecular reaction dynamics involving quantum mechanical tunneling [1-3] and roaming [4-5]. Experimental studies and complementary theoretical analysis show the importance of these dynamical pathways under controlled laboratory conditions as well as their impact in atmospheric chemistry.

### References

- [1] V. P. Barber, S. Pandit, A. M. Green, N. Trongsirawat, et al., *J. Am. Chem. Soc.* **140**, 10866 (2018).
- [2] V. P. Barber, A. S. Hansen, Y. Georgievskii, S. J. Klippenstein, et al., *J. Chem. Phys.* **152**, 094301 (2020).
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## Directly measuring the kinetics of once-elusive intermediates

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Understanding the networks of chemical reactions that govern technological and environmental questions, such as autoignition in combustion engines, heterogeneous catalysis, or formation of atmospheric aerosols often hinges on understanding the reactions of a few key intermediate species. These intermediates are formed by some reactions in the system and the course of their subsequent chemical transformations changes the behavior of the overall system. A central focus in understanding complex chemical systems is therefore the experimental characterization and quantification of reaction intermediates. I will focus on recent work that related to hydrocarbon oxidation chemistry in the troposphere and in combustion, describing how methods to independently produce these intermediates and follow their chemistry, combined with advanced theory and modeling, can guide our understanding of these oxidation systems.

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## MissIons: Missing ions in laboratory and space

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Ions play a key role in the chemical evolution of our universe. The process of star and planet formation is tightly connected to the presence and abundance of these species. Their spectra are diagnostic tools for various astrophysical environments and their temporal evolution. However, laboratory spectra of most ions relevant to astrophysics are not available. Moreover, predicted spectra from ab-initio theory are not nearly accurate enough to guide astrophysical searches. Therefore, laboratory spectra of molecular ions are needed. I will report on progress towards recording high-resolution spectra from the microwave to visible range using our unique and innovative methods in ion traps [1]. These methods are molecule specific through mass selection, many orders of magnitude more sensitive and less complex due to buffer gas cooling as compared to conventional spectroscopy methods.

Examples concern the first molecule observed in space,  $\text{CH}^+$  [2] but also ions which can play an important role in the chemical development producing more complex species, e.g.,  $\text{C}_3\text{H}^+$  [3],  $\text{C}_3\text{H}_2^+$  [4] and  $\text{CH}_3^+$  [5]. For many reasons  $\text{H}_3^+$ , including its deuterated siblings, is a corner stone in ion chemistry. It gives away its proton to most other species. As a result, protonation of more complex species, like methanol, could be another key towards the formation of complex organic species, molecules which are observed with today's telescopes but how they come into existence is under debate. I will discuss the tools to record the spectra and to understand the relevant reactions in the laboratory.

### References

- [1] B. A. McGuire, O. Asvany, S. Brünken, S. Schlemmer, *Nat. Rev. Phys.* **2**, 402 (2020).
- [2] J. L. Doménech, P. Jusko, S. Schlemmer, O. Asvany, *Astrophys. J.* **857**, 61 (2018).
- [3] S. Brünken, L. Kluge, A. Stoffels, O. Asvany, et al., *Astrophys. J. Lett.* **783**, L4 (2014).
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## Asymmetric photolysis of neutral amino acids in solid parahydrogen

T. Momose and B. Moore

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Asymmetric photolysis of chiral molecules induced by circularly polarized photons has attracted attention due to its potential connection to the extraterrestrial origin of homochirality in current biological systems. Numerous studies have explored the asymmetry in amino acids. However, these studies focused on samples in liquid or solid states, where amino acids predominantly exist in their zwitterionic form. In the unique conditions of interstellar space, such as gas phases or on grain surfaces, amino acids are likely more stable in their neutral form rather than the zwitterionic form. This makes the study of the asymmetry in the neutral form more pertinent to understanding the extraterrestrial origins of homochirality. Through matrix isolation spectroscopy, it has been demonstrated that amino acids can exist in their neutral forms within these matrices. Various studies by Prof. Y. P. Lee's group have demonstrated that parahydrogen is a particularly useful matrix host for photodissociation studies due to its diminished cage effect [1, 2, 3]. We applied parahydrogen matrix isolation spectroscopy to the photodissociation of amino acids, and found that UV photons near 200 nm lead to the dissociation of the alpha carbonyl C-C bond, forming the HOCO radical and destroying chirality [4]. When employing circularly polarized UV photons, we observed an asymmetry in the dissociation rate as high as 0.1 for neutral leucine, a significant finding given that photoexcitation asymmetry is typically less than 0.005 [5]. This degree of asymmetry, at 0.1, could result in an enantiomeric excess of over 10% at 90% reaction completion. Our study demonstrates that parahydrogen matrix isolation spectroscopy is a valuable method for investigating asymmetric photolysis of amino acids in their neutral form.

### References

- [1] C. -W. Huang, Y. -C. Lee, Y. -P. Lee, *J. Chem. Phys.* **132**, 164303 (2010).
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## Adventures in parahydrogen matrix isolation infrared spectroscopy

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The use of *para*-hydrogen (p-H<sub>2</sub>) as a host in matrix isolation studies really began in 1998 when Momose and Shida started using solid p-H<sub>2</sub> to record the infrared spectrum of unstable molecules such as radicals and ions [1]. Sparked by the eloquent high-resolution laser studies of solid p-H<sub>2</sub> by Oka and co-workers [2], there was growing interest in developing so-called quantum hosts such as liquid helium and solid p-H<sub>2</sub> for matrix isolation studies. In principle quantum hosts offer several advantages - sharp guest species linewidths, weak cage effect for *in situ* photolysis studies, and tunneling mobility - over classical noble gas matrices such that new low temperature phenomena can be explored.

Research in the Anderson group started in 2000 at the University of Wyoming where we made several discoveries: guest species induce IR activity in the solid p-H<sub>2</sub> host [3], mobile *ortho*-hydrogen (o-H<sub>2</sub>) molecules present at controlled proportions can be used to form guest-(o-H<sub>2</sub>)<sub>n</sub> clusters [4], and we identified and developed a two-step UV/IR photolysis scheme to selectively produce hydrogen atoms (H-atoms) in order to study low temperature bimolecular chemical reactions [5]. We have focused our subsequent studies on the details of H-atom reactions with various guest species in solid p-H<sub>2</sub>.

However, this talk will highlight some new results that I think nicely illustrate how quantum hosts differ from classical matrix hosts. From the beginning we have been interested in how *in situ* photochemistry can be utilized to create species that are difficult to generate any other way. In the current studies, we photolyze diborane (B<sub>2</sub>H<sub>6</sub>) at 193 nm to create two BH<sub>3</sub> fragments that easily escape the solvent cage and react with the p-H<sub>2</sub> host to generate BH<sub>5</sub>. The BH<sub>5</sub> chemical intermediate is a highly fluxional molecule and is thought to scramble the hydrogen atoms within the complex. Following the photolysis exposure, we observe recombination of the photofragments which indicate that BH<sub>3</sub> (or BH<sub>5</sub>) can diffuse through the p-H<sub>2</sub> matrix even at temperatures as low as 1.5 K. We learn how far the photofragments travel before equilibrating with the p-H<sub>2</sub> solid and at what separation distance they recombine with unit probability. I will also show that the BH<sub>5</sub> species catalyzes p-H<sub>2</sub> → o-H<sub>2</sub> nuclear spin conversion in highly enriched p-H<sub>2</sub> solids at liquid helium temperatures via a mechanism that must involve H<sub>2</sub>(v=1) vibrons. The fact that the BH<sub>5</sub> fragments are mobile and can recombine was unexpected and shows how matrix isolation studies can also be used to probe the peculiarities which arise from the dominance of zero-point effects in these weakly interacting, light mass, media.

### References

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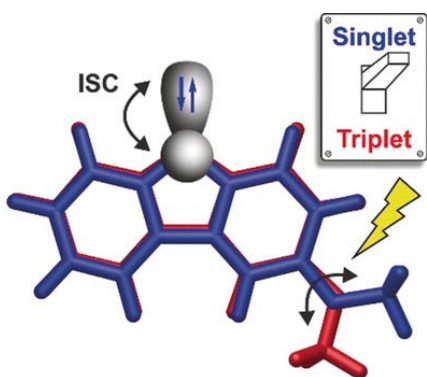
## Criegee intermediates and carbenes – controlling spin and reactivity of highly reactive molecules

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Carbonyl oxides, the Criegee intermediates, are highly reactive molecules that play a role in oxidation processes, including oxidation reactions in the troposphere. The properties of these species vary much with substituents. The first part of the lecture will give a short overview of the synthesis and isolation of Criegee intermediates in low-temperature matrices [1].

Carbenes are divalent carbon species which are significant trace constituents of the gas in the interstellar medium (ISM). These extremely reactive molecules can exist in two spin states: triplet as the parent carbene  $\text{CH}_2$  or singlet as cyclopropenylidene  $\text{C}_3\text{H}_2$ . Both carbenes were detected in the ISM. The triplet states react as diradicals, and the reaction with  $\text{O}_2$  leads to Criegee intermediates. In contrast, singlet states react as zwitterions exhibiting an entirely different reaction pattern. A paradigm of carbene chemistry is that reactions of carbenes are spin-specific, and that the intersystem crossing between the spin states occurs at a picosecond time scale. Thus, spin-equilibration precedes most chemical reactions.

Recently, we challenged this paradigm by isolating the same carbenes in both spin states as mixtures of singlet and triplet species [2, 3]. The intersystem crossing in these carbenes is exceedingly slow, leading to non-thermal spin distributions. The second part of the lecture will show examples of spin-bistable carbenes and discuss how this unusual behavior influences carbene reactivity.



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## Reversed fractionation of aqueous carbonate and bicarbonate at the air–water interface<sup>1</sup>

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In the course of our investigations of the adsorption of ions to the air-water interface, we previously reported the surprising result that doubly-charged carbonate anions exhibit a stronger surface affinity than do singly-charged bicarbonate anions. In contrast to monovalent, weakly hydrated anions, which generally show enhanced concentrations in the interfacial region, multivalent (and thus strongly hydrated) anions are expected to show much weaker surface propensity. Recently, we used resonantly enhanced deep-UV second harmonic generation spectroscopy to measure the Gibbs free energy of adsorption of both carbonate and bicarbonate anions to the air-water interface. Contrasting the predictions of classical electrostatic theory, and in support of our previous findings from X-ray photoelectron spectroscopy, we find that carbonate anions do indeed exhibit much stronger surface affinity than do the bicarbonate anions. Molecular dynamics simulation reveals that strong ion pairing of carbonate with sodium counter-cations in the interfacial region, resulting in formation of near-neutral “agglomerates”, is responsible for this counterintuitive behavior. These findings not only advance our fundamental understanding of ion adsorption chemistry, but will also impact important practical processes such as ocean acidification, atmospheric aerosol chemistry, and mammalian respiration physiology.

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## Spectroscopy of iron organometallic ions relevant for astrochemistry

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Organometallic ion complexes have been implicated as important species in astrochemistry, and suggested to be involved in the catalytic formation of large biomolecules or to be carriers of optical signals such as the diffuse interstellar bands (DIBs). Iron is by far the most abundant transition metal in space, and therefore its organometallic ions are particularly interesting. In the present work, we investigate the properties of iron cation complexes with acetylene or benzene molecules using a combination of molecular beams, mass spectrometry and laser spectroscopy.

Ion-molecule complexes of the form  $\text{Fe}^+(\text{C}_2\text{H}_2)_n$  and  $\text{Fe}^+(\text{benzene})_n$  are produced by laser vaporization in a pulsed-nozzle supersonic beam source. The ions are analyzed and selected by mass in a reflectron time-of-flight mass spectrometer. Vibrational spectroscopy measurements on the acetylene complexes are performed with infrared photodissociation spectroscopy, using an IR-OPO laser and the method of "tagging" with argon atoms to enhance dissociation yields [1]. UV-visible spectroscopy on  $\text{Fe}^+(\text{C}_2\text{H}_2)$ ,  $\text{Fe}^+(\text{benzene})$  and  $\text{Fe}^+(\text{benzene})_2$  is accomplished via photodissociation using a UV-visible OPO laser [2,3]. The energetic threshold where photodissociation first occurs provides the metal ion-ligand bond energy. Additional experiments employ the method of photofragment imaging to investigate the energetics of the cation- $\pi$  bonds which form in these complexes [2,3].

Infrared experiments establish that the  $\text{Fe}^+(\text{C}_2\text{H}_2)$  complex has a cation- $\pi$  structure, with the iron cation located in a symmetric position above the triple bond of acetylene. Charge-transfer interactions cause the C-H stretch vibrations to shift to lower frequencies compared to those in the free acetylene molecule. Electronic spectroscopy and photofragment imaging measurements are in agreement on the cation-molecular bond energies in these complexes, and the values obtained also agree with previous results from collisional dissociation experiments. The electronic spectra for both  $\text{Fe}^+(\text{C}_2\text{H}_2)$  and  $\text{Fe}^+(\text{benzene})$  quasi-continuous throughout the visible wavelength region, eliminating these ions as candidates to explain DIB spectra.

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## **Spectroscopy, dynamics, and absorption cross sections of free radical intermediates in the tropospheric oxidation of volatile organic compounds**

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Enormous amounts, of order 500 Tg/year, of volatile organic compounds are injected into the troposphere. Photo-initiated oxidation of these organics leads to numerous free-radical intermediates that drive complex chemistry that profoundly affects the world around us and the quality of the air we breathe. This talk will focus on one family of these intermediates, which are the peroxy radicals,  $\text{RO}_2$ , with the emphasis on those for which R is an alkyl group. These species have an electronic transition in the near infrared (NIR). Room temperature NIR spectra have been observed that allow detailed experimental spectra-structure relationships to be developed and show the dependence of spectral properties on the number of carbon atoms in the radical, and its isomeric and conformeric structure. Higher resolution rotationally resolved spectra of peroxy radicals cooled by free-jet expansion to near 10K also have been observed. Analysis of these spectra determine molecular parameters that depend on the molecule's precise geometric structure and distribution of its unpaired electronic spin density. The observed spectral widths probe the dynamics of the radicals when they are subjected to NIR radiation. The room-temperature spectrum can be used as a diagnostic for sensitive and selective measurement of radical concentrations for different  $\text{RO}_2$  species in an isomer- and conformer-specific manner. For this purpose, absorption cross sections must be determined. Calculation of these cross sections using quantum chemistry techniques is described and compared with empirical means for their determination.

## Sulfur from SO<sub>2</sub> photochemistry from C state excitation

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When SO<sub>2</sub> is dissociated in with 193-nm light a small amount of Sulfur atoms has been observed<sup>1</sup> under flow reactor conditions. This would indicate a new method for formation of O<sub>2</sub> in early earth atmosphere. We have cooled SO<sub>2</sub> into a molecular beam and observed both O atoms and S atoms via 2+1 resonantly enhanced multiphoton ionization following excitation of individual transitions of the C electronic state. Velocity mapped Ion imaging was used to detect the velocity of the S and O atoms. The results and their interpretation will be discussed.

### Abel-Inverted Velocity-Mapped Image of S<sup>+</sup> UV Excitation of SO<sub>2</sub> at 200.430 nm 2+1 REMPI of S at 308.203 nm

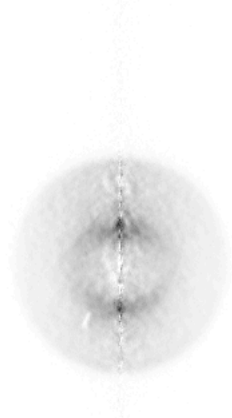


Figure 1: Image of S atoms from SO<sub>2</sub>.

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# Quantum-phase control of a polyatomic reaction under ambient conditions

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Mode-selectivity is a well-established concept in chemical dynamics. A polyatomic molecule possesses multiple vibrational modes; the mechanical couplings between them result in complicated anharmonic motions, defying a simple oscillatory description. Fermi-coupled vibration is a prototypical example, in which an energy-split eigenstate executes a coherent nuclei-motion comprising the characters of constituent normal modes with distinctive phases. Will this vibrational phase affect chemical reactivity? How to disentangle the phase effect from the amplitude effect? Here we report an experiment to address these questions in the reaction of Cl-atom with a pair of Fermi-states of  $\text{CH}_3\text{D}(\nu_1\text{-I}$  and  $\nu_1\text{-II})$ . We found that the reactivity ratio of  $(\nu_1\text{-I})/(\nu_1\text{-II})$  in forming the  $\text{CH}_2\text{D}(\nu = 0) + \text{HCl}(\nu)$  products deviates significantly from that permitted by the conventional reactivity-borrowing framework. Based on a proposed metric, this discrepancy can only be explained when the scattering interferences mediated by the  $\text{CH}_3\text{D}$  vibrational phases are explicitly considered [1], which expands the concept of vibrational control of chemical reactivity into the quantum regime—and under the ambient conditions.

In terms of more detailed state-to-state distributions, both the product vibrational state and the pair-correlated angular distributions in reactions with the two Fermi-paired  $\text{CH}_3\text{D}(\nu_1\text{-I}$  and  $\nu_1\text{-II})$  reactant states show striking similarities—only minor differences are noted. This ‘loss-of-memory’ finding is counterintuitive and in sharp contrast to the conventional wisdom that the more detailed differential cross sections should accentuate the differences shown in the integral cross sections even more. On the other hand, comparing to the corresponding dynamical attributes in the reaction with  $\text{CH}_3\text{D}(\nu_4=1)$ , where  $\nu_4=1$  denotes one quantum excitation of the anti-symmetric stretching mode, distinct mode-specific behaviors are clearly revealed [2, 3]. The precise mechanisms underpinning those perplexing observations are yet to be elucidated and call for future theoretical investigations.

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# **Invited Lectures**

# Optical binding and swarming of gold nanoparticles at solution interface

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Optical trapping enables 3D manipulation of single micro-objects and assembling of nanoparticles (NPs) at the focus in solution [1]. We found the assembling is extremely enhanced at solution interface; amino acid crystallization and assembling of supramolecule, protein, polystyrene NP, and so on. The assembly nonlinearly expands and reaches a few tens micrometer along the interface, although the trapping focus is in the order of 1  $\mu\text{m}$ . We named the phenomena “Optically Evolved Assembling” and have been studying their dynamics and mechanism [1, 2].

Gold NPs show a new phenomenon as in Figure 1. A few NPs are arranged periodically inside the trapping laser focus, then extending to the outside and evolving to dynamically fluctuating swarms [3]. This assembling and swarming can be interpreted in terms of optical binding and its network formation [4]. Particularly optical binding outside the focus is characteristic of optical trapping, which dynamics and mechanism will be discussed.

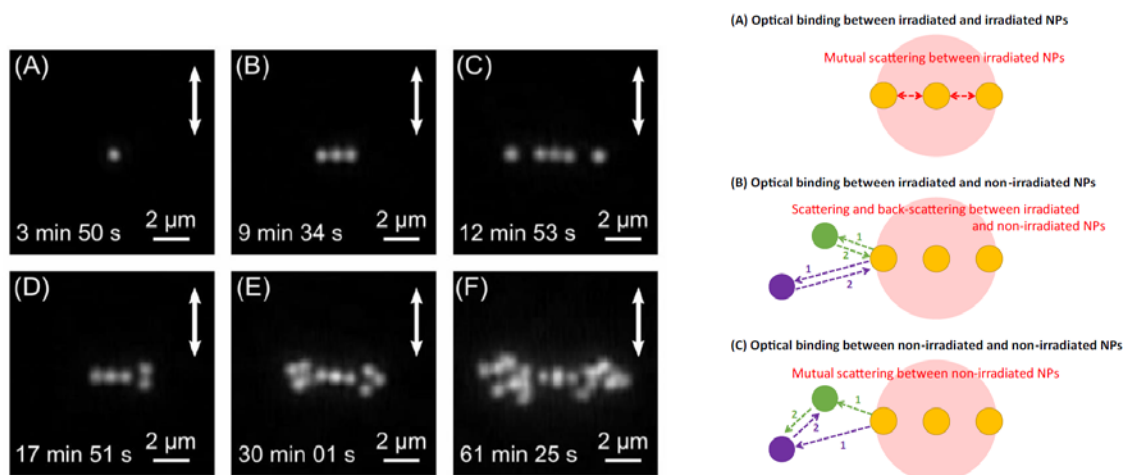


Figure 1. (LEFT) Light scattering images of gold nanoparticles of 400 nm diameter showing optically evolved assembling at glass/solution interface. The arrow indicates the polarization of the 1064 nm trapping laser. (RIGHT) Illustrations of optical binding inside and outside the trapping laser focus.

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## UV spectroscopy and reaction kinetics of Criegee intermediates

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Criegee intermediates (CIs) are very reactive carbonyl oxides which are formed in the ozonolysis of alkenes. CIs are thought to be important in the oxidation of atmospheric molecules including SO<sub>2</sub>, NO<sub>2</sub>, inorganic and organic acids, and even water. To better assess the roles of CIs of various structures in atmospheric chemistry, it is desired to know the trend of their reactivity. Our group has measured the UV spectra of a few important CIs and determined their absolute absorption cross sections. The intense UV absorption of CIs allows scientists to probe their reaction kinetics. We found that there are strong structure dependences in the thermal decomposition reactions of CIs and in their reactions with water molecules. Furthermore, there is a strong synergy effect in the CI reactions with hydrogen-bonding molecules. Vinyl substituted CIs are more stable due to the extended conjugation of the double bonds, which also affect the reactivity. The fates of various CIs in the atmosphere can be estimated based on their reactivity trend.

I will talk about the story of our research on CIs [1–5].

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# Absolute line strength measurements of transient free radicals with mid-infrared two-color time-resolved dual-comb spectroscopy

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Transient free radicals such hydroxyl (OH) and hydroperoxy (HO<sub>2</sub>) radicals play the important role in atmospheric chemistry. Quantification of the free radicals are important to further study the kinetics and mechanisms of many key atmospheric reactions. Here, a novel method to determination of transient free radicals using high-resolution time-resolved dual-comb spectroscopy will be reported [1–2]. By employing mid-infrared two-color time-resolved dual-comb spectroscopy [3–5], time-resolved spectral measurements can be achieved simultaneously in two molecular fingerprint regions 3~5 and 8~10 μm for determining multiple species such as precursor molecules, free radicals, and byproducts. With this new approach, in addition to studying the kinetics of bimolecular reactions involving OH and HO<sub>2</sub> radicals, the absolute line strength measurements of fundamental transitions of OH and HO<sub>2</sub> radicals are able to be achieved with a small uncertainty of <10% [5]. In the future work, the presented two-color time-resolved dual-comb spectroscopy also holds promise for investigations on the kinetics of radical–radical reactions.

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## Detection of the reaction products between the simplest Criegee intermediate and organic acids

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Carbonyl oxides, the so-called Criegee intermediates (CIs), are produced in the ozonolysis reactions of unsaturated hydrocarbons. The species play important roles in atmospheric chemistry. Nascent CIs possess a large amount of energy, and many of the CIs undergo unimolecular decay. However, a fraction of them is stabilized, and they can further react with many trace atmospheric species. In the present work, we have investigated the reactions of the simplest Criegee intermediate, CH<sub>2</sub>OO, with organic acids, HCOOH and CH<sub>3</sub>COOH, by observing rotational spectra of their adducts using Fourier-transform microwave spectroscopy.

As shown in Fig. 1, the reaction proceeds with almost no activation energies to produce adducts. In the case of reaction with HCOOH, hydroperoxymethyl formate (HPMF, HC(O)OCH<sub>2</sub>OOH) and/or hydroxylated ozonide (HSOZ) are considered to be produced. Similarly, reaction with CH<sub>3</sub>CHOO produces its methyl derivative, hydroperoxymethyl acetate (HPMA, CH<sub>3</sub>C(O)OCH<sub>2</sub>OOH). For the detection of HPMF, a gas mixture containing 0.3% of formic acid and 2% of oxygen diluted in Ar was passed through a container filled with liquid 1,1-diodomethane. A pulsed electric discharge with 900 V was used to induce reactions. For the detection of HPMA, formic acid was replaced by acetic acid.

Among four low lying conformers expected for HPMF, two low lying conformers were detected with intensity ratio for the lowest one to the next lowest to be 2.9:1 [1]. Similarly three conformers are expected for HPMA [2]. Two low lying conformers, P<sub>1</sub> and P<sub>2</sub> were detected with intensity ratio about 1.5:1. For the two conformers of HPMA, splittings due to the methyl top internal rotations were observed. Analyses using the XIAM program yielded the internal rotation barriers, V<sub>3</sub>, to be 120.2 cm<sup>-1</sup> and 146.2 cm<sup>-1</sup> for P<sub>1</sub> and P<sub>2</sub>. In addition to the adducts, their dehydrated products, formic anhydrides (CHOOCHO from HPMF and CH<sub>3</sub>COOCHO from HPMA) were weakly observed, showing the reaction further proceeds. However, under our present experimental conditions, they were fairly weak and reactions do not proceed so fast.

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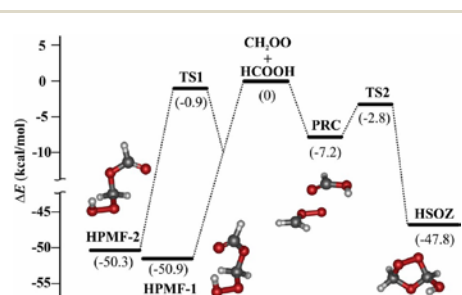


Fig. 1 Energy diagram for the CH<sub>2</sub>OO + HCOOH reaction

## Vibrational characterizations and reactions of geminal diols

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Hydrated aldehydes, forming the geminal diols, play important roles in the chemical reactions in aqueous aerosols. Gaseous IR spectrum of the simplest geminal diol, methanediol ( $\text{CH}_2(\text{OH})_2$ ), has been successfully monitored in hydration of gaseous formaldehyde [1] and the vapors of the aqueous formaldehyde solution [2], as shown in Fig. 1. Four IR spectra of isotopic analogues in aqueous solution were also reported [3]. Reactivity of  $\text{CH}_2(\text{OH})_2$  was compared with that of  $\text{CH}_3\text{OH}$  in the photolysis of aqueous nitrite solution probed with the step-scan FTIR [4]. Two OH groups of  $\text{CH}_2(\text{OH})_2$  can be treated as a water reservoir via the transformation between  $\text{H}_2\text{O}$  and  $\text{CH}_2\text{O}$  and facilitate the hydrolytic solvation reaction. Moreover, the photolysis of nitrite in presence of  $\text{CH}_2(\text{OH})_2$  was also examined by steady-state IR and Raman spectroscopy.  $\text{N}_2\text{O}$ ,  $\text{HCOO}^-$ , and  $\text{CO}_3^{2-}$  are the main products, without the generation of oxalate ( $\text{C}_2\text{O}_4^{2-}$ ) [5]. In addition to  $\text{CH}_2(\text{OH})_2$ , the IR spectra of geminal diols with two carbons via hydrations of glyoxal ( $\text{CHOCHO}$ ) to form monohydrate ( $\text{CHOCH}(\text{OH})_2$ ) and dihydrate ( $\text{CH}(\text{OH})_2\text{CH}(\text{OH})_2$ ) were also recorded in aqueous solution [6]. C–O stretching modes of dihydrate and  $d_4$ -dihydrate in aqueous solution were observed at *ca.*  $1075\text{ cm}^{-1}$ . Upon heating the solution containing  $(\text{CHO})_2$  and  $\text{D}_2\text{O}$ , a new peak appeared at  $1745\text{ cm}^{-1}$ , which was attributed to the C=O stretching mode of  $d_2$ -monohydrate ( $\text{CHOCH}(\text{OD})_2$ ). The preliminary result showed that the gaseous  $d_2$ -monohydrate reveals the rovibrational features in  $1750\text{--}1820\text{ cm}^{-1}$ . Successful IR characterizations of the geminal diols make it possible to investigate the relevant reactions of geminal diols in laboratory studies.

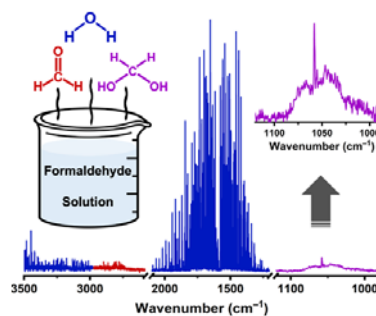


Fig. 1. IR spectrum of gaseous  $\text{CH}_2(\text{OH})_2$  [2].

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## Mass-selected UV/visible absorptions of $\text{CO}_2^+$ and aniline<sup>+</sup> in solid neon

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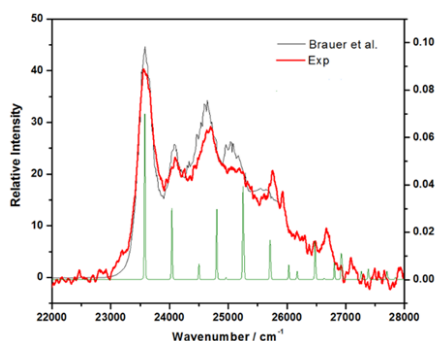
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The newly-built mass-selective matrix isolation system has been successfully employed to acquire IR and UV-visible absorption spectra of  $\text{CO}_2^+$  and aniline<sup>+</sup> isolated in solid Ne. The targeted cations are generated through electron impact ionization of precursors. Following generation, ion beam ions are extracted, deflected, and undergoing injection into a quadrupole mass filter, where most neutrals are eliminated. The ions of interest are then selected by  $m/e$  in the quadrupole mass filter and co-deposited with matrix atoms onto the cold substrate downstream.

The absorption spectrum of  $\text{CO}_2^+$  isolated in solid Ne at 3 K reveals a progression in the spectral region of 27800–33000  $\text{cm}^{-1}$ , corresponding to the electronic transition from the ground state to the first electronically excited state. The observed interval is determined to be 1130  $\text{cm}^{-1}$ , consistent with the previously reported value of the  $\nu_1$  mode of the  $A$  state [1]. In comparison to the band origin measured in the gas phase, the band origin is observed to be slightly red-shifted by approximately 373  $\text{cm}^{-1}$ . Notably, each progression band exhibits fine structures might be attributed to the rotational contour and splitting of the sublevels of the  ${}^2\Pi$  states. In the UV-visible absorption spectrum of aniline cations in solid Ne, intense progression observed in the spectral region 23000–28000  $\text{cm}^{-1}$  corresponds to the electronic transition from the ground state ( $X {}^2B_1$ ) to the  $B {}^2B_1$  state. A comparison of spectra recorded in helium droplets [2] and the present work is illustrated in Fig. 1.



**Fig. 1** Comparison of spectra of aniline<sup>+</sup> in helium droplet (black) and in solid Ne (red), and simulation with TD-B3LYP/cc-pVTZ (green).

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## Probing acidity of terminal OH sites in hydrogen bond networks by use of weak proton acceptors

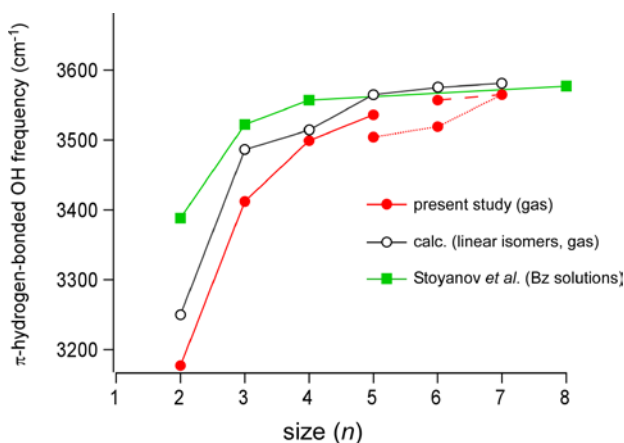
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An excess proton in a hydrogen bond (H-bond) network (*e.g.*, protic solvents) enhances the magnitude of surrounding H-bonds. The extent of such H-bond enhancement in the network is of great interest to understand the nature of the proton solvation.

To determine this extent of the enhancement, we measured infrared (IR) spectra of protonated methanol-benzene clusters ( $\text{H}^+(\text{MeOH})_n\text{-Bz}$ ,  $n = 2\text{-}7$ ) in the gas phase. In these clusters, the excess proton is located at the center of the H-bond network of MeOH, and Bz is weakly  $\pi$ -hydrogen-bonded to the terminal OH site of the  $\text{H}^+(\text{MeOH})_n$  moiety. The OH stretch frequency of the  $\pi$ -bound MeOH should reflect the acidity of the terminal OH site of the H-bond network. The red plot in Fig. 1 shows the observed  $\pi$ -H-bonded OH stretch frequency of  $\text{H}^+(\text{MeOH})_n\text{-Bz}$  in the gas phase. With increase of cluster size ( $n$ ), the OH frequency shifts to blue, indicating weakening of the acidity of the terminal site. The OH frequency becomes almost constant at  $n \sim 7$ , which corresponds to the extent of the H-bond enhancement with the excess proton. In other words, the excess proton is effectively solvated by surrounding  $\sim 7$  MeOH molecules. These results are consistent with the pioneering work by Stoyanov *et al.*, in which the  $\pi$ -H-bonded OH frequency of  $\text{H}^+(\text{MeOH})_n$  was measured in the benzene solutions (green plot in Fig.1) [2]. In the small sizes ( $n \leq \sim 5$ ), however, the  $\pi$ -H-bonded OH frequency shows large difference between the gas phase and Bz solution. The origin of this difference is discussed with the OH frequency measurements of  $\text{H}^+(\text{MeOH})_n\text{-(Bz)}_m$  ( $m = 2$  and  $3$ ) in the gas phase.

In addition, we found that the  $\pi$ -H-bonded OH stretch frequency shift of  $\text{H}^+(\text{MeOH})_n\text{-Bz}$  shows linear correlation with the clustering enthalpy change in  $\text{H}^+(\text{MeOH})_n + \text{MeOH} \rightarrow \text{H}^+(\text{MeOH})_{n+1}$  [3]. This suggests the Badger-Bauer rule (correlation between the OH frequency shift and H-bond formation enthalpy change) is held also in H-bond networks.



**Fig.1** The cluster size ( $n$ ) dependence of the  $\pi$ -H-bonded OH frequency in  $\text{H}^+(\text{MeOH})_n\text{-Bz}$ .

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## Fermi resonance in mid- and near-IR & from 1-D to 2D

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Vibrational motions of molecules are intrinsically “anharmonic” and complex vibrational features in mid-IR are often attributed to anharmonic coupling known as Fermi Resonance (FR)<sup>1</sup>. With the assistance of *ab initio* anharmonic algorithms (A<sup>3</sup>), we can construct simple vibrational exciton models without any fitting parameters to understand FR and analyze experimental spectra of solvated H<sub>3</sub>O<sup>+</sup> and CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> in mid-IR.<sup>2,3</sup> In this talk, we will present our recent developments to push A<sup>3</sup> to cover both mid- and near-IR and to enable simulation on both linear and non-linear spectroscopy.

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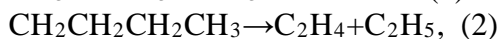
## Thermal decomposition of alkyl radicals and reactions of H atoms with alkanes

H. Matsui

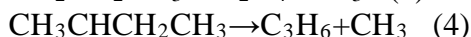
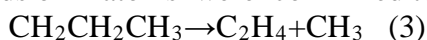
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Bond scission at  $\beta$ -C of alkyl radicals was quantitatively examined by monitoring H and I atoms produced from shock-heated C3-C6 alkyl iodides with using ARAS over the temperature range 900-1400 K.<sup>1</sup> Initial concentration of alkyl radicals was given by the concentration of I atoms, and the yields of H atoms were confirmed to be ca100 % for s-propyl and n-butyl radicals, i.e.,

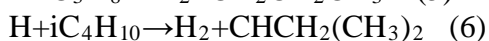


followed by  $\text{C}_2\text{H}_5 \rightarrow \text{C}_2\text{H}_4 + \text{H}$ . Reactions (1) and (2) complete immediately in the time scale of the shock tube measurements. In contrast, for n-propyl and s-butyl radicals, the yields of H atoms were confirmed to be very small.



because products of (3) and (4),  $\text{C}_2\text{H}_4$ ,  $\text{C}_3\text{H}_6$  and  $\text{CH}_3$ , are very stable in the temperature range of this study. Such a distinct difference on the production yield of H atoms was obscured for larger alkyl radicals; for 1- $\text{C}_5\text{H}_{11}$  and 1- $\text{C}_6\text{H}_{13}$  radicals, the yields of H atoms were 40-50 %. This is attributed to isomerization of 1-alkyls to 2-alkyls via the intramolecular H atom migration with the 5- and 6-membered rings.

By utilizing above experimental results, direct measurement of site-specific rates of the reactions H+C3,C4 alkanes were performed by monitoring evolution of H atoms over 1000-1200 K (P=2.0 bar), where, H atoms were supplied by thermal decomposition of  $\text{C}_2\text{H}_5\text{I}$ .<sup>2</sup> i.e.,



The measured rates of (5)-(7) were regarded as substantially reliable, because this experiment was conducted with using very low concentrations of sample gases ( $6-7 \times 10^{12}$  atom/cm<sup>3</sup>), and reference signals (production rate of H from decomposition of  $\text{C}_2\text{H}_5\text{I}$ , and background absorption by excess alkanes at H-Lyman  $\alpha$  line) were monitored separately to improve the reliability. Reported theoretical calculations<sup>3-5</sup> were compared with the present experimental results: the site-specific rates of (5) and (6) by the theoretical calculations were confirmed to be in reasonable agreement with the present experimental results, but the observed rates of (7) were 56-72 % of the theoretical ones. Contribution of steric-hindrance was discussed to explain the disagreement.

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## Water catalysis in gas phase reactions?

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Some studies have mentioned the possibility of water catalysis for gas phase reactions in the atmosphere, where  $A+B+H_2O \rightarrow C+H_2O$  is faster than  $A+B \rightarrow C$  in atmospheric conditions. For this catalytic effect to be relevant, the enthalpic stabilization by the additional water molecule has to overcome the entropic penalty of associating three reactants versus two reactants. In this talk, we will take a look at several reactions where water molecules can and cannot catalyze the reaction.

Criegee intermediates (CIs) are reactive carbonyl oxides,  $R_1R_2COO$ , produced in the atmosphere by the reaction of  $O_3$  and alkenes. At atmospheric relevant conditions, it was found that the reaction of the simplest CI,  $CH_2OO$ , with one water molecule is slow, but the reaction involving two water molecules is very fast and is one of the dominant pathways for  $CH_2OO$  decomposition in the atmosphere. We performed theoretical rate coefficient calculations based on transition state theory with an anharmonic vibrational effect as well as tunneling corrections to rationalize the effect of the second water. To understand the errors in our calculations, we compared the transition state energies by various quantum chemistry methods ranging from single to multireference methods. Furthermore, in opposition to previous experimental studies that focused on the effect of two water molecules, we will show that three water molecules can be an important reaction pathway for  $CH_2OO$  and water vapor in atmospheric conditions.<sup>1</sup>

Another important atmospheric reaction is the hydrogen abstraction reaction of OH radical from methanol. Experimental studies in Teflon bags reported that water molecules can promote the reaction. Using theoretical calculations based on accurate quantum chemistry energies, we show that for the  $OH+CH_3OH \rightarrow CH_2OH+H_2O$  reaction, the addition of the extra water molecule does not promote the reaction.<sup>2</sup>

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## Study the triplet electronic states using step-scan time-resolved Fourier transform near-infrared spectroscopy

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Triplet transitions of light emitting materials, including Rose Bengal, tris(2-phenylpyridine)iridium(III) ( $\text{Ir}(\text{ppy})_3$ ), tris(1-phenylisoquinoline)iridium(III) ( $\text{Ir}(\text{piq})_3$ ), and bis[2-(4,6-difluorophenyl)pyridinato-C<sub>2</sub>,N](picolinato)iridium(III) (FIrpic), were studied using step-scan time-resolved Fourier-transform near-infrared (FTNIR) spectroscopy. We excited the samples to their singlet excited states by 355 nm nanosecond laser and then molecules underwent efficient internal conversions (IC)/intersystem crossings (ISC) to their triplet manifolds. Upon excitation of Rose Bengal, a transient absorption band appeared at  $9400\text{ cm}^{-1}$  (in methanol solution), and this band is reassigned to the  $T_3 \leftarrow T_1$  transition based on the corresponding time evolution and the time-dependent density functional theory (TD-DFT) calculations. For  $\text{Ir}(\text{ppy})_3$ ,  $\text{Ir}(\text{piq})_3$ , and FIrpic, the most intense transient absorption bands were observed at  $7700$ ,  $7500$ , and  $7500\text{ cm}^{-1}$  and assigned to  $T_7 \leftarrow T_1$ ,  $T_6 \leftarrow T_1$ , and  $T_6 \leftarrow T_1$  transitions, respectively. For  $\text{Ir}(\text{ppy})_3$ , the most intense band involved transitions between different triplet metal-to-ligand charge transfer states ( $^3\text{MLCT}$ ), while for  $\text{Ir}(\text{piq})_3$  and FIrpic, they mainly involved a metal-center to  $^3\text{MLCT } d+\pi \leftarrow d$  transition. Based on the TD-DFT calculations and the observed short lifetime data, the observed  $T_1$  states were assigned to  $^3\text{MLCT}$ . Detailed triplet investigations make it possible to further unveil the energetics of light emitting materials, which are essential for excitonic energy utilization in radiative processes.

## Electric field effects on structure, dynamics and function in molecules, molecular system and biological system

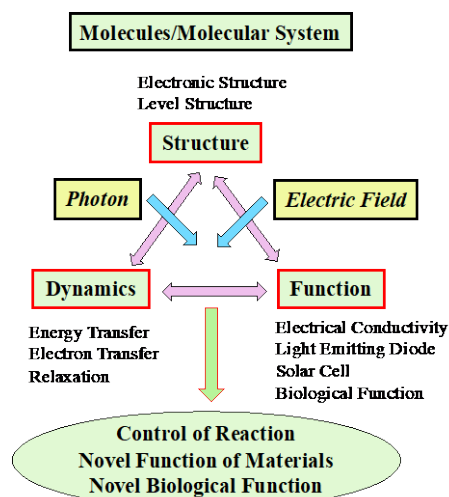
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Control of the dynamics of molecules and molecular systems is extremely important to create novel functions in materials and biological systems. The use of light (photon) along with the application of the electric field as a tool to give external stimuli has many advantages which originate from the characteristics of interaction among photons, molecules, and electric fields. Through the experiments of external electric field effect on absorption, photoluminescence and/or conductivity, it was shown that molecular structure (orientation), molecular dynamics, and material functions are well affected by application of electric field.<sup>[1-6]</sup> Since biological system is composed of molecules, dynamics and function in biological system are also expected to be affected by application of electric field, which can be examined by using fluorescence microscopic method.

In the present talk, the effects of nanosecond pulsed electric field on the dynamics and function of live cells, which have been examined by using fluorescence microscopy including autofluorescence lifetime imaging, are introduced with a special attention to the difference of the electric field effects between cancerous and normal cells.<sup>[7,8]</sup>



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# **Poster Presentations**

## The rate coefficient of *syn-trans*-MVKO with HCOOH investigated with a quantum-cascade laser system

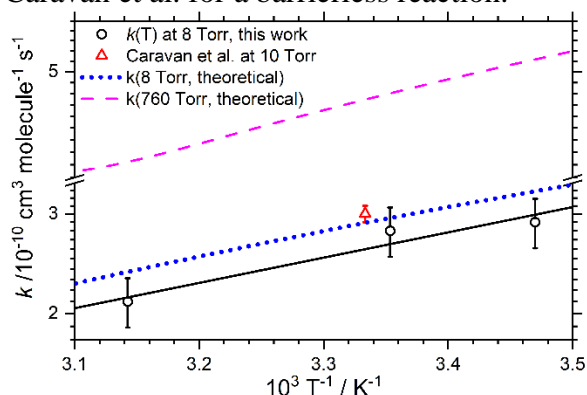
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The reaction of the methyl-vinyl-substituted Criegee intermediate, methyl vinyl ketone oxide (MVKO), with HCOOH is considered to be important in atmospheric chemistry due to its prospective contribution to the decay of MVKO and the potential for the formation of aerosol. In this study, we employed a tunable cw external-cavity quantum-cascade laser system coupled with a Herriott multipass absorption cell to record the spectrum of *syn-trans*-MVKO in region 916.4–915.6 cm<sup>-1</sup>. We integrated the absorption band of *syn-trans*-MVKO from 915.83–915.81 cm<sup>-1</sup> (Q-branch of  $\nu_{25}$ , CH<sub>2</sub> wagging mode) and recorded the temporal behavior at various concentrations of HCOOH. We found a significant pressure dependence for the rate coefficients, from 1.7×10<sup>-10</sup> to 2.6×10<sup>-10</sup> cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> for total pressure at 0.5 to 33 Torr at 298 K. These rate coefficients agree with the only experimental value 3.0×10<sup>-10</sup> cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> investigated with a multiphoton ionization mass spectrometer at 10 Torr and 300 K and the theoretical prediction of (0.8–3.9)×10<sup>-10</sup> cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> in pressure range 0.8–38 Torr at 300 K reported by Caravan et al.<sup>1</sup> We also performed temperature-dependence experiments from 288–315 K at total pressure 8 Torr. The rate coefficient of *syn-trans*-MVKO with HCOOH can be described by an Arrhenius expression  $k(T) = A \times \exp(-E_a/RT)$  with a pre-exponential factor  $A$  of  $(8.5 \pm 0.7) \times 10^{-12}$  molecule cm<sup>3</sup> s<sup>-1</sup> and an activation energy  $E_a$  of  $-8.5 \pm 2.2$  kJ mol<sup>-1</sup>. The negative temperature dependence agrees with the theoretical prediction reported by Caravan et al. for a barrierless reaction.<sup>1</sup>



Arrhenius plot for the rate coefficient of *syn-trans*-MVKO with HCOOH at 8 Torr. The black circles represent rate coefficients measured at this work and fitted with an Arrhenius expression  $k(T) = (8.5 \pm 0.7) \times 10^{-12} \exp[(-8500 \pm 2200)/RT]$  molecule cm<sup>3</sup> s<sup>-1</sup>. The red triangle represents a rate coefficient reported by Caravan et al.<sup>1</sup> at 10 Torr and 300 K; the blue dotted line and pink dashed line represent predicted temperature dependence at 8 Torr and 1 atm, respectively.

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## Pure rotational spectra and characteristics of triatomic free radicals: ClSO and ClSS

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Pure rotational transitions of the ClSO radical have been observed by Fourier-transform microwave (FTMW) spectroscopy.[1] The *a*-type and *b*-type transitions, for both  $^{35}\text{Cl}$  and  $^{37}\text{Cl}$  isotopologues, were detected, and the observed very complicated fine and hyperfine components were well-assigned. The intensities of the observed spectra for the two isotopologues correspond to the ratio of the isotope abundances for  $^{35}\text{Cl}$  and  $^{37}\text{Cl}$ . A total of 21 molecular constants were determined precisely for both  $^{35}\text{ClSO}$  and  $^{37}\text{ClSO}$ , including the rotational constants, the centrifugal distortion constants, the electronic spin-rotation constants, the nuclear spin-rotation constants, the magnetic hyperfine constants, and the quadrupole coupling constants of chlorine. The molecular constants show ClSO to have the  $^2A''$  electronic ground state with the out-of-plane unpaired electron. The spin density of the chlorine atom is about 10%, which is similar to that of the fluorine atom for FSO, about 8%.

The ClSS radical is a member of the thiosulfeno radicals (XSS, X = H, F, Cl). The rotational spectrum of ClSS was observed by Fujitake *et al.*[2] using a millimeter- and submillimeter-wave spectrometer. The rotational constants, the centrifugal distortion constants, and the spin-rotation constants have been determined, while no hyperfine splitting was observed. In the present study, low-*N* rotational transitions with completely resolved hyperfine splitting were observed using FTMW spectroscopy, and the hyperfine constants of chlorine were determined.

Results of the ClSO and ClSS radicals are compared with other triatomic radicals with similar structures, the XSS, XSO, and XOO radicals with X = H, F, and Cl, leading to a conclusion that the ClSO and ClSS radicals are more like FSO and FSS, respectively, but fairly different from the FOO and ClOO radicals.

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## ***In situ* and *real-time* vibrational spectroscopic characterizations of the photodegradation of nitrite in the presence of methanediol**

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Nitrite ( $\text{NO}_2^-$ ) is a common inorganic matter in cloud droplets or aqueous aerosols, and its photolytic product hydroxyl radical (OH) and nitric oxide (NO) are the potential reactants to oxidize the organic compounds, such as methanediol ( $\text{CH}_2(\text{OH})_2$ ). Nevertheless, the photodegradation process of nitrite in the presence of methanediol has not been well characterized. In this work, the nitrite aqueous solution containing methanediol is exposed to 365 nm LED and the fate of reactants and products are probed simultaneously via vibrational spectroscopy, as shown in Fig.1(a). The depletions of nitrite and methanediol and the formations of nitrous oxide ( $\text{N}_2\text{O}$ ) and formate ( $\text{HCOO}^-$ ) were observed in the infrared spectra. Besides, the gain or loss features are more obvious with increasing concentrations of methanediol and the irradiation flux of the 365 nm LED. Additionally, the carbonate ( $\text{CO}_3^{2-}$ ) appears in the time-evolved Raman spectra. According to the literature [1] and theoretical calculations, the reaction mechanism is proposed in Fig.1(b).  $\text{CH}(\text{OH})_2$ ,  $\text{CO}_2^-$  and  $\text{NOCO}_2^-$  could be the possible intermediates in the photodegradation of nitrite in the presence of methanediol. Through vibrational spectroscopy and theoretical calculations, a reasonable mechanism is established, which facilitates the understandings of the roles of nitrite and methanediol simultaneously in the aqueous environment under irradiation.

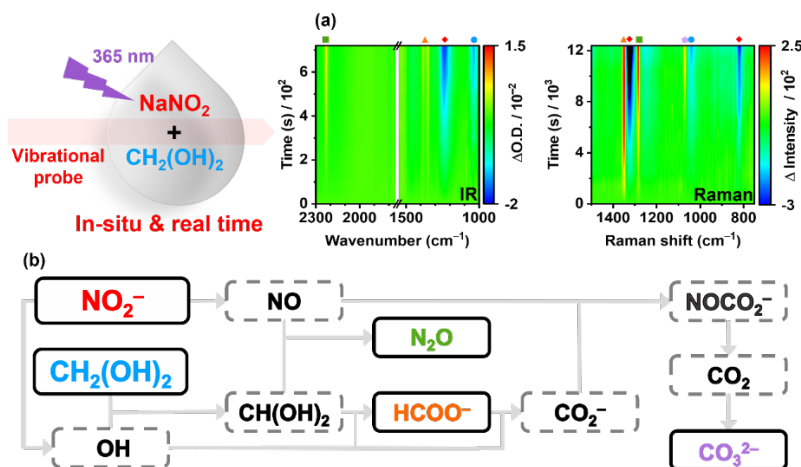


Fig. 1. (a) The time-evolved difference infrared and Raman spectra of the aqueous mixture of  $\text{NaNO}_2$  and  $\text{CH}_2(\text{OH})_2$  upon 365 nm continuous photoexcitation. (b) Proposed mechanism of the photodegradation of nitrite in the presence of methanediol. [2]

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## High resolution spectroscopy of HO<sub>2</sub> radical and its self-reaction kinetics

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HO<sub>2</sub> radical is a key species that involves in oxidative reactions in different regions of atmosphere [1]. In this work, HO<sub>2</sub> radical is generated via photolysis of the Cl<sub>2</sub>/CH<sub>3</sub>OH/O<sub>2</sub> flowing mixtures with laser pulse at 351 nm. After photolysis, the Cl atoms can be generated and reacted with CH<sub>3</sub>OH to form HCl and CH<sub>2</sub>OH radicals. Subsequently, CH<sub>2</sub>OH can react with excessive O<sub>2</sub> in the system to produce HO<sub>2</sub> and HCHO. By simultaneous monitoring both HCl and HO<sub>2</sub> utilizing synchronized two-color dual-comb time-resolved spectroscopy near 3.3 and 8.9 μm, respectively [2,3], the line intensity of HO<sub>2</sub> transitions could be determined accurately based on the well-defined line intensity of HCl transitions [4]. Furthermore, the self-reaction rate coefficient of the HO<sub>2</sub> can be obtained in this work as well.

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## Determination of the rate coefficient of the reaction OH + HO<sub>2</sub>

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The hydroxyl radical (OH) and the hydroperoxyl radical (HO<sub>2</sub>) are both important oxidants in the atmosphere in removing trace gases such as NO<sub>x</sub> [1]. In a recent experiment, the rate coefficient between OH and HO<sub>2</sub> radicals was reported to be  $(1.00 \pm 0.32) \times 10^{-11}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> [2], however, it is one order of magnitude slower than the previous value by Assaf *et al.*,  $(1.02 \pm 0.06) \times 10^{-10}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> [3]. In this work, we studied the title reaction by simultaneously measuring the time-dependent spectra of OH and HO<sub>2</sub> near 2.9 and 8.9 μm, respectively, before and after 248-nm photolysis of the H<sub>2</sub>O<sub>2</sub>/N<sub>2</sub> flowing mixtures. The rate coefficient of the reaction OH + HO<sub>2</sub> can further be determined by analyzing the concentration time traces of both OH and HO<sub>2</sub> with kinetic simulations and compared with the previous experiments.

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## Using spatially differentiated velocity map imaging in the study of large molecule photodissociation

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We have constructed a new modified velocity map imaging (VMI) method, which retains a high-velocity resolution and can distinguish signals from the dissociative ionization background. The modified VMI combines the high-velocity resolution of VMI with the long pump-probe delay time used in multi-mass ion imaging.<sup>1</sup>

We moved the crossing point of a pump laser beam with the molecular beam a few centimeters upstream, increasing the pump-probe delay time and expanding the size of recoiled photofragments sphere in the velocity mapping region. The probe beam ionizes only fragments whose velocities in the center-of-mass frame are parallel to the probe laser beam. These ions are accelerated to the detector by the ion optics based on velocity mapping. They form a line-shaped image, not a circle-like image. (See Fig. 1) The length of the image does not depend on the size of the photofragment sphere in which the fragments were distributed but only on the velocity of the fragments.

Meanwhile, the probe laser beam ionizes the hot parent molecules, which absorb the pump laser but do not yet dissociate completely and produce ionic fragments whose velocities are distributed in all directions (i.e., dissociative ionization). They form a circle-like image. This circle-like image overlaps with the line-shaped image when the ions have equal  $m/z$  values. The signal (line-shaped image) and background (circle-like image) can therefore be distinguished according to the shape of the images.

We first applied the modified VMI with the 118 nm photoionization in the 266 nm photodissociation of iodotoluenes and chlorotoluenes. Interferences by undissociated hot parent molecules in the slow dissociation rates of these large molecules (number of atoms > 10) in the ground state were observed. Here, we demonstrate the validity of the new proposed VMI<sup>2,3</sup> with the spatial map to differentiate the actual signal from the background.

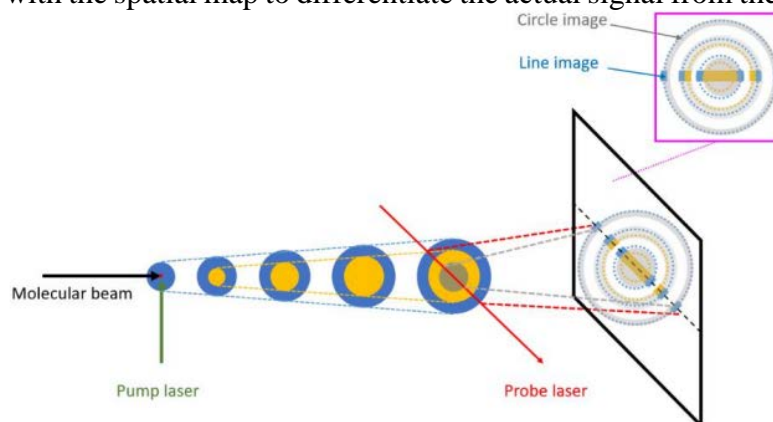


Fig. 1 The spatially differentiated VMI.

# FTMW spectroscopy of the $^{13}\text{C}/^{18}\text{O}$ -substituted tropolone and the determination of tunneling splitting.

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Tropolone has the symmetric potential for the proton tunneling with barrier height of  $h_b \sim 4100 \text{ cm}^{-1}$  and the ground state is split into a doublet with the separation of  $\Delta E_0 = 29.134 \text{ GHz}$  or  $0.9738 \text{ cm}^{-1}$ . [1] When one of the C/O atoms is substituted to the  $^{13}\text{C}/^{18}\text{O}$  isotope, the proton tunneling occurs between the  $^{13}\text{C}$ -4 and -6 forms (also  $^{13}\text{C}$ -3 and -7,  $^{13}\text{C}$ -1 and -2 and  $^{18}\text{O}$ -8 and -9) although they have asymmetric potential due to the difference in the zero point energy (ZPE). The difference in ZPE is small ( $0.1\sim 2.0 \text{ cm}^{-1}$ ), but it will hinder the proton tunneling substantially.

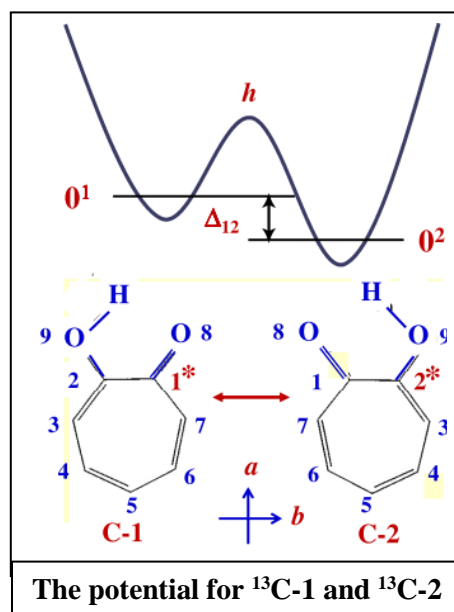
In the present study, Fourier-transform microwave (FTMW) spectroscopy has been applied for the  $^{13}\text{C}/^{18}\text{O}$ -substituted tropolone to observe the tunneling-rotation transitions as well as the pure rotational transitions. From the observed tunneling splitting  $\Delta E_{ij}$  ( $0.9800 \sim 1.6824 \text{ cm}^{-1}$ ), the differences in ZPE  $\Delta_{ij}$  are derived to be  $-0.110, -0.565, -1.369$  and  $1.404 \text{ cm}^{-1}$  for the  $^{13}\text{C}$ -46, -37, -12, and  $^{18}\text{O}$ -89 species to agree well with the DFT calculation, where the signs mean  $^{13}\text{C}$ -6,  $^{13}\text{C}$ -7,  $^{13}\text{C}$ -2 and  $^{18}\text{O}$ -8 forms have the higher energy.

The state mixing ratio of the tunneling  $i$ - and  $j$ -states decreases drastically from (44: 56 %) to (8: 92 %) for the  $^{13}\text{C}$ -46 to  $^{18}\text{O}$ -89 species with increase in the asymmetry  $\Delta_{ij}$  of the potential function, indicating that the  $^{18}\text{O}$ -8 and  $^{18}\text{O}$ -9 forms are almost localized as two different isotopologues. Observed tunneling-rotation interaction constants  $F_{ij}$  decrease from  $16.001$  to  $9.224 \text{ cm}^{-1}$  as the differences in ZPE  $\Delta_{ij}$  increase. On the other hand, the diagonal tunneling-rotation interaction constants  $F_u$  characteristic to the species with  $C_s(M)$  symmetry increase as  $1.767\sim 13.70 \text{ cm}^{-1}$  for the  $^{13}\text{C}$ -46~ $^{18}\text{O}$ -89 species to be explained well by the mixing ratio of the proton tunneling states.

The dynamics of the proton tunneling was also studied to obtain the barrier height to be  $h_b = 4116 \text{ cm}^{-1}$  for the normal species and the differences in ZPE  $\Delta_{ij}$  are obtained to agree well with the above results in the perturbation theory.

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## Studying reaction of aerosol with formaldehyde under different relative humidity via aerosol optical tweezers

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Methanediol ( $\text{CH}_2(\text{OH})_2$ ), the simplest geminal diol, is crucial in both atmospheric and space chemistry, can be produced by the hydration reaction of  $\text{CH}_2\text{O}$  and  $\text{H}_2\text{O}$ .

Aerosol optical tweezers (AOT) are the technique that can trap particles in focused laser beams. In this work, we utilize AOT combining with Raman spectroscopy, to study the kinetics of the reaction of aqueous NaCl micro-droplets with gaseous formaldehyde.

Raman spectroscopy is a tool to determine various physical and chemical properties. E.g. ionic strengths, viscosities, diffusion coefficients, and methanediol concentration.

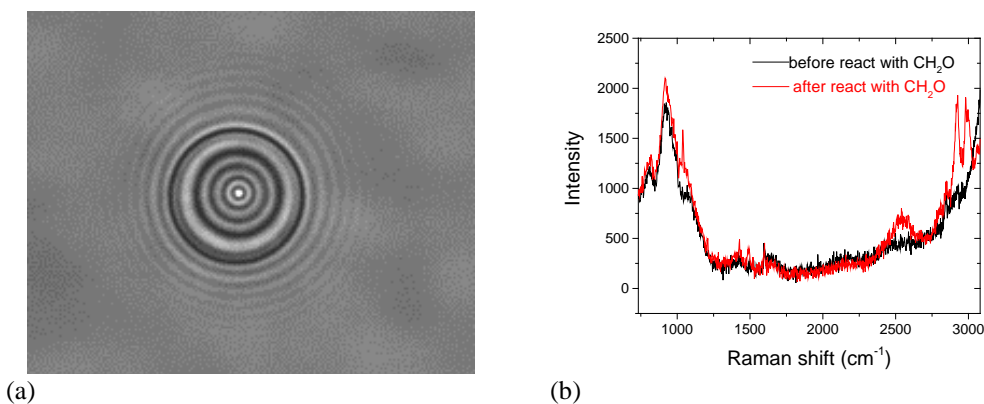


Fig. 1. (a) Microscopic image of the aerosol.

(b) The Raman spectrum of the reaction between before and after reacting with formaldehyde.

We utilized Raman spectrometer to monitor the hydration reaction of  $\text{CH}_2\text{O}$  and  $\text{H}_2\text{O}$ , which leads to the generation of gaseous  $\text{CH}_2(\text{OH})_2$ . The relative signal value of molecular characteristic peaks in Raman spectrum can be used for qualitative and quantitative analysis. In addition, the whispering gallery mode that appears in the spectrum can calculate the particle size and refractive index of the aerosol.

Chemical bonds and symmetrical molecules have spectral information of special vibrations, we observed band centers of the trans-OCO asymmetric stretching vibration mode at  $1045 \text{ cm}^{-1}$ , the  $\text{CH}_2$  scissoring vibration mode at  $1495 \text{ cm}^{-1}$ , the  $\text{CH}_2$  symmetric stretching and asymmetric stretching vibration modes of at  $2912 \text{ cm}^{-1}$  and  $2982 \text{ cm}^{-1}$ .

The study of Raman characterization of methanediol promotes further investigation on the related reactions of geminal diols in atmospheric chemistry and astrophysics.

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## Rate coefficients of CH<sub>3</sub>CHI with O<sub>2</sub> and *syn-/anti*-CH<sub>3</sub>CHOO with HCl investigated with an IR/UV dual probe system

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The reactions between Criegee intermediates and hydrogen chloride (HCl) play a significant role in the atmosphere, particularly in polluted urban areas, because of their large rate coefficients. We employed a tunable cw external-cavity quantum-cascade laser coupled with a Herriott absorption cell to record the high-resolution spectra of CH<sub>3</sub>CHOO, produced by photolyzing a gas mixture of 1,1-diiodoethane/O<sub>2</sub>/HCl with laser light at 248 nm. We also employed a 335-nm UV laser to probe the Criegee intermediate at the same time to measure its concentration. By monitoring the  $\nu_{10}$  bands of *syn*-CH<sub>3</sub>CHOO in region 883.13–883.15 cm<sup>-1</sup>,<sup>1</sup> we recorded the temporal evolution of the *syn*-CH<sub>3</sub>CHOO conformer and measured the rate coefficient of *syn*-CH<sub>3</sub>CHOO + HCl at 298 K under total pressures of 4–8 Torr. The measured bimolecular rate coefficient was determined to be  $(4.8 \pm 1.3) \times 10^{-11}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>, which is nearly identical to a value  $(4.8 \pm 1.0) \times 10^{-11}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> reported by Liu et al.,<sup>2</sup> who employed the laser-induced fluorescence detection of unimolecular decomposition product OH. We also monitored the high-resolution spectra of the  $\nu_7$  mode of *syn*-CH<sub>3</sub>CHOO in region 1277.0–1283.0 cm<sup>-1</sup>; the temporal profile indicated that a stable product, likely *anti*-CEHP,<sup>3</sup> also contribute to the absorption. The preliminary results showed that the overall rate coefficient of the reaction *syn-/anti*-CH<sub>3</sub>CHOO + HCl is  $k_{\text{HCl}} = (8.7 \pm 1.0) \times 10^{-10}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 10–16 Torr and 298 K. During the course of our investigation, we found that the rate coefficient of the formation reaction CH<sub>3</sub>CHI + O<sub>2</sub> → CH<sub>3</sub>CHOO + I,  $(3.4 \pm 0.7) \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>, is ~2.5 times smaller than that reported by Howes et al.<sup>3</sup> and Sheps et al.<sup>4</sup> who employed mass spectrometry and UV absorption, respectively.

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## The microwave spectra of ethanesulfonic acid and its monohydrate

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Ethanesulfonic acid ( $\text{CH}_3\text{CH}_2\text{SO}_2\text{OH}$ ) is an alkylsulfonic acid that has uses as a pharmaceutical intermediate and a catalyst of polymerization and alkylation. Sulfonic acids/water aerosols are known for playing a part in the destruction of the ozone. For this reason, the study of how sulfonic acids interact with water in the gas phase is critical. The high-resolution rotational spectra of ethanesulfonic acid and its monohydrate were studied using both broadband chirped pulse and cavity-based Fourier transform microwave spectrometers over the frequency range of 5–18 GHz for the first time. The rotational constants and the centrifugal distortion constants have been determined for the ethanesulfonic acid monomer. The quantum chemical calculations were carried out using MP2 and B3LYP density functional theory (DFT) with an aug-cc-pVTZ basis set. The rotational constants from the optimized geometric structures were in good agreement with the experimental values. Neither the large amplitude motion of the hydroxyl hydrogen flipping nor the methyl group internal rotation were observed in the monomer spectrum. The energy barrier of the methyl group internal rotation was calculated to be 12 kJ/mol. The preliminary results on the rotational constants and centrifugal distortion constants of the monohydrate of ethanesulfonic acid are also presented. The structure of the monohydrate is stabilized by two hydrogen bonds formed between ethanesulfonic acid and the water molecule.

## Absolute photodissociation cross sections of thermalized methyl vinyl ketone oxide (MVKO) and methacrolein oxide (MACRO) were measured

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Methyl vinyl ketone oxide (MVKO) and methacrolein oxide (MACRO) are generated from the ozonolysis of isoprene in the atmosphere. Both MVKO and MACRO react with atmospheric gases such as SO<sub>2</sub>, and their unimolecular reactions can generate OH radical, the most important oxidant in the atmosphere. [1–2] The absolute photodissociation cross sections of MVKO and MACRO are important parameters which can be used to estimate the photolysis of MVKO and MACRO in the atmosphere and the concentrations of MVKO and MACRO in the laboratory experiments with the UV absorption spectroscopy.

Our group used a 352 nm excimer laser pulse to photodissociate MVKO and MACRO, and measured the remained fraction with the UV absorption spectroscopy. The broad band probe light and the 352 nm laser pulse were separated with 355 nm longpass filters. The peaks of the absolute photodissociation cross sections were determined to be  $(3.70 \pm 0.74) \times 10^{-17} \text{ cm}^2$  for MVKO at 371 nm and  $(3.04 \pm 0.58) \times 10^{-17} \text{ cm}^2$  for MACRO at 397 nm. We used these values to estimate the synthetic yields of MVKO and MACRO generated with the photolysis of the precursors in our experiments, and the deduced values are  $(0.22 \pm 0.10)$  for MVKO (at 30–700 torr and 299 K) and  $(0.043 \pm 0.019)$  for MACRO (at 500 torr and 299 K).

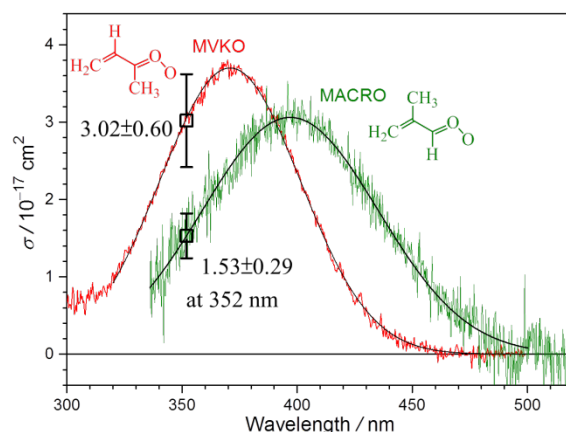


Fig. 1. The absolute photodissociation cross sections of MVKO (red) and MACRO (green). We determined the cross sections at 352 nm and scaled the reported UV absorption spectra. [1–2]

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# Spectral studies of the reaction of the Criegee intermediate methyl vinyl ketone oxide (MVKO) with HC(O)OH using a step-scan time-resolved Fourier-transform infrared absorption spectrometer

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Methyl vinyl ketone oxide [MVKO, (C<sub>2</sub>H<sub>3</sub>)(CH<sub>3</sub>)COO] is one of the Criegee intermediates produced when atmospheric isoprene undergoes ozonolysis. The reactions between Criegee intermediates with HC(O)OH lead to the formation of secondary organic aerosols and impact the atmospheric composition [1].

In this work, we recorded time-resolved infrared absorption spectra of transient species produced upon irradiation at 248 nm of a flowing mixture of (*Z*)-(CH<sub>2</sub>I)HCC(CH<sub>3</sub>)I/HC(O)OH/O<sub>2</sub> at 298 K. The majority of MVKO produced in this reaction has the *syn-trans* conformation. Bands near 1726, 1430, 1378, 1347, 1213, 1169, 1033, and 987 cm<sup>-1</sup> were assigned to the hydrogen-transferred adduct 2-hydroperoxybut-3-en-2-yl formate [HPBF, (C<sub>2</sub>H<sub>3</sub>)(CH<sub>3</sub>)C(OCHO)OOH]; its conformation could not be definitively assigned. The observed wavenumbers and relative intensities agree with the anharmonic vibrational wavenumbers and IR intensities predicted with the B3LYP/aug-cc-pVTZ method. We also calculated the potential-energy scheme of this reaction with the CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ method. Our observation indicates that the reaction of MVKO and HC(O)OH follows the pathway with the smallest barrier to form HPBF. Unlike other hydrogen-transferred adducts produced from the reaction of HC(O)OH with CH<sub>2</sub>OO or CH<sub>3</sub>CHOO, HPBF does not undergo dehydration because the central carbon atom in HPBF, which is connected to a methyl group and a vinyl group, does not have a hydrogen atom available for abstraction by OH, preventing it from undergoing dehydration.

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## Infrared spectroscopic investigation of radical cations of hydrocarbons and its clusters

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Hydrocarbons and their derivatives are ubiquitous in chemistry and our environments. Neutral hydrocarbons are aprotic and generally regarded as inert substances. On the other hand, properties of radical cations of hydrocarbons have poorly been investigated, so far. We have previously reported with IR spectroscopy that the acidity of CH bonds of pentane is highly enhanced in the cationic state. Thus, properties of radical cations of hydrocarbons are largely different from those of their neutrals. The ionization-induced isomerization of pentane dimer is investigated by IR spectroscopy based on vacuum-ultraviolet photoionization detection and quantum calculations. The ionized pentane dimer isomerizes to the cationic structure where hydrogen atoms intermolecularly form the semi-covalent bond. The monomer and dimer cations of 1-heptene are also investigated, spectroscopically. The ionized 1-heptene cyclizes through the formation of the covalent bond through the intermolecular proton transfer, while its dimer cation intermolecularly forms covalent bonds. These results indicate that the radical cations of these hydrocarbons are highly reactive. The properties and reactivities of these radical cations, and the reactions pathways of their ionization-induced reactions are discussed based IR spectroscopy, quantum calculations, and theoretical reaction path searches.

## Investigation of HBr elimination in the photolysis of bromobenzene at 266 nm using repetitive scan FT-IR spectroscopy and DFT calculations

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Halobenzenes are widely used as an intermediate in various industries for the production of herbicides, dyestuff, and rubber. These chemicals are also used as a high-boiling solvent in many industries as well as in the laboratory. These activities could be a potential source of C<sub>6</sub>H<sub>5</sub>X (X = F, Cl, Br, I) in the troposphere. The fate of excited C<sub>6</sub>H<sub>5</sub>X has been studied for a long time due to its role in photochemical reactions, combustion processes, and atmospheric chemistry [1-3]. The photodegradation of C<sub>6</sub>H<sub>5</sub>X has significance in environmental protection since nascent halogen atoms destroy the ozone layer in the stratosphere. Also, there is a possibility of the formation of hydro-halogenated product (HX) upon degradation of C<sub>6</sub>H<sub>5</sub>X in addition to the C–X bond fission [4]. This primary HX product can take part in acid rain in the troposphere. Therefore, it is crucial to understand the mechanism of the degradation which gives a detailed mechanism of different reactions in combustion processes and atmospheric photochemistry.

In this work, the photolysis of C<sub>6</sub>H<sub>5</sub>Br in the gas phase has been studied at 266 nm using repetitive scan FT-IR spectroscopy [5,6] and density functional theory. Upon 266 nm photolysis of C<sub>6</sub>H<sub>5</sub>Br, rovibrational lines were observed in the region 2720.5 - 2361.2 cm<sup>-1</sup>, at 3317.8/ 3262.7 cm<sup>-1</sup> and 1346.2/1301.2 cm<sup>-1</sup>. These infrared features are assigned to the HBr and C<sub>2</sub>H<sub>2</sub>, respectively. Identification of C<sub>2</sub>H<sub>2</sub> but not expected HBr co-product *ortho*-benzyne (*o*-C<sub>6</sub>H<sub>4</sub>) indicates, *o*-C<sub>6</sub>H<sub>4</sub> further degraded into C<sub>2</sub>H<sub>2</sub> + C<sub>4</sub>H<sub>2</sub>. B3PW91/aug-cc-pVTZ calculated and CBS-QB3 corrected potential energy surfaces for the possible degradation channels of C<sub>6</sub>H<sub>5</sub>Br showing that HBr elimination is expected to be slightly lower as compared to the primary C–Br bond fission, however, their experimental branching ratio was determined to be 1 : 1. The RRKM rate of HBr elimination of C<sub>6</sub>H<sub>5</sub>Br at 266 nm was found to be 8.1 × 10<sup>3</sup> s<sup>-1</sup> and compared with the HCl and HF elimination rates in C<sub>6</sub>H<sub>5</sub>Cl [6] and C<sub>6</sub>H<sub>5</sub>F [2], respectively.

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# Investigation of excited state relaxation of hemicyanine dye

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Cyanine dyes are widely utilized in various applications, such as biological labeling, and among them, hemicyanine dyes have also attracted much attention. Hemicyanines consist of a conjugated system between two nitrogens, with one side forming an open chain and the other side adopting a cyclic structure. It is commonly used in photodynamic therapy [1]. Its excited state relaxation process is not yet fully comprehensive. Cao et al. calculated all possible internal rotations in a typical hemicyanine molecule for the excited state relaxation [2]. They proposed that the relaxation pathway involves the rotation of the aniline-ethylene bond. We employed time-correlated single photon counting (TCSPC) and fluorescence up-conversion techniques to investigate the excited state relaxation process of dianisole aminostyryl pyridine with bromide substitution (DAPy-Br) in solution. The excitation wavelength is 515 nm, which pumps the molecule to high vibrational levels of the first excited state. High polar solvent DMSO and the low-polarity solvent *p*-dioxane were used. As shown in Figure 1, the fluorescence of DAPy-Br in DMSO has three decay components 0.03 ps, 0.68 ps, and 2.5 ps while in *p*-dioxane, 0.03 ps, 3.8 ps, 34.3 ps, and 613 ps were observed. Those two short components were due to vibrational relaxation and other ultrafast processes like solvation. In DMSO, possible conversion to a twisted intramolecular charge transfer TICT state in 2.5 ps, causing a rapid relaxation of  $S_1$ . In *p*-dioxane, relaxation via internal rotation to other conformations is possible.  $\tau_5$  is the fluorescence decay of  $S_1$ .

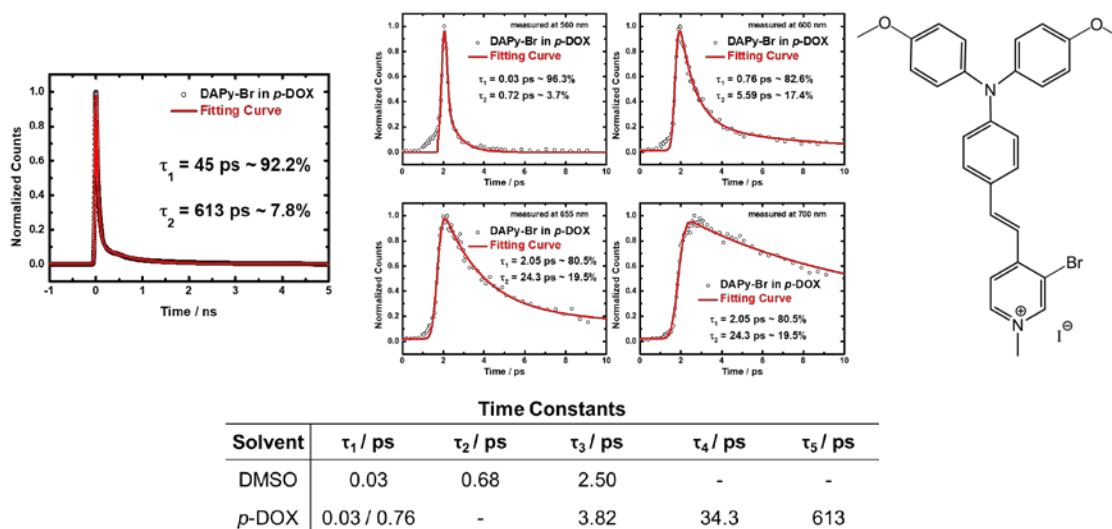


Fig. 1. The structure of DAPy-Br and time-resolved results of DAPy-Br in *p*-dioxane.

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## A perturb-then-diagonalize algorithm for high-dimensional anharmonic vibrational analysis

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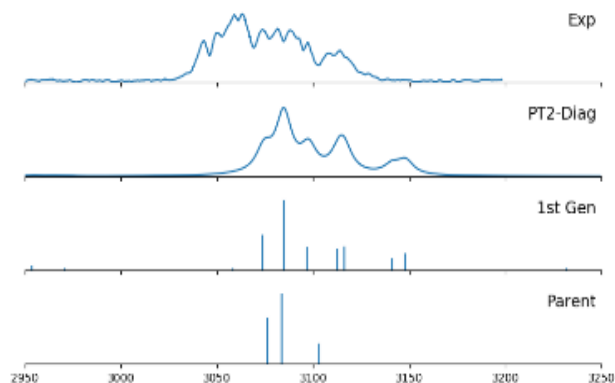
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Recent developments in infrared action spectroscopy, such as IRMPD and IRPD spectroscopy, have unlocked the potential to measure high-resolution vibrational spectra of molecule species. These advanced techniques have unveiled anharmonic phenomena, including Fermi Resonance and Combination bands, which were previously forbidden in harmonic approximations. To interpret these experimental spectra accurately, explicit treatments of anharmonic vibrational analysis have become essential.

Currently, two primary methods are employed for anharmonic vibrational analysis. The perturbative approach, such as vibrational second-order perturbation theory (VPT2), is typically faster but can suffer from accuracy issues, especially when encountering resonance conditions. In contrast, the variational approach, such as vibrational configuration interaction (VCI), offers improved accuracy in such cases but lacks scalability. To address this challenge, a potential solution lies in the reduced-dimensional approach, where specific vibrational modes are chosen for explicit anharmonic analysis, assuming they are uncoupled from the remaining modes.

In our research group, we have implemented a VCI-based method on a quartic potential energy surface (PES) capable of analyzing ~40 high-frequency vibration modes previously. However, this capability falls short when dealing with larger molecules. Moreover, incorporating low-frequency modes significantly increases the number of required eigenstates, worsen the situation even when considering only ~25 modes. To overcome this limitation, we have devised a novel approach that combines the strengths of both perturbative and variational methods, resulting in a perturb-then-diagonalize technique. Through this approach, we have performed efficient vibrational analyses on some azine systems, completing a 30-modes analysis in just a few minutes.



The C-H stretching region in the IR spectra of F-Bz. The perturb-then-diagonalize method find the most relevant basis kets, shrinking a  $20000^2$  VCI Hamiltonian into a  $29 \times 29$  matrix. The interaction between each basis kets are also visualized using this way.

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## Infrared spectroscopy and theoretical structure analyses of the protonated 2,2,2-trifluoroethanol and ethanol mixed clusters

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We investigated the development of the hydrogen-bonded (H-bond) structures and the influence of fluorination in the protonated alkyl alcohols [1-4]. Because fluorine is the electron-withdrawing substituent, the fluorine substitution of the alkyl groups decreases the proton affinity of the hydroxyl group. It reduces the stability of the double acceptor sites in the H-bond network, which is the crucial factor in forming the cyclic H-bonded network. As shown in the protonated 2,2,2-trifluoroethanol (TFE) clusters [4], the linear H-bond persists up to 5 TFE molecules. On the other hand, H<sup>+</sup>(ethanol)<sub>5</sub> presents the cyclic H-bond signature. In this work, we review the impact of fluorination by mixing  $m$  TFE and  $n$  ethanol molecules for  $m + n = 5$ . Using the Basin-Hopping structure search algorithm, we sampled the mixed cluster structures to represent the essential H-bonded structures in the IRPD experiment. Both simulated IR spectra and the tagged-atom effect are also discussed in this work.

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## Infrared spectra of isomers of protonated and hydrogenated phenanthridine isolated in solid *para*-hydrogen

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Large polycyclic aromatic hydrocarbons (PAH) and polycyclic aromatic nitrogen heterocycles (PANH) have been proposed to be potential carriers responsible for the unidentified infrared (UIR) emission bands in the interstellar medium.<sup>1</sup> The nitrogen atom in PANH induces a blue shift of the CC-stretching mode of the PAH, occurring around 6.3  $\mu\text{m}$ . In addition to PANH, several H<sup>+</sup>PAH and H<sup>+</sup>PANH also exhibit blue shifts.<sup>2</sup> Therefore, the CC-stretching band of the H<sup>+</sup>PANH might agree better with the UIB band at 6.2  $\mu\text{m}$  and H<sup>+</sup>PANH might be potential candidates that contribute to the UIR bands.

We report the infrared (IR) spectra of two isomers of protonated phenanthridine (H<sup>+</sup>C<sub>13</sub>H<sub>9</sub>N) and seven isomers of mono-hydrogenated phenanthridine (HC<sub>13</sub>H<sub>9</sub>N), produced upon electron-bombardment of a mixture of phenanthridine (C<sub>13</sub>H<sub>9</sub>N) and *para*-hydrogen (*p*-H<sub>2</sub>) during matrix deposition at 3.2 K. IR spectra of protonated species C<sub>13</sub>H<sub>9</sub>NH<sup>+</sup> was observed. In addition to the hydrogenation on the N atom of C<sub>13</sub>H<sub>9</sub>N to form C<sub>13</sub>H<sub>9</sub>NH, mono-hydrogenation at six carbon sites to form 1-, 2-, 3-, 7-, 9-, and 10-HC<sub>13</sub>H<sub>9</sub>N, respectively, were also observed. To confirm the spectral identification of hydrogenated phenanthridine, additional experiments on a C<sub>13</sub>H<sub>9</sub>N/Cl<sub>2</sub>/*p*-H<sub>2</sub> matrix were performed; the matrix was irradiated at 365 nm to generate Cl atoms, followed by IR irradiation to generate H atoms via Cl + H<sub>2</sub> ( $\nu = 1$ )  $\rightarrow$  HCl + H; the H atoms reacted with C<sub>13</sub>H<sub>9</sub>N via quantum tunneling. In these experiments, six hydrogenated phenanthridine species, except the one hydrogenated at the carbon site 3, were clearly observed. Spectral groupings were achieved according to the behaviors of lines upon secondary photolysis at various wavelengths, chosen according to the vertical electronic transitions of various isomers of HC<sub>13</sub>H<sub>9</sub>N predicted with the TD-B3LYP/6-311++G(d,p) method. The spectral assignments were supported via comparison of the experimental results with the vibrational wavenumbers and IR intensities of possible isomers predicted with the B3LYP/6-311++G(d,p) method. All spectra of H<sup>+</sup>C<sub>13</sub>H<sub>9</sub>N and HC<sub>13</sub>H<sub>9</sub>N are new.

For H<sup>+</sup>C<sub>13</sub>H<sub>9</sub>N, major observed lines are at 6.22, 12.53 and 12.8  $\mu\text{m}$ ; the CC-stretching band of C<sub>13</sub>H<sub>9</sub>NH<sup>+</sup> was observed at 6.22  $\mu\text{m}$ , blue shifted from that of the corresponding PAH, 10-C<sub>14</sub>H<sub>11</sub><sup>+</sup>. For HC<sub>13</sub>H<sub>9</sub>N, major lines were observed at 13.43, 13.16, and 13.55  $\mu\text{m}$  for C<sub>13</sub>H<sub>9</sub>NH, 9-HC<sub>13</sub>H<sub>9</sub>N, and 2-HC<sub>13</sub>H<sub>9</sub>N, respectively. Based on the overall spectral pattern, these protonated and hydrogenated species are unlikely to be the carriers of the UIR bands, characterized by emission bands near 3.3, 6.2, 7.7, 8.6, 11.2, and 12.0  $\mu\text{m}$ .

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## A model for extended red emission: Far-UV-induced photoluminescence in graphene

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Extended Red Emission (ERE) is a broad feature in the spectral region of 500–900 nm commonly observed in various circumstellar and interstellar environments. Despite well-established observational constraints for ERE [1], the definitive identification of carriers and associated processes adhering to these constraints remains elusive. We propose a plausible two-step model involving far-ultraviolet (UV)-irradiated single-layer graphene (SLG), considered as large polycyclic aromatic hydrocarbons, to address these constraints. This model is supported by laboratory experiments. The far-UV-treated SLG, which produces structural defects and graphene quantum dots, exhibits a photoluminescence excitation spectrum that extends from the far-UV to the UV–visible region, thus meeting the requirements of far-UV light and high photon-conversion efficiency. Additionally, a photoluminescence band shifting from ~585 nm to ~750 nm for high-dose-exposed SLG aligns with the observed red shift of the ERE band in regions under greater far-UV radiation density [2,3].

Moreover, a N-doped graphene thin film and quantum dots can also be prepared by exposing graphene to far-UV light in the presence of N<sub>2</sub>. A new photoluminescence band is observed at 380 nm, exhibiting an asymmetric band shape. This newly observed PL band bears resemblance to the unidentified blue luminescence detected in the red rectangle nebula [4], suggesting N-doped graphene might be responsible for the origin of the blue luminescence.

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## Infrared spectra of protonated methane isolated in solid *para*-hydrogen

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CH<sub>5</sub><sup>+</sup> is a fluxional molecule. In the lowest-lying structure of CH<sub>5</sub><sup>+</sup>, two hydrogen atoms and the carbon atom are connected by two electrons and denoted as a 3-center-2-electron (3c-2e) bond.<sup>1</sup> In 1999, Oka reported the first IR absorption spectrum of gaseous CH<sub>5</sub><sup>+</sup> in the C–H stretching region without assignments.<sup>2</sup> Later, Asvany et al. recorded broad absorption features of gaseous CH<sub>5</sub><sup>+</sup> at 110 K in the full IR region.<sup>3</sup> In 2015, Asvany et al. reported the high-resolution action spectra of gaseous CH<sub>5</sub><sup>+</sup> at 4 and 10 K in the 2880–3120 cm<sup>-1</sup> region and provided some tentative quantum-number assignments.<sup>4</sup> Boo et al. reported broad IR features of CH<sub>5</sub><sup>+</sup>(H<sub>2</sub>)<sub>1–3</sub> in an ion trap in region 2800–3100 cm<sup>-1</sup> and, along with molecular dynamic calculations, revealed that the tagging H<sub>2</sub> slows down the hydrogen scrambling in CH<sub>5</sub><sup>+</sup>.<sup>5</sup>

We produced CH<sub>5</sub><sup>+</sup> by electron bombardment of the CH<sub>4</sub>/*para*-H<sub>2</sub> matrix during deposition and recorded its IR absorption spectrum. After deposition for 5 h, the CH<sub>4</sub>/*para*-H<sub>2</sub> matrix was either maintained in darkness for 27 h or irradiated at 3244 nm with an OPO laser for 40 min. After these processes, lines of CH<sub>5</sub><sup>+</sup> decreased in intensity either because of the neutralization-dissociation by trapped electrons or dissociation by IR light; the latter was observed in the previous action spectrum. We observed bands at 1176, 2342, 2651, and 3064 cm<sup>-1</sup>, consistent with those of CH<sub>5</sub><sup>+</sup>(H<sub>2</sub>)<sub>1–3</sub> predicted by Esser et al.<sup>6</sup> Our results also agree with the theoretical prediction and the experimental results by Asvany et al.<sup>3</sup> except that our bands are much narrower and the antisymmetric stretching band of the 3c-2e-bonded CH<sub>2</sub> was shifted from 2472 to 2342 cm<sup>-1</sup> due to the significant interaction of CH<sub>5</sub><sup>+</sup> with H<sub>2</sub>. Alternatively, we produced CD<sub>4</sub>H<sup>+</sup> by electron bombardment of the CD<sub>4</sub>/*para*-H<sub>2</sub> matrix. The preliminary results showed five absorption bands at 970, 1177, 2179, 2225, and 2384 cm<sup>-1</sup>, which are consistent with the theoretical prediction and the experimental results by Ivanov et al. for CD<sub>4</sub>H<sup>+</sup>.<sup>7</sup> Similar to the work of CH<sub>4</sub>/*para*-H<sub>2</sub>, we observed much narrower bands, and the tentatively assigned stretching band of the 3c-2e-bonded CDH was significantly shifted from 2603 to 2384 cm<sup>-1</sup>.

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## Electronic spectra of protonated and hydrogenated isoquinoline isolated in solid *para*-hydrogen

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Diffuse interstellar bands (DIB), electronic absorption bands in the visible to near IR, have drawn attention since their first discovery in 1922. Polycyclic aromatic nitrogen heterocycles (PANH) and their cationic, protonated, and hydrogenated derivatives have been proposed to contribute to the unidentified infrared bands (UIR). Thus, they might also be promising candidates as the DIB carriers. However, laboratory spectra of these species suitable for comparison to astronomical observations are scarce.

Using the unique properties of solid *para*-hydrogen (*p*-H<sub>2</sub>) as a matrix host, we recorded the fluorescence excitation and dispersed fluorescence spectra of protonated isoquinoline (*iso*-C<sub>9</sub>H<sub>7</sub>NH<sup>+</sup>). We located the 0<sub>0</sub><sup>0</sup> band of the S<sub>1</sub> – S<sub>0</sub> transition of *iso*-C<sub>9</sub>H<sub>7</sub>NH<sup>+</sup> at 28097 cm<sup>-1</sup>; this suggests a blue shift of ~ 54 cm<sup>-1</sup> with respect to the gas-phase [1,2] due to the *p*-H<sub>2</sub> environment. The dispersed fluorescence spectrum was recorded over the range 350–420 nm after excitation at 349.8 nm and shows a progression with spacing of ~ 500 cm<sup>-1</sup>. We monitored fluorescence emission as a function of excitation wavelength in region 320–370 nm to record the excitation spectrum. To analyse our experimental results and assign the observed peaks to individual vibronic transitions, we performed Franck-Condon Hertzberg-Teller simulations on the basis of optimized geometries and harmonic frequencies obtained from (TD-)DFT calculations. In addition, we observed the fluorescence emission of at least two isomers of hydrogenated isoquinoline in the range 510–620 nm. We tentatively located the 0<sub>0</sub><sup>0</sup> bands of their S<sub>1</sub> – S<sub>0</sub> transitions at about 18494 cm<sup>-1</sup> and 19444 cm<sup>-1</sup> for 4-*iso*-HC<sub>9</sub>H<sub>7</sub>N and 8-*iso*-HC<sub>9</sub>H<sub>7</sub>N, respectively.

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## UV-induced photochemical reactions on water-covered carbonaceous grains: Dust thickness and structure effects

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In cold dense region, cosmic dust grains are predominantly composed of carbonaceous and siliceous material with the water-rich ice coverage. These grains provide a surface area for diverse photochemical reactions that leads to the formation of simple and complex molecules. Previous studies have demonstrated the catalytic effects of dust grains (<sup>[1]</sup>Brucato et al. 2006 and <sup>[2]</sup>Potapov et al. 2019) and recently research <sup>[3]</sup>Chuang et al. 2023 reported the possible interface reaction between H<sub>2</sub>O and carbonaceous dust to the formation of CO and CO<sub>2</sub>. In this work, we investigate the formation efficiency with various dust thickness and the chemical structure effects.

The laser ablation method was utilized to produce the two types of carbonaceous dust grains, namely amorphous carbonaceous (a-<sup>13</sup>C) and hydrogenated amorphous carbonaceous (HA<sup>13</sup>C). Subsequently, water ice was deposited onto the <sup>13</sup>C dust grains and exposed the UV light provided by NSRRC. The experimental results indicated a clear dust thickness dependence, implying more reaction sites available for H<sub>2</sub>O ice on thicker dust grains. As for the efficiency on HA<sup>13</sup>C and a-<sup>13</sup>C, the photochemical reaction is stronger on the HA<sup>13</sup>C dust grains but the production rate is significantly declined after repeating the same experiments on the processed dust sample, credited to the transformation from aliphatic-rich to aromatic-rich structures. The UV-induced structure transformation was demonstrated by the <sup>[4]</sup>Gadallah et al. 2012 as well.

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## Infrared spectra of isomers of protonated and hydrogenated phenol isolated in solid *para*-hydrogen

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Phenol (C<sub>6</sub>H<sub>5</sub>OH) is a fundamental building block of many bio-molecules. It was detected in the interstellar space in 2013.<sup>1</sup> Since proton sources are abundant in the outer space, it is expected that protonated phenol, H<sup>+</sup>C<sub>6</sub>H<sub>5</sub>OH, is likely to be formed in the interstellar space. The infrared photo-dissociation spectral studies of H<sup>+</sup>C<sub>6</sub>H<sub>5</sub>OH-Ar<sub>n</sub> in region 3600 – 2800 cm<sup>-1</sup> revealed that protonation of C<sub>6</sub>H<sub>5</sub>OH occurs at the oxygen, *para*-, and *ortho*-carbon positions.<sup>2</sup> The reaction of H + C<sub>6</sub>H<sub>5</sub>OH has been studied in supersonic expansion experiments after electric discharge at a temperature of 100–200 K. The detection of *ortho*-HC<sub>6</sub>H<sub>5</sub>OH, *ortho'*-HC<sub>6</sub>H<sub>5</sub>OH, and tentatively *meta*-HC<sub>6</sub>H<sub>5</sub>OH have been reported.<sup>3</sup>

Using the *para*-hydrogen (*p*-H<sub>2</sub>) matrix isolation method, we have recorded the infrared (IR) spectra of two isomers of protonated phenol (H<sup>+</sup>C<sub>6</sub>H<sub>5</sub>OH) and four isomers of hydrogenated phenol (HC<sub>6</sub>H<sub>5</sub>OH), produced upon electron-bombardment during matrix deposition of a mixture of C<sub>6</sub>H<sub>5</sub>OH and *p*-H<sub>2</sub> at 3.2 K. The IR signals of H<sup>+</sup>C<sub>6</sub>H<sub>5</sub>OH diminished when the matrix was maintained in darkness for 14 h because of the neutralization of cations with trapped electrons, whereas those of HC<sub>6</sub>H<sub>5</sub>OH increased in intensity. Grouping of observed spectral lines was achieved according to the behavior of secondary photolysis at various wavelengths, which were chosen according to the vertical electronic transitions of various isomers of protonated and hydrogenated phenols predicted with the TD-B3LYP/6-311++G(d,p) method. Lines of various groups identified through secondary photolysis were assigned according to the comparison with the quantum-chemically calculated IR spectra predicted with the B3LYP/6-311++G(d,p) method.

Two protonated species with lowest energies, *ortho*- and *ortho'*-H<sup>+</sup>C<sub>6</sub>H<sub>5</sub>OH, were identified. Hydrogenation products *meta'*-, *para*-, *meta*-, and *ortho*-HC<sub>6</sub>H<sub>5</sub>OH were also identified. The *ortho'*-HC<sub>6</sub>H<sub>5</sub>OH, which has the second lowest energy, was not observed. This might be because the barrier for isomerization from *ortho'*-HC<sub>6</sub>H<sub>5</sub>OH to *ortho*-HC<sub>6</sub>H<sub>5</sub>OH, 13.1 kJ mol<sup>-1</sup>, is small, so that *ortho'*-HC<sub>6</sub>H<sub>5</sub>OH was converted to *ortho*-HC<sub>6</sub>H<sub>5</sub>OH under our experimental conditions.

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## Experimental investigations on the behavior of free radicals on the surface of icy grain analogues

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Molecular clouds are the birthplace of stars and are characterized by very low temperatures as low as 10 K and low density ( $\sim 10^3$  molecules  $\text{cm}^{-3}$ , dominated by  $\text{H}_2$ ). Regardless of such an extreme condition unfavorable for chemical reactions, more than 200 kinds of species have been identified in molecular clouds. It has been well known that chemical reactions on icy grain surfaces play an important role in producing these variety of molecules with large abundances. Because of low temperatures, tunneling reactions involving hydrogen atoms and radical-radical reactions, which tend to be barrierless, are critically important. However, studying the behavior of radicals (e.g., their diffusion on the surface) is so difficult that many experimental studies could detect only products and were forced to guess the mechanisms of their formation. We have developed a method to detect free radicals, in situ, on icy grain analogues [1,2]. This method combines photostimulated desorption (PSD) and resonance enhanced multiphoton ionization (REMPI): the PSD-REMPI method. Because the PSD-REMPI method is highly sensitive, species-selective, and surface-selective method and its intensity is proportional to the surface number density of target species, we can study the behavior of radicals on the surface of icy grain analogs.

We have recently applied the PSD-REMPI method to studying the surface diffusion of hydroxyl (OH) radical [3] and carbon atoms [4], which are considered abundant on the icy grain surface and important for the formation of interstellar molecules. From experiments, we determined the activation energy for their surface diffusion on amorphous solid water. Considering the lifetime of icy grains ( $10^5$  years) and typical sizes (diameter  $\sim 100$  nm), we suggested that the diffusive reactions of OH radical and carbon atom are activated at temperatures above 36 and 22 K, respectively.

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## The photodesorption of OH radical triggered by visible light

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The hydroxyl (OH) radical plays an important role in forming various species both on the ice dust surface and in the gas phase in cold interstellar regions. The photodesorption of OH from ice induced by UV and X-ray photons has been studied for decades, while that by visible photons has not been investigated because both a water molecule and an OH radical were considered to be transparent in the visible region. Recently, the desorption of OH adsorbed on the ice surface was found to be induced by a photon at 532 nm, following photoabsorption by OH strongly bonded on ice via three hydrogen bonds with neighboring H<sub>2</sub>O molecules [1]. In our experiments, OH radicals on ice were desorbed and detected by a combination of photostimulated desorption (PSD) and resonance-enhanced multiphoton ionization (REMPI) methods. The PSD laser provided the visible photons for the photodesorption process, and the selectively ionized OH by 2+1 REMPI process was eventually detected by the time-of-flight (TOF) mass spectrometer. The electronic A-X transition of isolated OH happens at 308 nm [2], however, the quantum chemical calculations revealed that the transition in the range extended to 600 nm is possible for OH radicals adsorbed on the ice surface. In this study, we investigated the photodesorption of OH adsorbed on water ice at the wavelengths from 410 to 700 nm, which is the first wavelength-dependent result at the visible range. Furthermore, by measuring the photodesorption cross section, we obtained insight into the relationship between photon absorption and the population of OH adsorption sites on the H<sub>2</sub>O surface.

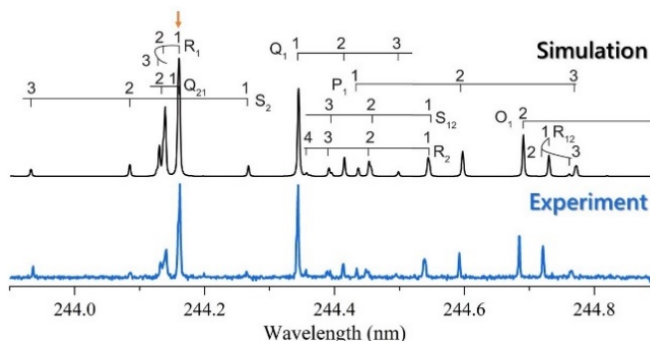


Fig. 1. The 2+1 REMPI spectra of OH radical in the transition of  $D^2\Sigma^-(v' = 0) \leftarrow X^2\Pi(v'' = 0)$  from both simulation and experiment results<sup>[1]</sup>. The arrow shows the selected R<sub>1</sub> (J = 1) branch to probe photodesorption.

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## Production of HO•CHC(O)H, HOCH<sub>2</sub>•CO, and HOCH<sub>2</sub>CH<sub>2</sub>O• in the reaction H + glycolaldehyde [HOCH<sub>2</sub>C(O)H] in solid *p*-H<sub>2</sub> and its implication in astrochemistry

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Glycolaldehyde (HOCH<sub>2</sub>C(O)H, GA), the simplest and the first sugar detected in interstellar medium (ISM), was proposed as a potential starting material for the synthesis of various complex sugar molecules, including ribose, crucial to the origin of life. Intermediates derived from GA, including hydroxyl-vinoxy radical [HO•CHC(O)H], hydroxy acetyl radical (HOCH<sub>2</sub>•CO), and 2-hydroxy ethoxy radical (HOCH<sub>2</sub>CH<sub>2</sub>O•) could be the prospective sources for the formation of higher order sugars. However, the detailed mechanisms involved in the formation complex sugars via GA-mediated radicals under interstellar milieu are still unclear. We employed *para*-hydrogen (*p*-H<sub>2</sub>) to investigate the reaction between H atoms and GA at 3.2 K; *p*-H<sub>2</sub> serves as not only a quantum-solid matrix host for effective H tunneling but also a medium for effective *in-situ* production of H-atoms. To generate H atoms, we performed UV photolysis at 365 nm on a matrix co-deposited with a mixture of GA/*p*-H<sub>2</sub> and Cl<sub>2</sub> to produce Cl atoms, followed by IR irradiation to promote the reaction Cl + H<sub>2</sub> (*v* = 1) → H + HCl. According to the orientation of O–H and C=O bonds, GA has 4 conformers; *Cis-cis* (*Cc*) conformer is found to have the least energy among all due to the intramolecular H-bonding. IR irradiation employed during H-atoms generation was also responsible for the *Cc* → *Tt* conformational conversion; which intricates the H + *Cc*-GA reaction. Therefore, H + *Tt*-GA reaction was performed in which conformational conversion was achieved initially by irradiating the matrix at 2827 nm (*v*<sub>OH</sub> fundamental of *Cc*-GA) prior to its reaction with H atoms. In both reactions, H + *Cc*-GA and H + *Tt*-GA, several channels including H-abstraction on the CH<sub>2</sub> and the C(O)H moieties to produce HO•CHC(O)H and HOCH<sub>2</sub>•CO, further H-abstraction on the C(O)H moiety of HOCH•C(O)H to produce HOCHCO (hydroxyketene), H-addition to the carbon atom of carbonyl moiety of GA to form HOCH<sub>2</sub>CH<sub>2</sub>O•, and H-induced fragmentation to form •CH<sub>2</sub>OH + H<sub>2</sub>CO were observed. Importantly, we are able to differentiate *Cc* and *Tt* conformers of associated products observed in both reactions. The assignments of all these products were supported by comparing experimental results with vibrational wavenumbers of possible products predicted with the B3LYP/aug-cc-pVTZ method.

## In situ electron diffraction analysis of nanoscale ice formed by neon matrix sublimation at cryogenic temperatures

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The structure of nanoscale ice (H<sub>2</sub>O) is important to understand the origin of its unique physicochemical properties that deviates from bulk phases. For example, on the surface of interstellar dust grains, the morphology of nanoscale ice affects the reaction rate of radicals [1]. Moreover, the vapor pressure of nanoscale ice can become three to ten orders of magnitude larger than that of bulk crystalline ice [2].

Nanoscale ice can be prepared by deposition of a water vapor onto a cold substrate (vapor-deposition). The formation of ice without a long-range ordered structure (amorphous water) is explained by kinetic effects due to the high deposition rate at low temperatures. Recently, the formation of crystalline ice is found by infrared spectroscopy even at cryogenic temperatures through sublimation of the water/neon (H<sub>2</sub>O/Ne = 1/1000) matrix [3]. However, the crystalline structure of the ice is still unknown.

Using newly developed reflection high energy electron diffraction (RHEED), we found almost no hexagonal stacking sequences in the crystalline ice formed by neon matrix sublimation at 13 K, in contrast to the crystalline ice prepared by annealing vapor-deposited amorphous water at 143 K (Fig.1) [4]. The formation of low hexagonal stacking sequences in nanoscale ice at ultra-high supercooling degrees is qualitatively in line with the size-dependence of stable configuration of water clusters [5].

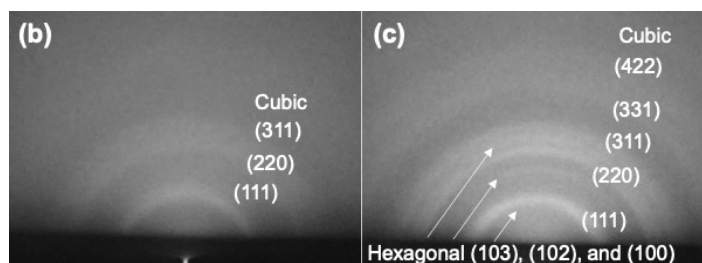


Fig.1. RHEED images of nanoscale ice obtained by neon matrix sublimation at 13 K (left), and nanoscale ice obtained by annealing vapor-deposited amorphous water at 143 K (right).

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## Exploring multiphase ion-neutral reactions: The preliminary studies on $\text{CO}_2^+$ with $\text{H}_2$ in solid $\text{H}_2$

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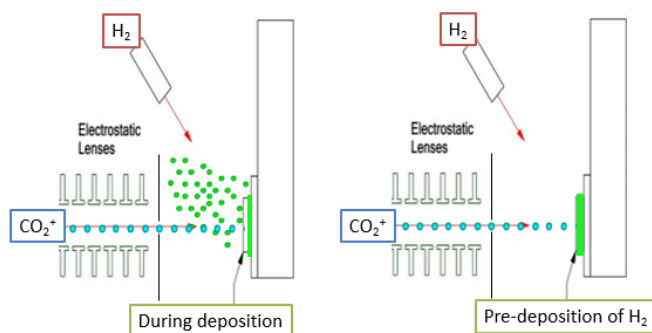
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Ion-neutral reactions have become a critical area of research, playing a significant role in astrochemistry, plasma physics, atmospheric chemistry, combustion, and flame processes. In astrochemistry, specifically, modeling chemical reactions in the interstellar medium (ISM) necessitates experimental data acquired in the laboratory to ensure reliability. While previous experimental techniques primarily focused on studying gaseous ion-neutral reactions, the ISM is highly heterogeneous, exhibiting a wide range of temperatures and densities. Therefore, laboratory studies of ion-neutral reactions in multiphase environments, facilitated by newly developed instrumentation, are essential to yield unprecedented data.

In this preliminary study,  $\text{CO}_2^+$  cations are deliberately selected with a specific kinetic energy to collide with  $\text{H}_2$  molecules during deposition, as illustrated in Fig. 1. After a 6-hour deposition, IR absorption spectra of the matrix sample are recorded. In contrast to the sole formation of  $\text{HOCO}^+$  from the ion-neutral reaction of  $\text{CO}_2^+ + \text{H}_2$  in the gas phase, various products are identified, encompassing both ionic and neutral species. Apart from the predominant  $\text{HOCO}^+$ , cationic species, including  $\text{H}^+(\text{CO}_2)_2$  and  $(\text{CO}_2)_2^+$ , and anionic species, such as  $\text{CO}_2^-$ ,  $\text{HCO}_2^-$ , and  $\text{HOCO}^-$ (?), as well as neutral species, including  $\text{HOCO}$ ,  $\text{HCO}$ ,  $\text{HCOOH}$ , and  $\text{CO}$ , are existing in solid  $\text{H}_2$ . The possible reaction routes in the gas phase and/or solid phase will be discussed.



**Fig.1** Experimental schemes for explore ion-neutral reactions in the multiphases.



## The formation of complex organic molecules via energetic electrons irradiation of astrophysical ices

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In astrophysical environments, H<sub>2</sub>O is the predominant molecule within interstellar ice, and CO stands out as both one of the most prevalent molecules and a vital carbon source for the creation of complex organic molecules (COMs). Additionally, NH<sub>3</sub> holds significant importance as a source of nitrogen for COMs formation. Over the past few decades, various energy sources, such as vacuum ultraviolet (VUV), soft X-rays, and heavy ions, have been employed to study the energetic processes within H<sub>2</sub>O+CO+NH<sub>3</sub> ice mixtures. These investigations have led to the observation of the formation of several COMs, including formamide (HCONH<sub>2</sub>), urea (NH<sub>2</sub>CONH<sub>2</sub>), and carbamic acid (NH<sub>2</sub>COOH) [1–3]. However, one critical energy regime has been notably absent from discussion: low-energy electrons with energies below 1000 eV, which are commonly produced through cosmic ray interactions with gas molecules in dense interstellar clouds. In this study, we irradiated CO+NH<sub>3</sub> and H<sub>2</sub>O+CO+NH<sub>3</sub> ice mixtures with 1000 eV electrons, focusing on the influence of H<sub>2</sub>O on the formation of products. Our investigation includes the examination of OCN<sup>-</sup> and HNCO, which play pivotal roles in the synthesis of COMs.

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## New insights into H atom reactions of astrophysical significance through *para*-H<sub>2</sub> matrix isolation

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The unique characteristics of a *para*-H<sub>2</sub> matrix, including the sharp spectral lines of the molecules isolated in this medium, the diminishing of cage effects, and the efficient diffusion of H atoms through quantum tunneling, have established *para*-H<sub>2</sub> matrix isolation as a valuable tool for modeling H atom reactions in cold, dark astrophysical environments, particularly in dense molecular clouds. The groundwork laid by the groups of Anderson [1] and Lee [2], who elucidated the facile generation of H atoms in *para*-H<sub>2</sub>.

At low temperatures, unsaturated molecules can absorb H atoms, while H atoms can abstract one or more H atoms from a molecule, resulting in the formation of H<sub>2</sub>. Employing the *para*-H<sub>2</sub> matrix isolation method, in collaboration with Yuan-Pern Lee, our investigations have revealed the existence of a dual-cycle mechanism connecting HNCO and NH<sub>2</sub>CHO [3]. This finding may explain the observed correlation in the column densities of these species in various astrophysical objects.

Subsequent to this discovery, our research group has constructed a novel experimental setup, VIZSLA [4], suitable for various laboratory astrochemistry experiments, including the investigation of low-temperature H atom reactions both in *para*-H<sub>2</sub> matrix and in astrophysical analogue ices. Using VIZSLA, we have delved into various H atom absorption and H atom abstraction cycles with relevance to astrophysics. These cycles not only establish chemical links among species in the Interstellar Medium (ISM) but also play a role in the formation of interstellar H<sub>2</sub>. This poster will provide a summary of the experimental studies conducted by our group over the past three years, shedding light on several astrophysically important chemical processes.

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## Electronic spectroscopy of polycyclic aromatic hydrocarbons in solid *para*-hydrogen

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Whilst well over 500 Diffuse Interstellar Bands (DIB) have been catalogued since their first discovery in 1922, so far, only the buckminsterfullerene cation  $C_{60}^+$  has been confirmed as the carrier of two DIB at 9577.5 and 9632.7 Å. [1,2] Large polycyclic aromatic hydrocarbons (PAH) and their cationic, protonated, and hydrogenated derivatives are considered particularly promising candidates. Electronic absorption spectra of these molecules suitable for a comparison to astronomical observations, however, are rarely available.

*para*-Hydrogen (*p*-H<sub>2</sub>) has frequently been employed as a matrix host to study the IR spectra of PAH and their derivatives. The spectra generally exhibit only small matrix shifts in line with the “softness” of the *p*-H<sub>2</sub> host. Over the past years, we have recorded dispersed fluorescence and fluorescence excitation spectra of several neutral, protonated, and hydrogenated PAH and PANH in solid *p*-H<sub>2</sub> to assess the properties of *p*-H<sub>2</sub> as a matrix isolation for electronic spectroscopy and its potential to aid *inter alia* in the search for the DIB carriers.

In our contribution, we present an excerpt of this work in three examples:

Ovalene (C<sub>32</sub>H<sub>14</sub>) has been discussed as potential DIB carrier and a system exhibiting anomalous fluorescence from higher excited singlet states. Combining experiment and theory, we found, however, that the lowest excited singlet state (*S*<sub>1</sub>) was previously assigned erroneously; we report the fluorescence emission and excitation spectra as well as fluorescence lifetimes of the true *S*<sub>1</sub> state. *peri*-Hexabenzocoronene (*peri*-HBC, C<sub>42</sub>H<sub>18</sub>) has rarely been studied before. We provide a first full assignment of the vibrational structure of the fluorescence emission and excitation spectra centered around the *S*<sub>1</sub>–*S*<sub>0</sub> origin band located ~22075 cm<sup>-1</sup> in solid *p*-H<sub>2</sub>. Our first results on protonated coronene (H<sup>+</sup>C<sub>24</sub>H<sub>12</sub>) indicate a red shift of the *S*<sub>1</sub>–*S*<sub>0</sub> origin induced by *p*-H<sub>2</sub> of ~40 cm<sup>-1</sup> compared to a red shift of ~7 cm<sup>-1</sup> in solid Ne. [3] This is in line with the small but consistent red shifts <100 cm<sup>-1</sup> we observed for the electronic transitions of other neutral and hydrogenated PAH in solid *p*-H<sub>2</sub>.

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## Nuclear spin conversion of methane in condensed layers at low temperatures

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Molecules including hydrogen nuclei, i.e., protons, in the rotationally symmetric positions are classified into the nuclear spin isomers, according to their resultant spin ( $I$ ). Because the symmetry restriction with respect to the permutation of the protons, each isomer occupies only specific rotational levels. This coupling between the rotation and nuclear spin allows us to distinguish the isomers by rotationally-resolved spectroscopy such as infrared and Raman spectroscopy. The conversion between the isomers is suppressed in the isolated state, but is promoted in condensed systems, where the excess rotational energy is dissipated. The conversion mechanism of fundamental molecules, such as H<sub>2</sub> [1], H<sub>2</sub>O [2], and CH<sub>3</sub>OH [3], has attracted much interest in the fields of the physical chemistry, astronomy, and industry [4].

In the case of methane, there are three kinds of nuclear spin isomers: ortho ( $I = 1$ ), meta ( $I = 2$ ), and para ( $I = 0$ ). Methane is a spherical top molecule, and its rotational energy is dependent on the rotational quantum number  $J$  as  $E_{\text{rot}} = BJ(J + 1)$ , where  $B$  denotes the rotational constant. The  $J = 0$  ( $J = 1$ ) level is occupied only by the meta (ortho) isomer while the ortho and para states are degenerate at the  $J = 2$  level. Because of this degeneracy, the conversion between ortho and para proceeds considerably fast, with the result that only the ortho-meta conversion has been observed in matrices of rare gases [5,6] and para hydrogen [7]. On the other hand, the nuclear spin conversion between three kinds of the isomers has recently been observed in the lower-temperature phase of crystalline methane [8]. In this presentation, the infrared spectroscopic study on the ortho-meta-para conversion in crystalline methane is demonstrated, comparing with previous matrix-isolation studies.

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## Interstellar ice-dust interactions: UV-induced $^{13}\text{CO}_2$ formation on $^{13}\text{C}$ -Dust with $\text{H}_2\text{O}$ ice deposited at various temperatures

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In the laboratory astrophysics/astrochemistry, most research groups utilize substrate like  $\text{CaF}_2$  or Au, which do not react with ice molecules from a chemical perspective. However, in realistic scenario, these ice molecules usually condensed on carbon- or silicate-based dust, forming interstellar ice. Therefore, the reactions occurring at the ice-dust interface have been taken into consideration in recent years. Under the exposure to various energy sources, such as X-rays, photons, and electrons, dusts may provide C or Si atoms, thereby facilitating the formation of larger molecules. Among them, the carbonaceous dust (C-dust) is much more interested by the scientists because it could potentially supply the necessary C atoms for the complex organic molecules (COMs) or their precursors.

Previous research groups have investigated the formation of CO and  $\text{CO}_2$  from ice covering C-dust under various energetic sources at low temperatures<sup>[1][2]</sup>. However, although some studies<sup>[3][4]</sup> discussed the temperature effect on the C-dust/ice interaction during the irradiation, they didn't constrain the deposition temperature. In this study, we deposited  $\text{H}_2\text{O}$  ice, one of the most abundant interstellar ices, onto the  $^{13}\text{C}$ -dust at different temperatures ranging from 13 K to 130 K. Subsequently, an ultraviolet (UV) source generated by the microwave-discharge hydrogen-flow lamp (MDHL) was employed to irradiate the samples under 13 K. From the formation yield of  $^{13}\text{CO}_2$ , the mobility of  $\text{H}_2\text{O}$  ice within the  $^{13}\text{C}$ -dust could be determined. Furthermore, the effective sites provided by  $^{13}\text{C}$ -dust for  $\text{H}_2\text{O}$  ice was examined by varying the thickness of  $\text{H}_2\text{O}$  ice.

Following the UV irradiation, the  $\text{H}_2\text{O}$  ice deposited at higher temperatures can lead to a higher  $^{13}\text{CO}_2$  formation yield. This indicates that the  $\text{H}_2\text{O}$  molecules can occupy more sites within  $^{13}\text{C}$ -dust as the deposition temperatures increased. The results will be presented in the poster.

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## Photochemical reaction of CH<sub>4</sub> in N<sub>2</sub>-rich environment

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Nitriles have been observed on planets such as Triton, Pluto, and Eris, suggesting their formation may involve the photochemical reactions of N<sub>2</sub> and CH<sub>4</sub> in mixed ices. To study this phenomenon, we conducted a series of experiments in environments enriched with N<sub>2</sub>, focusing on the photochemical reactions of CH<sub>4</sub> after exposure to vacuum ultraviolet (VUV).

The experimental procedure involved depositing CH<sub>4</sub>:N<sub>2</sub> ice mixture onto a CaF<sub>2</sub> substrate cooled to 12.5 K, followed by irradiation with VUV photons generated by a microwave-discharged hydrogen-flow lamp (MDHL). The results indicate that N<sub>2</sub> plays a suppressive role in the production of C<sub>2</sub>H<sub>6</sub> and C<sub>3</sub>H<sub>8</sub>, with the production of C<sub>3</sub>H<sub>8</sub> reaching zero at a CH<sub>4</sub>:N<sub>2</sub> ratio of 1:50. Additionally, a positive correlation was observed between the concentration of N<sub>2</sub> and the generation of HCN. Furthermore, N<sub>2</sub> inhibits the photodesorption of CH<sub>4</sub>, with complete suppression observed when N<sub>2</sub> exceeds 80%. This study expands our understanding of the photochemical behavior of CH<sub>4</sub> in N<sub>2</sub>-rich environments, revealing intricate VUV photochemical processes occurring in astrophysical environments.

## Electronic absorption spectra of 4-phenanthridine cations: A theoretical study

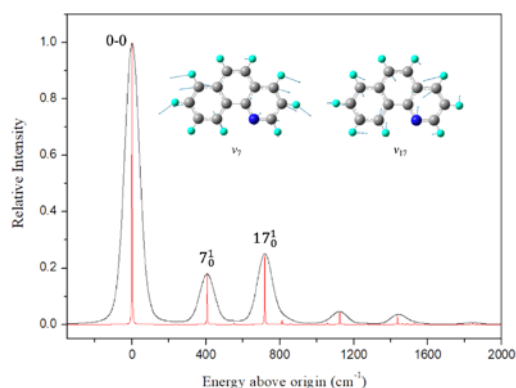
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Infrared studies have suggested that the sub-group of nitrogen-substituted PAHs, exhibit spectral features similar to those of PAHs, potentially contributing to unidentified spectral bands. The importance of PANHs in photon-dominated regions, as the spectra of PANH cations were not merely useful, but required, to fit the 6.2 and 11  $\mu\text{m}$  emission features observed towards NGC 7023 [1]. However, based on the general properties derived from the spectra of these small nitrogen-substituted PAHs, the larger PANH cations [2] emerge as strong candidates for Diffuse Interstellar Bands (DIB) carriers. This is attributed to the anticipated positions of their electronic transitions in the UV-visible spectrum and the narrowness of their spectral bands. Optimization of excited and ground state structures for 4-phenanthridine cation was conducted using Complete Active Space Self-Field (CASSCF), Time-Dependent Density Functional Theory (TDDFT) calculations, and absorption spectra simulations via one-photon excitation equations. The absorption spectrum of the  $\pi\pi^*$  transition of 4-C<sub>13</sub>H<sub>9</sub>N<sup>+</sup> was simulated using the displaced harmonic oscillator approximation and Franck–Condon approximation [3,4]. The simulated spectrum is presented with Franck-Condon factors plotted as a function of the excitation energy and calculated excited state frequencies, highlighting the main vibrational progressions  $\nu_7$  and  $\nu_{17}$ . The indicates that the electronic transition of the D<sub>1</sub> state calculated in the adiabatic representation effectively includes a contribution from the adiabatic vibronic coupling through Franck-Condon factors perturbed by harmonic oscillators.



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## Elucidating structure and properties of charged sugars/glycosaminoglycans using neural network potential

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Glycosaminoglycans (GAGs) are the family of negatively charged polysaccharides with variable sulfation that are the predominant constituent of the extracellular matrix. Their pivotal role in essential biological processes, influencing cellular properties, tissue development, remodeling, homeostasis, and disease progression have been highlighted. The GAGs are made of repeating disaccharide units of a hexuronic acid, galactose in keratan sulfate, a hexosamine, and acetylated hexosamine throughout a regular alternation of 1–4 and 1–3 glycosidic linkages. Due to these characteristic sequence microheterogeneity, high negative charge density, and the isomeric nature of the building blocks, GAGs are challenging to characterize. As the chemical space of GAGs is too large to fully cover by experimental methods, theoretical spectra computed from DFT structures may be required to bridge this gap. In this study, we make a structure exploration for the building block of GAGs, including sulfated Idouric or Glucuronic acid, Glucosamine, acetylated Glucosamine, and acetylated Galactosamine [IdoA2S, GlcA2S, GlcNS, GlcNac3S, GalNac4S e.t.c]. [1] This process can be accelerated by neural network potential (NNP) by means of SchNet. [2-3] The study demonstrated that knowledge could be transferred among the saccharide families; the structural search is initiated from our structure database of the mono-saccharides, and the NNP can be transferred to the sulfated saccharides quickly. With an efficient scheme, the iterative NNP training and preliminary structure search can be done within a few days.

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## Controlling C-C coupling reactivity through pore shape engineering of B-doped graphyne family

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Graphyne is an interesting carbon allotrope characterized by  $sp$ - $sp^2$  hybridized carbon bonds, which allow for structure variability. Though there are studies evaluating the electrical and mechanical properties of various structures, studies utilizing its structural variety toward catalyst applications are minor. In electrocatalytic  $\text{CO}_2$  reduction reactions (CRR), producing valuable  $\text{C}_{2+}$  products, such as  $\text{C}_2\text{H}_4$  or  $\text{C}_2\text{H}_5\text{OH}$ , under mild conditions is still challenging. The bottleneck has been assigned to the carbon-carbon (C-C) coupling reaction, such as  $2^*\text{CO} \rightarrow ^*\text{OCCO}$ . In this reaction, one requires strong binding to the catalyst to enhance neighboring CO concentration, but at the same time, one needs to have low C-C coupling barriers making the OC-CO bond. Following our previous study, which showed B-doped  $\gamma$ -graphyne can be a catalyst for ethanol production, we conducted theoretical investigations on a range of B-doped graphyne families using density functional theory. Out of the 15 different structures studied, four, 4,12,2-, sR-,  $\gamma$ -, and 6,6,12-graphynes, show promising potential for CRR. B-doped 4,12,2-graphyne had a very low C-C coupling barrier of 0.34 eV with strong  $2^*\text{CO}$  adsorption (-2.5 eV). Furthermore, our research revealed a correlation between the heat of reaction ( $2^*\text{CO} \rightarrow ^*\text{OCCO}$ ) and the average pore area around the acetylenic linker reaction site. Smaller pores give a favorable orientation of two CO molecules, resulting in low reaction barriers.

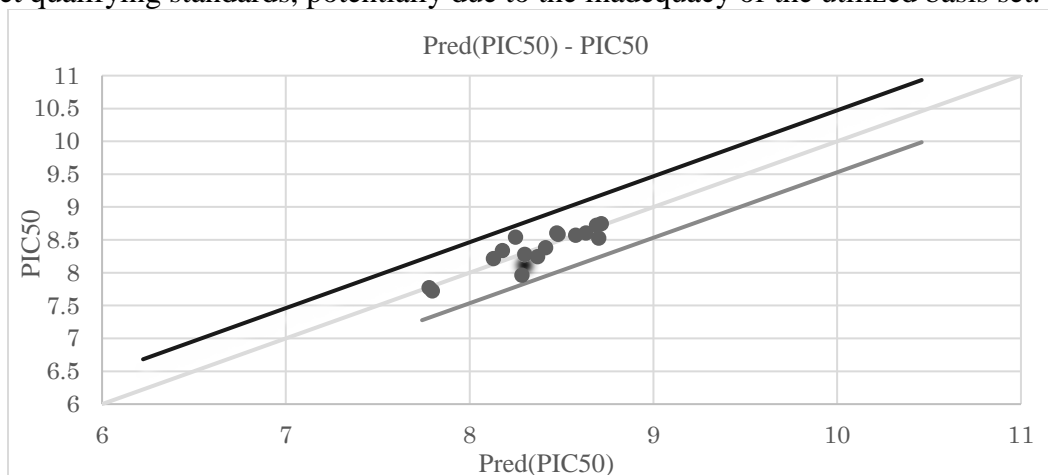
## Using DFT and MLR to build a QSAR model for studying nitrogen-mustard compounds

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The dipeptide-alkylated nitrogen-mustard compound is a new kind of nitrogen-mustard derivative with a strong anti-tumor activity, which can be used as a potential anti-osteosarcoma chemotherapy drug. In this study, Quantum parameters (structures, energies) have been calculated using the DFT/BP86 method in conjunction with basis set def2-TZVP. The quantum chemical parameters acquired as independent variables have been combined with specific experimental biochemical values, serving as dependent variables, to establish a dataset for constructing the model. The depicted results in the figure illustrate the successful construction of a QSAR model employing 8 independent variables, effectively describing and predicting the biological activity within the research system. The QSAR prediction model obtained  $R^2 = 0.797$ ;  $Q^2 = 0.796$ ;  $R^2\text{-test} = 0.242$ . The statistical metrics indicate that the linear multivariate regression method, employing quantile parameters, can serve as a viable theoretical model for predicting the activity of substances investigated in this research. The system exhibits moderate reliability; however, the  $R^2\text{-test}$  index does not meet qualifying standards, potentially due to the inadequacy of the utilized basis set.



Graph of predicted activity against experimental data

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## A neural network accelerated target search to study the dissociations in Di-saccharides

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Exploring the reactions of carbohydrates is challenging in computational chemistry. Because of high flexibility, disaccharides have millions of conformers, making reaction exploration difficult. As the neural network potential (NNP) has a thousand times acceleration and a similar accuracy to the DFT methods, an NNP-accelerated target search scheme was performed to study the collision-induced dissociations in saccharides. [1-2]

The target search scheme includes the transition state (TS) structure sampling, NNP training, and the candidates labeling for the low-lying TS. Taking advantage of the mono-saccharide studies, the *attach & rotate* sampling protocol utilizes their structures and pathways as a starting point. The initial guesses of disaccharides can be generated by attaching two mono-saccharide conformers with the glycosidic rotations. Considering the pathways do not exist in mono-saccharides, the second TS structure sampling is applied to the structural adjustment of the minima candidates. After sampling, a small batch of the initial structures is calculated and used iteratively in the SchNet NNP training. A decent NNP with an MAE of 5 kJ/mol is obtained and applied in the TS exploration.

The NNP-TSs can be further utilized in the feature analysis of random forest (RF) algorithms to search the candidates for low-lying TS from the complete set of initial structures. The features of ring puckering configuration, dihedral glycosidic bond angles, sodium ion coordination, and hydrogen bonds are analyzed. The RF model labels 20% of the initial structures as candidates, which includes more than 85% of the initial structures for the low-lying TS. The neural network accelerated target search aggressively improves the efficiency in the search of low-lying TS and makes the exploration for a disaccharide possible in a few days. By patching the NNP, the new reaction pathways can be quickly adapted and explored. The search scheme can transfer the "knowledge" among the saccharide family by reusing the NNP and structural database. With the "knowledge" accumulated, the oligosaccharide computational study becomes feasible.

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LabRAM Odyssey Nano



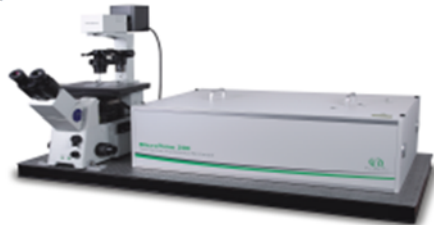
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SPEX SamplePrep



- + 研磨量 10ml/罐, 攪拌量 25ml/罐。  
(SPEX 8000D 一次放兩罐)
- + 多方向振動研磨, 快速球磨, 每分鐘馬達轉速 1425 ~ 1725 RPM
- + 可連接 TIMER 程式多段控制操作。
- + 採用萬向頭三度空間研磨不會造成研磨罐內產生軌跡, 造成樣品污染。

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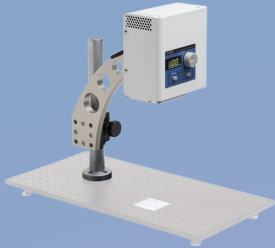
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太陽光模擬器



雷射



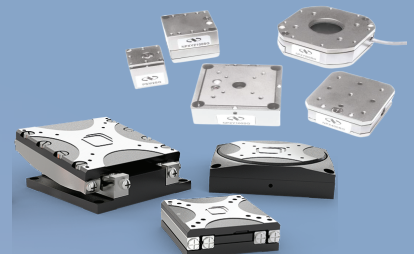
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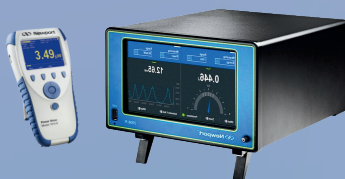
單光儀 & 光譜儀



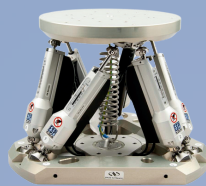
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## UniDRON

共軛焦顯微拉曼光譜儀 (Raman)  
光激螢光光譜儀 (PL)  
時間解析螢光光譜 (TRPL)  
原子力顯微鏡 (AMF-Raman)



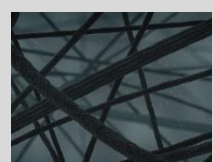
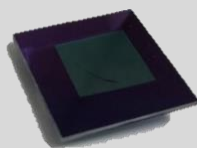
## XperRAM

2D快速掃描 (2D scan)  
拉曼影像/螢光壽命影像/光電流影像  
(Raman/FLIM/PC image)  
電池充放電原位分析 (In-situ Raman)



## UTA Lithography

無光罩曝光 (Maskless)  
自由繪製圖型 (Pattern design easily)  
微米等級線寬 (Micron line width)



訂製二維材料, 粉體/晶體/薄膜  
石墨烯/奈米碳管/TMDC/MXene  
二維材料轉印  
二維材料轉印設備 E1-T



# Acknowledgments



國立陽明交通大學  
NATIONAL YANG MING CHIAO TUNG UNIVERSITY



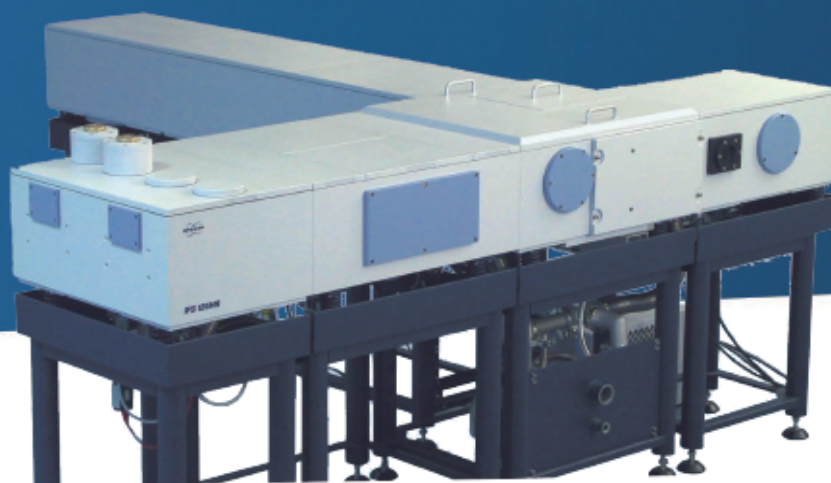
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FT-IR Research SPECTROMETER

# VERTEX 80v IFS 125HR



## VERTEX 80v

The VERTEX 80 and VERTEX 80v spectrometers are the high-end research instruments in the VERTEX series. Their innovative optics design results in the most powerful bench top purge and vacuum spectrometers available. They offer broadest spectral range from the UV/VIS region ( $50000\text{ cm}^{-1}$ ) to the FIR/THz region ( $5\text{ cm}^{-1}$ ), highest spectral and temporal resolution and an unmatched level of flexibility. The versatile VERTEX 80/80v systems provide with their PEAK technology the right solution for all high-end research applications.

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VERTEX 80v



IFS 125HR