

# Molecules as probes of activity in obscured luminous galaxies

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Chemistry of the molecular interstellar medium (ISM) can be used to distinguish between AGN and starburst-driven activity in heavily extinguished nuclei. It is a potentially powerful tool to help track evolution of activity, probing the interplay between activity and ISM properties and to explore the starburst-AGN relation. For example, the chemistry of the ISM near an intense X-ray source such as an AGN (an XDR, X-ray Dominated Region) is expected to show a different chemical signature than that of an evolved starburst characterized by PDRs (Photon Dominated Regions). Young star formation dominated by dense, warm and shielded gas will have properties different from both XDRs and PDRs.

Interpreting extragalactic mm- and sub-mm molecular line emission involves disentangling excitation and radiative transfer effects (e.g. optical depth, radiative excitation, absorption) from those of chemistry. As an example of the challenges and rewards of studies of the molecular ISM of luminous galaxies I will discuss the prototypical ULIRG (Ultra Luminous IR Galaxy) Arp220 and observations/models of HNC, HCO<sup>+</sup> and H<sub>3</sub><sup>+</sup>O. Furthermore, the unusually luminous HC<sub>3</sub>N line emission towards the IR-bright, but otherwise inconspicuous, S0 galaxy NGC4418 (Fig. 1) will be discussed. Herschel studies of IR-luminous galaxies will be presented as well as a recent 3-mm line survey carried out with the IRAM 30m EMIR instrument.

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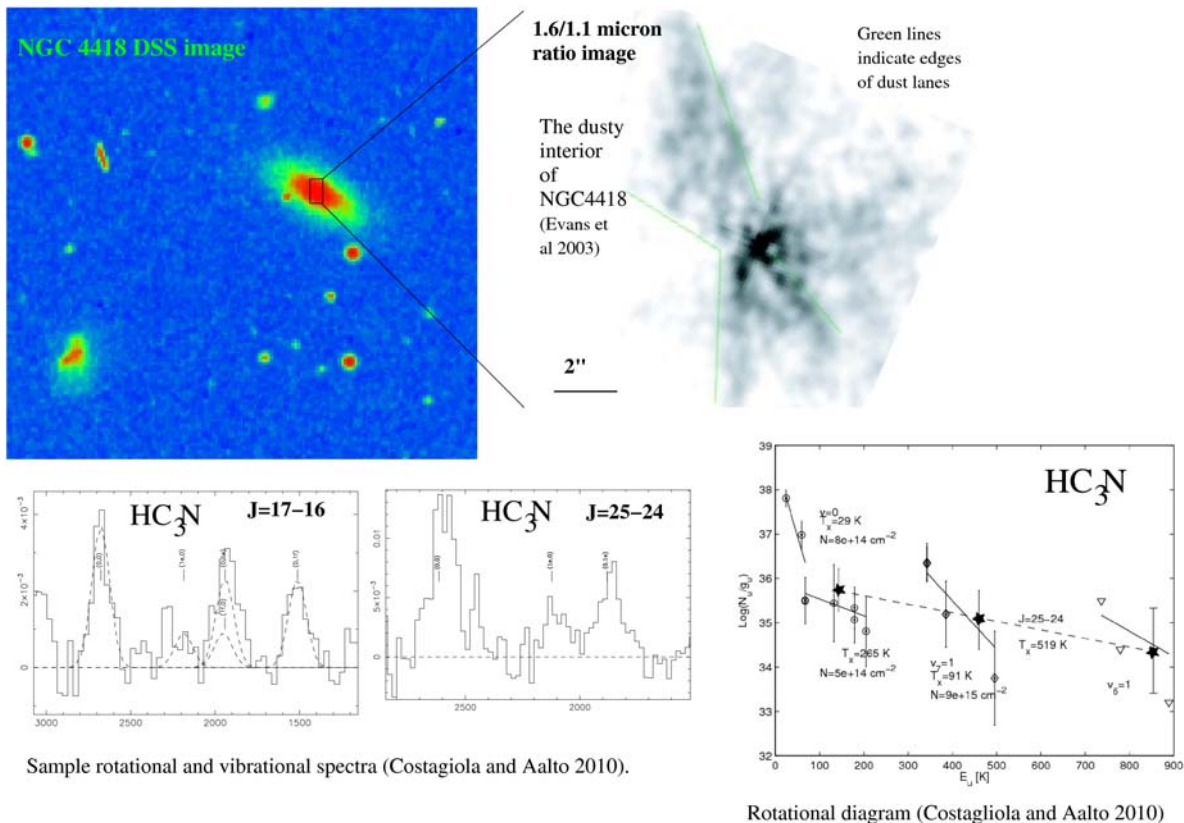


Figure 1: Sample HC<sub>3</sub>N spectra and rotational diagram of NGC4418. Note the prominent vibrational lines and the multiple temperature components in the rotational diagram.

## AKARI observations of ice absorption bands towards edge-on YSOs

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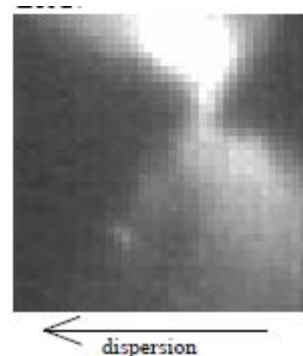
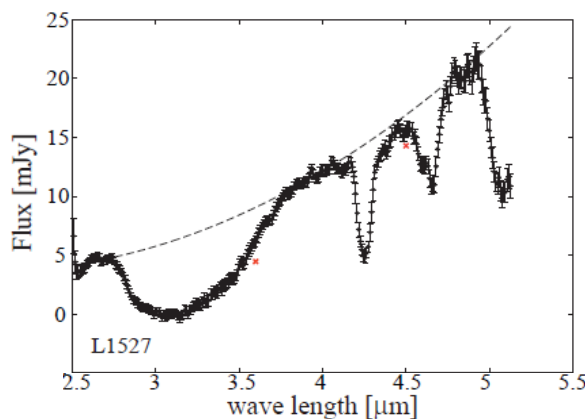
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Circumstellar disks and envelopes of low-mass young stellar objects (YSOs) contain significant amount of ice. Such icy material will evolve to be volatile components of planetary systems, such as comets in our solar system. In order to investigate the composition and evolution of circumstellar ice of low-mass YSOs, we have observed ice absorption bands at near infrared (NIR) towards 8 YSOs ranging from class 0 to class II, among which 7 are associated with edge-on disks.

Slit-less spectroscopic observations are performed using grism mode of Infrared Camera (IRC) on board AKARI, which enables us to obtain full NIR spectra from 2.5  $\mu\text{m}$  to 5  $\mu\text{m}$ , including the CO<sub>2</sub> band and blue wing of the H<sub>2</sub>O band, which are not accessible from the ground. We developed procedures to reduce the spectra of targets with nebulosity. The spectra are fitted by the polynomial to derive the absorption spectrum, which then is fitted by the laboratory database of ice absorption bands considering the instrumental line profile and spectrum resolution of the grism.

Towards the Class 0-I sources, absorption bands of H<sub>2</sub>O, CO<sub>2</sub>, CO and XCN are clearly detected. Column density ratios of CO<sub>2</sub> ice and CO ice relative to H<sub>2</sub>O ice are 15-28 % and 13-46 %, respectively. If XCN is OCN<sup>-</sup>, its column density is as high as 2-6 % relative to H<sub>2</sub>O ice. Weak features of <sup>13</sup>CO<sub>2</sub>, HDO, C-H band, and gaseous CO are detected as well. OCS ice absorption is detected towards IRC-L1041-2. Towards class II stars, H<sub>2</sub>O ice band is detected. We also detected H<sub>2</sub>O ice, CO<sub>2</sub> ice and tentative CO gas features of the foreground component of class II stars.



# Spectral Lines of Carbon Chain Molecules in a Star Forming Region L1527 between 29 and 90 GHz

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We have studied molecular spectral lines of carbon chain molecules in a star forming region L1527 between 29 and 90 GHz by using the 45m telescope of the Nobeyama Radio Observatory (NRO). H<sub>2</sub>CCO, HCCCHO, SO and isotopic species of HCN and HC<sub>3</sub>N have been detected for the first time in L1527.

Using integrated intensities of the detected rotational lines of  $J_{Ka,Kc} = 4_{0,4}-3_{0,3}$ ,  $4_{1,4}-3_{1,3}$  and  $4_{1,3}-3_{1,2}$  of H<sub>2</sub>CCO, column densities of ortho and para H<sub>2</sub>CCO were estimated to be  $3.8 \times 10^{12}$  and  $2.0 \times 10^{12}$  cm<sup>-2</sup>, respectively, with an assumption of an excitation temperature of 12.3 K [1a]. These values give an ortho to para ratio of 1.8(-0.1, +0.7) which is less than the ortho to para ratio of 3.0 at the high temperature limit. The small ratio might suggest that H<sub>2</sub>CCO in L1527 comes off from the grain surfaces.

Column densities of HC<sup>13</sup>CCN and HCC<sup>13</sup>CN were obtained based on the assumption of the excitation temperature of 12.3 K [1a] as shown in Table 1. Isotopic ratios, [Normal Species]/[<sup>13</sup>C Species], were derived from a comparison with the reported column density of the normal species HC<sub>3</sub>N [1b]. Since the isotopic ratios in L1527 were similar to those in TMC-1 [2], the chemical reaction producing HC<sub>3</sub>N in L1527 can be similar to those suggested in TMC-1 as follows [2]:

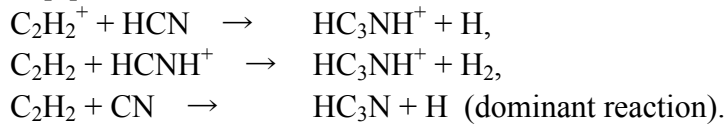


Table 1: Column densities and isotopic ratios of HC<sub>3</sub>N in TMC-1 and L1527

Isotopic Species	Column Density(cm <sup>-2</sup> )	[Normal Species]/[ <sup>13</sup> C Species]
TMC-1 [2]		
H <sup>13</sup> CCCN	$(2.0 \pm 0.2) \times 10^{12}$	$79 \pm 11$
HC <sup>13</sup> CCN	$(2.1 \pm 0.2) \times 10^{12}$	$75 \pm 10$
HCC <sup>13</sup> CN	$(2.9 \pm 0.3) \times 10^{12}$	$55 \pm 7$
L1527		
H <sup>13</sup> CCCN	-	-
HC <sup>13</sup> CCN	$3.3 \times 10^{11}$	$80 \pm 6$
HCC <sup>13</sup> CN	$5.8 \times 10^{11}$	$50 \pm 4$

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# **The mesoscale morphologies of ice films: Porous and biomorphic forms of ice under astrophysical conditions**

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I present the results of experiments in which we grow submicrometer- to millimeter-thick ice films at temperatures of 6 to 220 K at low pressures in situ in a cryo environmental scanning electron microscope. We find that ice films show pronounced morphologies at the mesoscale similar to those previously described in films of ceramics, semiconductors, and metals; materials with quite different material properties to ice. Our experiments are aimed at revealing the mesoscale morphologies of amorphous and crystalline ice with regard to astrophysical environments, as the conditions in which the ice films grow in our experiments are those under which exists most extraterrestrial ice. The porosity on the mesoscale of many of the morphologies is notable in this regard; a further intriguing finding is that these ice films can emulate biological forms.

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# UV/EUV photolysis of polar and nonpolar molecules' effect on methane containing ice mixture

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UV/EUV photolysis of  $N_2+CH_4$ ,  $H_2O+CH_4$  and  $N_2+CH_4+H_2O$  ice mixtures at 17K have been investigated in this work. IR spectra show that  $C_2H_6$  and  $C_3H_8$  production yields are slower in nonpolar molecule ( $N_2$ ) containing ice mixtures, and lots of H atoms dissociated from  $CH_4$  molecules will recombine with CCCN molecules to form HNCCC in  $N_2+CH_4$  ice mixture. That makes the absorbance feature of HNCCC at  $2205\text{ cm}^{-1}$  is stronger than CCCN at  $2194\text{ cm}^{-1}$ [1]. Besides, all CCN bearing molecules which were formed via UV/EUV photolysis of  $N_2+CH_4$  ice mixture converted into  $OCN^-$  while polar molecule ( $H_2O$ ) was the starting component of ice mixture. This result shows that CN bearing molecules prefer to interact with OH radical to form HNCO and subsequently interacts with  $H_2O$  to form  $OCN^-$ .

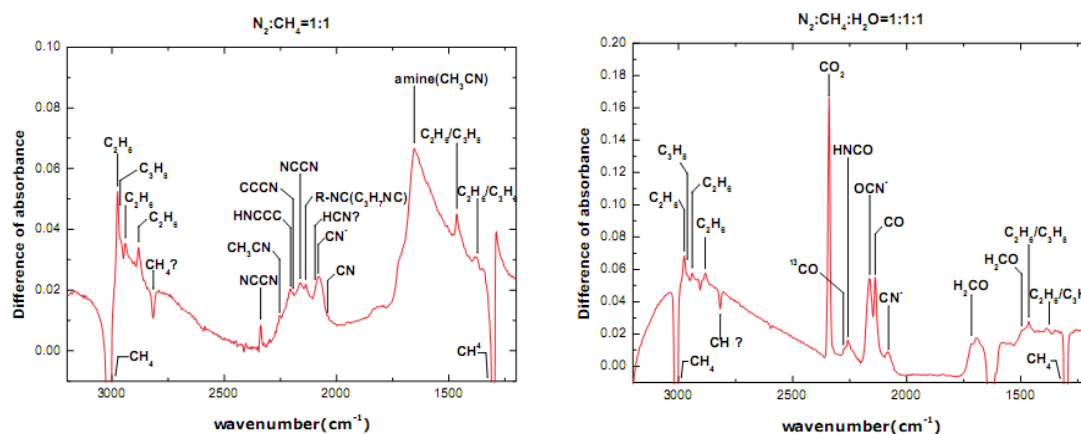


Figure 1: IR spectra of  $N_2:CH_4= 1:1$  and  $N_2:CH_4:H_2O = 1:1:1$  after UV/EUV irradiation.

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## HOCO<sup>+</sup> toward Sgr B2 Complex

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A number of rotational lines of protonated carbon dioxide, HOCO<sup>+</sup>, have been observed mostly at frequencies above 80 GHz in interstellar clouds. In this conference, we report the identification of the lowest rotational transition 101-000 of HOCO<sup>+</sup> at 21.383 GHz toward Sgr B2, and a detection of emission of the next lowest transition 202-101 at 42.766 GHz toward GCM0.77-0.06, using the Nobeyama 45m telescope.

Protonated carbon dioxide (HOCO<sup>+</sup>) has been identified in interstellar clouds since 1981 [1]. Although millimeter-wave thermal lines of this molecule are considerably weak and difficult to detect in general, they are found in a few different environments in the Galaxy, for example, toward the translucent clouds [2], in the Galactic Center [3], and toward a low-mass protostar [4], and moreover, toward the center of the galaxy NGC 253 [5]. This molecular ion can be used as a measure of the abundance of CO<sub>2</sub> which is not observable directly at radio wavelengths.

Several years ago, we have identified the weak thermal line U42.767 seen toward the Galactic Center to the HOCO<sup>+</sup> 202-101 transition, and made a map of this thermal line in the 30' x 30' area of Sgr A\* [6]. Because the frequency of this transition is close to the frequency of the SiO v=2 J=1-0 transition (42.821 GHz), so that the observations can simultaneously be made with SiO maser surveys with the Nobeyama 45-m telescope [7,8].

No observation of the lowest rotational transition 101-000 of HOCO<sup>+</sup> has been reported till today, because the line is severely blended with a recombination line H67alpha at 21.386 GHz. We reanalyzed the spectral line data toward Sgr B2 complex at this frequency, which were taken using Nobeyama 45m telescope in 2004 and were archived. Subtracting the averaged line profile of H66alpha and H68alpha from the H67alpha profile, we obtained the difference spectrum, which shows a clear emission of the 101-000 transition of HOCO<sup>+</sup>. We also report the detection of unexpectedly strong HOCO<sup>+</sup> emission toward the Galactic Center molecular cloud GCM0.77-0.06 at 42.766 GHz.

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# A hybrid moment equation approach to gas-grain chemistry

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Complementary to the gas phase chemistry, chemical processes happening on the grain surfaces are important for the overall interstellar matter repository. Due to their discrete and stochastic nature, however, usually surface chemistry cannot be accurately modeled by the rate equations. Various methods have been proposed, including the modified rate equation approach (Caselli et al. 1998; Garrod 2008), master equation approach with cutoff (Stantcheva et al. 2002), moment equation approach with cutoff (Lipshtat and Biham 2003; Barzel and Biham 2007), multiplane approach (Barzel et al. 2007), and the exact Monte Carlo approach (Vasyunin et al. 2009). The Monte Carlo approach would produce the most accurate results if it is repeated for many times; however, it is computationally heavy, and eventually impractical when a large chemical network is being modeled. On the other hand, a consistent and automatic algorithm is needed to handle a generic system in which both the gas phase and grain surface processes are included. In the present work, we propose a moment equation approach in which the generating function machinery is used to generate the equations automatically (up to any prescribed order), and a cut-off-and-switch scheme is implemented to approximate the infinite system of equations. Comparisons are made between the results of this method and those from the exact Monte Carlo simulations for several commonly used systems. The agreement is usually satisfactory, while the speed of our method is not much slower than the rate equation approach. Further issues include the numerical stability of this method (when higher order moments are included), how to control the errors quantitatively, and how to select those mostly needed terms to limit the number of variables and lower the computational burden.

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## Near-Infrared Image of Circular Polarization in the Orion Nebula

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We report a wide image of circular polarization (CP) in the Orion nebula. Near infrared circular polarimetry of the nebula was conducted using the SIRIUS camera [1] and its polarimeter (SIRPOL) on the 1.4-m IRSF telescope at the South African Astronomical Observatory.

The CP image in the  $K_s$  band (2.14  $\mu\text{m}$ ) reveals that a high CP region is spatially extended ( $\sim 0.4$  pc) around the massive star-forming region, the Orion Becklin-Neugebauer(BN)/Kleinman-Low(KL) nebula [2]. The degrees of CP range from +17% to  $-5\%$ . On the other hand, other regions, including the linearly polarized Orion bar, show no significant CP, in contrast with the linear polarization (LP) image [3].

The detected degrees of CP are the highest among the previously observed young stellar objects (YSOs). To explore the production mechanism of CP in a YSO, we investigate correlations of CP, LP, and  $H - K_s$  color, in the BN/KL region from the obtained images [4].  $H - K_s$  color representing extinction is well correlated with CP. We derive a simple relation between dichroic extinction, color excess, CP, and LP, assuming a model for a YSO with aligned non-spherical dust grains. The observed correlation between the Stokes parameters and the color excess agrees with the derived relation, and suggests a major contribution of dichroic extinction to the production of CP in this region.

From the viewpoint of astrobiology, our results also provide the implication for the origin of the terrestrial life. The terrestrial living material consists almost exclusively of one enantiomer, left-handed amino acids and right-handed sugars. The origin of biomolecular homochirality is a longstanding mystery that is critical to understanding the origin and development of life. Our result reveals that the significant CP extends over a region  $\sim 400$  times the size of the solar system [2]. If our solar system formed in a massive star-forming region like the Orion nebula and was irradiated by CP radiation, then enantiomeric excesses could have been induced, through asymmetric photochemistry, in the parent bodies of the meteorites. These would be subsequently delivered to Earth, and could then have played a role in the development of biological homochirality on Earth.

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## Carbon Isotope and Isotopomer Fractionation in Cold Dense Cloud Cores

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<sup>13</sup>C should be useful to investigate chemistry of carbon bearing species. Recent observations in TMC-1 indicated that the molecular abundances of carbon isotopomers are different. Takano et al. (1998) observed HC<sub>3</sub>N and found HCC<sup>13</sup>CN is more abundant than HC<sup>13</sup>CCN and H<sup>13</sup>CCCN, which indicates three carbon atoms are not equivalent in HC<sub>3</sub>N. Sakai et al. (2007; 2010) reported the abundance ratios of C<sup>13</sup>CS/<sup>13</sup>CCS = 4.2 and CCH/<sup>13</sup>CCH = 1.6. Again, these results indicate two carbon atoms are not equivalent in CCS and CCH. They pointed out there are two possible processes to cause these fractionation: (i) the formation path ways of the species and (ii) the exchange of the <sup>13</sup>C position after formation of molecules by isotopomer-exchange reactions.

We construct the gas-grain chemical network model which includes carbon isotopes (<sup>12</sup>C and <sup>13</sup>C). Temporal variations of molecular abundances, the carbon isotope ratios (<sup>12</sup>CX/<sup>13</sup>CX) and the isotopomer ratios (<sup>12</sup>C<sup>13</sup>CX/<sup>13</sup>C<sup>12</sup>CX) of CCH and CCS in cold dense cloud cores are investigated by numerical calculations.

We reproduce the observed C<sup>13</sup>CH/<sup>13</sup>CCH ratio in TMC-1; isotopomer-exchange reaction, <sup>13</sup>CCH + H → C<sup>13</sup>CH + H. However, the C<sup>13</sup>CS/<sup>13</sup>CCS ratio is lower than observed in TMC-1. We propose the isotopomer-exchange reaction, <sup>13</sup>CCS + H → C<sup>13</sup>CS + H + 15K. In the model with this reaction, we reproduce the observed C<sup>13</sup>CS/<sup>13</sup>CCS, CCS/C<sup>13</sup>CS and CCS/<sup>13</sup>CCS ratio simultaneously.

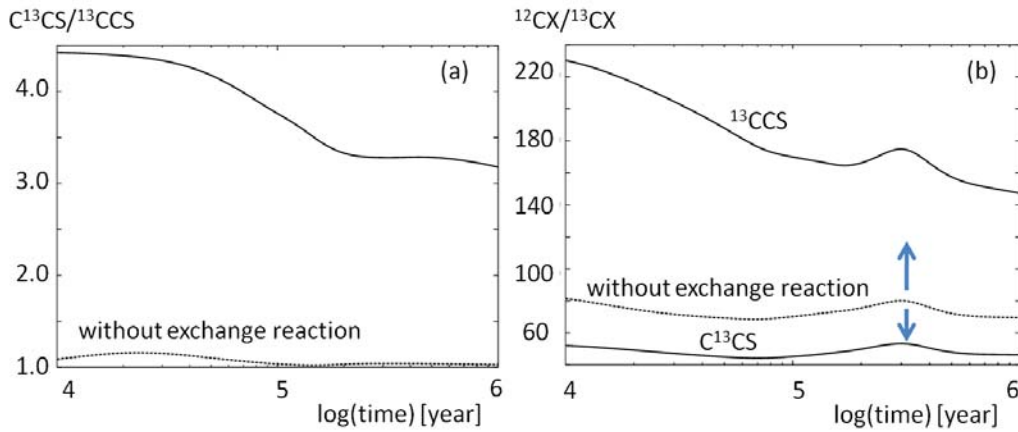


Figure 1: Temporal variation of (a) isotopomer ratios: the C<sup>13</sup>CS/<sup>13</sup>CCS ratio and (b) isotope ratios of CCS: the CCS/<sup>13</sup>CCS and CCS/C<sup>13</sup>CS ratios. Solid lines show ratios in the model with the reaction, <sup>13</sup>CCS + H → C<sup>13</sup>CS + H + 15K. Dashed line shows the isotope ratio of CCS in the model without the reaction. The density is n<sub>H</sub> = 10<sup>5</sup> cm<sup>-3</sup>.

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## Dissociative Recombination and the build-up of complex molecules in the Interstellar Medium

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methanol, ethanol, dimethyl ether and formic acid are produced in the gas-phase or on grain surfaces. As gas-gas production pathways very often ion-neutral reactions leading to the protonated form of the species followed by dissociative recombination to yield the final product have been invoked.

In the case of methanol, a feasible gas-phase production process is unlikely. The rate of radiative association of  $\text{CH}_3^+$  and  $\text{H}_2\text{O}$  leading to  $\text{CH}_3\text{OH}_2^+$  has been found to be far too low to explain the observed methanol abundances [1] and, on top of that, only a minor fraction of methanol (3 %) is produced in the dissociative recombination of the latter ion [2]. Introduction of these new findings into state-of-the-art model calculations of dark clouds yielded that the proposed gas-phase mechanism is by far insufficient to explain the observed methanol abundances. On the other hand, successive hydrogenation of CO on icy grain surface by H atoms has been found to produce methanol [3].

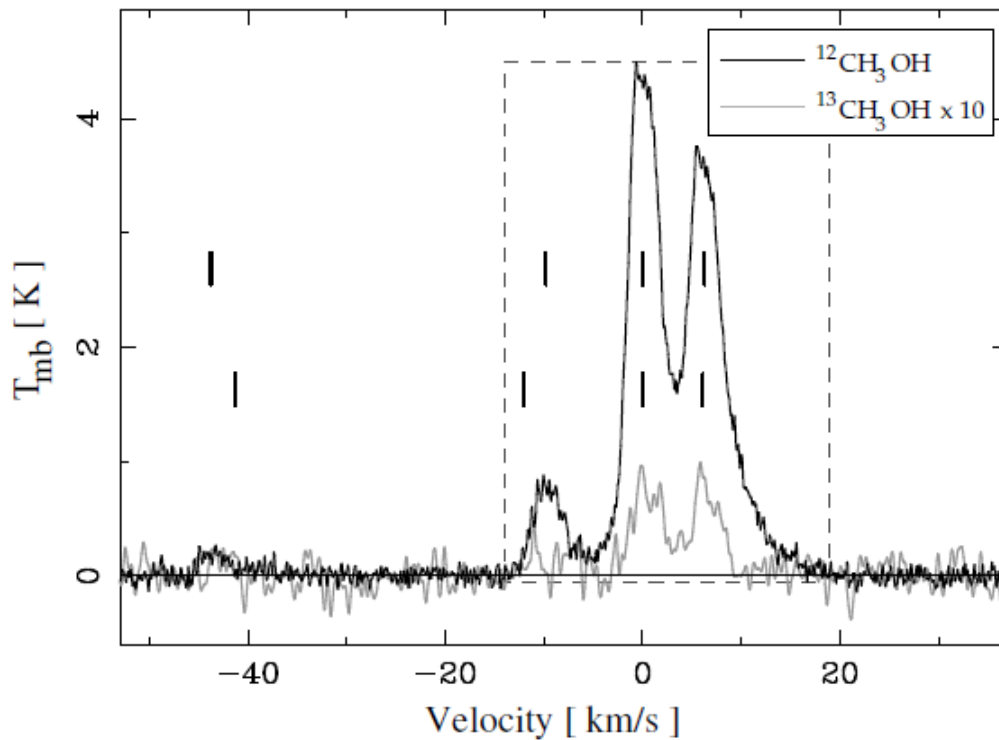


Figure 1: Spectra of the 2-1 rotational line group of  $^{13}\text{CH}_3\text{OH}$  (black) and  $^{12}\text{CH}_3\text{OH}$  (gray) around 96 GHz

It now remains to be proven by direct observation that interstellar methanol really originates from grain surfaces. This can be done by the so-called, isotope labelling a posteriori, which was first suggested by Charnley et al. [4]. The method is based on the fact that  $^{13}\text{C}$  is preferably accumulated in CO at low temperature, which in turn results in a  $^{13}\text{C}$  deficiency in other molecules forming from ion-neutral reactions in the gas-phase [5]). Assuming that this selective fractionation remains unaltered by the processes of adsorption and desorption, the  $^{12}\text{C}/^{13}\text{C}$  ratio in various molecules could be used to distinguish between formation from CO on cold grains and gas-phase formation.

We therefore performed observations of the  $^{12}\text{C}/^{13}\text{C}$  ratio for  $\text{C}^{18}\text{O}$  and methanol in several massive young stellar objects, one pair of compact HII regions and one source hosting several young stellar objects. The 2-1 rotational line groups of the 2 isotopomers around 96 GHz were observed using the 20m telescope at Onsala Space Observatory. (see Fig. 1). With one exception (where the  $^{12}\text{C}$  molecule lines are very probably optically thick) the agreement of the  $^{12}\text{C}/^{13}\text{C}$  ratio on the two compounds is excellent. This points to a surface origin of interstellar methanol, which is also corroborated by the fact that a strong correlation of abundances between methanol and formaldehyde has been found in several star-forming regions [6].

Furthermore, the role of dissociative recombination in the formation of other, more complex molecules detected in star-forming regions like ethanol, dimethyl ether and ethanol will be discussed.

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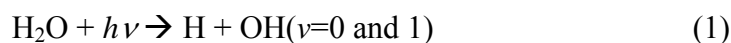
## Formation of oxygen molecules following vacuum ultraviolet photodissociation of amorphous solid water

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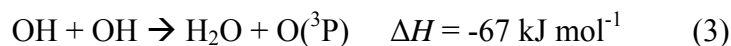
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The effect of radiation on water ice has intrigued many scientists in the fields of interstellar chemistry and planetary ice science as well as reaction dynamics, since water is the predominant component of interstellar icy grain mantles in dense molecular clouds and small solar system bodies such as comets. Oxygen molecule is known to be a product when water ice is irradiated with photons, electrons, or with energetic ions. These experimental studies indicate that VUV photodissociation of amorphous solid water (ASW) leads to secondary reactions that result in molecular oxygen formation on or in ASW. Photodissociation of H<sub>2</sub>O in the first absorption band of water ice (130–165 nm) involves mainly two primary processes.



For the electronically ground O(<sup>3</sup>P) production, two different formation mechanisms were proposed: the exothermic recombination reaction of OH, and the photodissociation of OH on the ASW surface.[1]



From the fact that OH( $\nu=0$  and 1) and O(<sup>3</sup>P) are formed with large excess energy via reactions (1), (3) and (4), O<sub>2</sub>(X<sup>3</sup>Σ<sub>g</sub><sup>-</sup>) and O<sub>2</sub>(a<sup>1</sup>Δ<sub>g</sub>) can be produced via subsequent reactions (5) and (6) in the 157 nm photolysis of ASW.[2]



Measurements of the translational and internal energy distributions of the photoproducts generated from photodissociation of ASW allow assessment of possible secondary reactions on/in ASW from reaction dynamics point of view. In the present work, we have investigated the kinetic and internal energy distributions of O<sub>2</sub>(X<sup>3</sup>Σ<sub>g</sub><sup>-</sup>,  $\nu=0$ ) and O<sub>2</sub>(a<sup>1</sup>Δ<sub>g</sub>,  $\nu=0$ ) following 157 nm photodissociation of ASW at 90 K using the resonance-enhanced multiphoton-ionization (REMPI) method.[3]

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# Modeling Chemistry in the Accretion Disk of an Active Galactic Nucleus

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Understanding the processes of galaxy formation, mass accretion onto a supermassive black hole and its connection to star formation are of great interest in astrophysics. It is useful to know the condition of the interstellar medium in different types of galaxies such as ultra-luminous infrared galaxies (ULIRGs), active galactic nuclei (AGN), and starburst galaxies. Some molecules have been proposed as probes of AGN/starburst activity in galaxies. For example, Kohno [1] found that a higher  $\text{HCO}^+/\text{HCN}$  intensity ratio is favored in starburst galaxies than in AGN-dominant galaxies. Enhanced HCN and CN intensity and abundances are observed in AGN-dominant galaxies. A higher HCN abundance and some complex molecules are observed in ULIRGs [2][3].

We model the chemistry in the molecular disk around an AGN using the condition of NGC 1068. We include the ionization by X-rays from the AGN core, cosmic-rays from the supernovae and stellar winds. The effect of UV-photons is also discussed. We used the OSU high temperature chemical network [4]. X-ray penetration is dependent on the disk structure, and we tried to vary this structure. In most cases, the effect of X-rays at radii  $>10\text{pc}$  can produce slightly less than the observed abundance of CN over the total hydrogen, which is  $(0.2-1) \times 10^{-7}$  at the 70 pc scale[5]. The HCN abundance is enhanced with high temperature in the inner disk, and our results produce equal to or more than the value suggested by Usero et al., which is  $(0.8-1) \times 10^{-7}$ [6]. If there is a dense midplane that X-rays cannot penetrate into, complex molecules such as  $\text{C}_2\text{H}_2$  and  $\text{HC}_3\text{N}$ , are enhanced at the very inner part of the AGN-disk due to the high temperature. The advent of ALMA will resolve some of these molecules in higher resolution and may provide useful information on the disk structure and the star-formation activities.

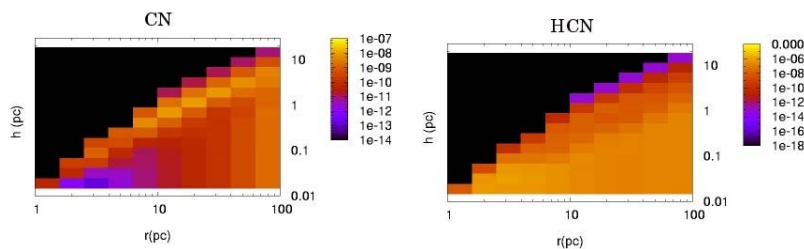


Figure 1: The fractional abundances of CN and HCN at different radius and height from the AGN core are shown.

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## Some Early Results from the HIFI Instrument on the *Herschel Space Observatory*

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*The Herschel Space Observatory* was sent into orbit in May 2009 in order to study the sky in the submillimeter-wave and far infrared. The observatory is now orbiting the earth at the so-called second Lagrangian point (L2) of the Earth-Sun system. The 3.5-meter dish sends radiation to three detectors, one of which is a high spectral-resolution spectrometer known as HIFI (Heterodyne Instrument for the Far Infrared), while the other two – PACS (Photoconductor Array Camera and Spectrometer) and SPIRE (Spectral and Photometric Imaging Receiver) – are cameras and imaging spectrometers. HIFI operates in 6 bands, ranging from 480 GHz to over 1900 GHz in frequency. The first period of observations was devoted to 7 Key Programs, which had been selected before launch and involved many astronomers and astrochemists, such as myself. Currently, proposals have been submitted for the first open-time portion of the mission (OT1), with each proposal having a team of perhaps 10 people, far smaller than the make-up of the Key Program groups.

Molecular observations using HIFI consist of both emission and absorption line studies. At the higher frequencies accessible to HIFI, critical densities for emission can be very large, and so absorption becomes competitive as long as there is a continuum to absorb. Emission lines have been detected from the usual suspects, especially hot cores rich in weeds such as methyl formate. Interestingly though, the density of lines is lower than seen at millimeter-wave frequencies. Even in Orion KL, absorption can be seen against the quasi-continuum emission. The absorption lines include those of HF, and two most improbable ions OH<sup>+</sup> and H<sub>2</sub>O<sup>+</sup>, which are known to react with abundant H<sub>2</sub> on every collision. Models explaining their existence indicate that the matter is in a most violent state.

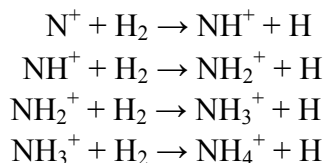
For continuum sources more distant than Orion, such as the galactic center, absorption is present both from cooler portions of the primary source and from diffuse matter in the spiral arms between the galactic center and us. In fact, there can be so many sources that the absorption spectra need not be resolved. Absorption studies of the spiral arm clouds show CH<sup>+</sup>, CH, CN, CCH, HCO<sup>+</sup>, HF, OH<sup>+</sup>, H<sub>2</sub>O<sup>+</sup>, and H<sub>3</sub>O<sup>+</sup>; here, though, it is somewhat easier to understand the presence of the two strange ions if H  $\gg$  H<sub>2</sub> in abundance. A new molecule detected is protonated HCl, or H<sub>2</sub>Cl<sup>+</sup>, although the density of its environment is unclear. Although water is a prosaic molecule, its detection and study are clearly important for astrobiological considerations. Deuterated isotopomers seen in the spiral arm clouds include ND and D<sub>2</sub>O. Although detailed gas-grain PDR models have not yet been run, it is difficult to understand the high abundance of ammonia without including surface chemistry. From the measurement of diverse ortho/para ratios for H<sub>2</sub>O, H<sub>2</sub>O<sup>+</sup>, D<sub>2</sub>O, and NH<sub>3</sub>, astrochemists hope to understand the physical conditions better, although the analysis of ortho/para ratios is itself a source of much debate. These and other important studies in old stars and external galaxies will be discussed as time permits.

# Ammonia formation by the successive hydrogenation of N atom trapped solid N<sub>2</sub> at low temperature

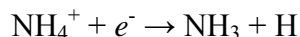
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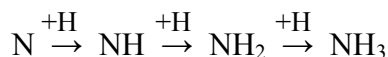
A high abundance of ammonia molecules (NH<sub>3</sub>) has been observed in the gas phase but also solid phase in molecular clouds. In the gas phase reaction, the combination process of the successive H atom abstraction reactions



and the dissociative recombination reaction



has been proposed as the formation process of NH<sub>3</sub>. However, it was indicated that this process is inefficient especially in cold molecular clouds [1], because the first abstraction reaction were reported to be the endothermic reaction [2,3]. In the gas-grain reactions, the successive hydrogenation of N atom



has been proposed. Since the grain (solid) surface performs as the third body and adsorbs excess energy of the chemical reactions, these simple addition reactions can proceed. In addition, these reactions are predicted to be fast reactions due to the radical-radical reaction. Thus, it has been expected that the high abundance of NH<sub>3</sub> requires the synthesis on the grain surfaces. However, the formation of NH<sub>3</sub> by the surface reactions has been little conducted quantitatively.

We performed the experiments of the NH<sub>3</sub> formation by the H atoms exposure of N atoms in solid N<sub>2</sub> at 10 K. The formed NH<sub>3</sub> was observed by the Fourier transform infrared absorption spectrometry. We will discuss the formation mechanism of NH<sub>3</sub> on/in solid N<sub>2</sub> at low temperature.

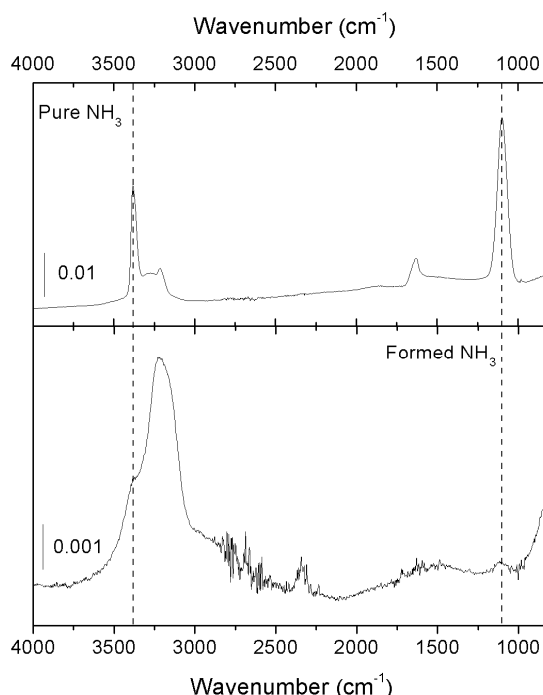


Figure 1: (top) Infrared absorption spectra for reference of solid NH<sub>3</sub> at 10 K. (bottom) Absorption spectra of the formed NH<sub>3</sub> by the H atoms exposure of N atoms in solid N<sub>2</sub> at 10 K. Dashed lines indicate the identified absorption bands of NH<sub>3</sub>.

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## Extremely high-velocity HCN emission from L1448C

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A class 0 protostar L1448C was mapped with the SMA in the HCN J=4–3, CS J=7–6, HCO<sup>+</sup> J=4–3, SO J<sub>K</sub>=8<sub>8</sub>–7<sub>7</sub>, and <sup>29</sup>SiO J=8–7 lines at an angular resolution of 2 arcsecond. The HCN, CS and HCO<sup>+</sup> emission mainly comes from three regions; one is centered at the position of the northern protostar L1448C(N), the second one is around the position of another protostellar source L1448C(S), and the third one is at ~7" south of L1448C(S).

The HCN spectra observed around L1448C(N) show broad wings that extends to  $\pm 30$  km s<sup>-1</sup> from the cloud systemic velocity and separate secondary peaks at extremely high velocities (EHV) of  $\pm 50$  km s<sup>-1</sup>. The terminal velocity of the EHV HCN emission is comparable to those of the SiO J=8–7 and CO J=3–2 [1]. However, the EHV HCN emission is localized on the compact region of  $\pm 2$ " from the protostar, and does not show the elongated jet-like morphology. The EHV emission is also shown in the SO and <sup>29</sup>SiO lines. The spatial distributions of the EHV emission in these lines are elongated along the jet axis, suggesting that these components are the dense part of the jet at the base. The CS and HCO<sup>+</sup> lines are much narrower than the HCN line, and show no hint of EHV component.

The HCN line observed near L1448C(S) shows a steep edge at the cloud systemic velocity and a broad redshifted wing that extends to  $+60$  km s<sup>-1</sup>. This line profile strongly suggest that the dynamical interaction between the energetic outflow from L1448C(N) and dense gas envelope around L1448C(S). The SO and <sup>29</sup>SiO lines observed here exhibit EHV component at  $+60$  km s<sup>-1</sup> without lower velocity wing component, suggesting that the emission of these lines arises from the jet impacting on the dense gas. On the other hand, the CS and HCO<sup>+</sup> lines exhibit narrow line width of  $\sim 2$  km s<sup>-1</sup> centered at the systemic velocity, and are likely to come from the L1448C(S) envelope.

The third component at ~7" south of L1448C(S) is seen in the maps of HCN, CS, and HCO<sup>+</sup>. As in the case of the L1448C(S) component, this component appears near the cloud systemic velocity in the CS and HCO<sup>+</sup>, while at  $\sim 10$  km s<sup>-1</sup> redshifted velocity in the HCN.

Our results suggest that the HCN emission is significantly enhanced in the regions where the energetic jet traced by the SO and <sup>29</sup>SiO lines impacts on the dense ambient gas observed in the CS and HCO<sup>+</sup> lines. The origin of the compact EHV HCN component might be the strong shocks in the jet beam at the base.

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# Computational Molecular Spectroscopy: Fe-containing Molecules of Astrochemical Interest

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Although Fe is known to have a large cosmic abundance comparable to those of Mg and Si, the only iron-containing molecules so far detected in the cosmic environment are FeH in sunspots [1] and FeO toward Sgr B2 [2,3]. In 1994, we made a preliminary *ab initio* calculation on FeCO as a candidate for observation in interstellar space [4], but attempts by Kasai *et al* to detect it in space failed [5,6]. Then we started *ab initio* calculations on several Fe-containing molecules of astrochemical interest, including FeC [7], FeN [8], FeS, FeCO, FeNC [9], FeCN [10], FeOH [11,12].

We discuss here the molecular properties of  $\tilde{X}^6\Delta$  FeNC,  $\tilde{X}^6\Delta$  FeCN, and  $\tilde{X}^6A'(^6\Delta)$  FeOH. The last two of these have not yet been observed spectroscopically, and hence the predicted spectra are shown in Fig. 1 and Fig. 2, respectively. The *ab initio* calculations are done at the level of MR-SDCI+ $Q+E_{\text{rel}}$ /[Roos ANO (Fe), aug-cc-pVQZ (C, N, O, H)].

The equilibrium structures of FeNC and FeCN are *linear*. The equilibrium structure of FeOH is *bent* with a barrier of 273  $\text{cm}^{-1}$  at linearity, which is just above the bending zero-point energy of 194  $\text{cm}^{-1}$ , so that  $\tilde{X}^6A'$  FeOH is a *quasi-linear* molecule. The geometrical constants of these molecules are given in Table 1.

The Fe atoms in these three molecules are bound to their ligands through an ionic bond, so that the bending potentials are shallow and give large amplitude bending motion. We have calculated ro-vibrationally averaged bond lengths for various

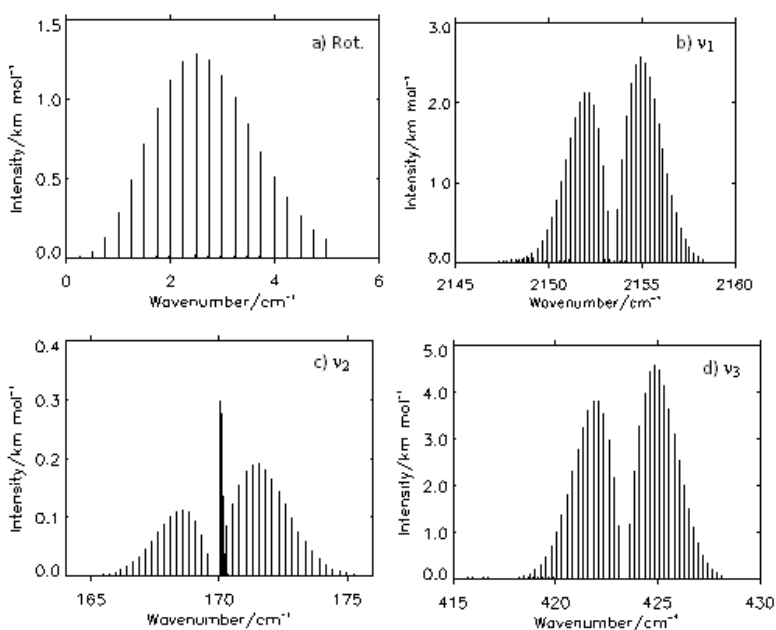


Fig. 1 Predicted spectra for the  $\tilde{X}^6\Delta$  FeCN: (a) rotation spectrum, (b)  $\nu_1$  (at 2153  $\text{cm}^{-1}$ ), (c)  $\nu_2$  (at 170  $\text{cm}^{-1}$ ), and (d)  $\nu_3$  (at 423  $\text{cm}^{-1}$ ), simulated at 12 K [10].

Table 1 *Ab initio* calculated molecular constants at the MR-SDCI+ $Q+E_{\text{rel}}$  level.

Molecule	$B_0$ / $\text{cm}^{-1}$	$10^8 D_J$ / $\text{cm}^{-1}$	$r_e(\text{M-ligand})$ / $\text{\AA}$	$r_e(\text{C-N})$ or $r_e(\text{O-H})$ / $\text{\AA}$	Bond angle /degrees	$\langle \hat{\rho} \rangle_0$ ( $\delta \hat{\rho}$ ) <sup>a)</sup> /degrees
$\tilde{X}^6\Delta$ FeNC <sup>b)</sup>	0.14274	4.84	1.9354	1.1823	180.0	13(7)
Exp. [13]	0.14447(13)		2.01(5), $r_0$	1.03(8), $r_0$	180.0	
$\tilde{X}^6\Delta$ FeCN <sup>c)</sup>	0.12380	4.12	2.0484	1.1681	180.0	10(5)
$\tilde{X}^6A'$ FeOH <sup>d)</sup>			1.8059	0.9520	134.2	39(14)

a) The bond angle deviation from linearity with quantum dynamical uncertainty in parentheses.

b) Ref. [9]. c) Ref. [10]. d) Refs. [11,12].

vibrational states as expectation values in terms of variational MORBID wavefunctions. The  $r_0$  structure and the bond angle supplement  $\langle\bar{\rho}\rangle_0$  (i.e. the angle deviation from linearity) thus determined are included in Table 1.

It should be noted that even for a linear molecule, whose equilibrium structure is linear, the ro-vibrationally averaged structure deviates substantially from linearity due to the large amplitude bending motion. It should also be noted that, for the quasi-linear molecule  $\tilde{X}^6A'$  FeOH, the  $\langle\bar{\rho}\rangle_0$  value is quite close to the equilibrium bond angle. Whether the molecule is linear or quasi-linear or bent can be distinguished by the Yamada-Winnewisser quasilinearity parameter  $\gamma_0$  [14],

$$\gamma_0 = 1 - 4 \times \frac{E(v_2=|l_2|=1) - E(v_2=|l_2|=0)}{E(v_2=2, |l_2|=0) - E(v_2=|l_2|=0)}$$

It was found that for the linear molecules FeNC and FeNC,  $\gamma_0 \approx -1.0$ , and for the quasi-linear molecule FeOH,  $\gamma_0 = 0.1$ . Thus, at the early stage of the analysis of the experimentally obtained infrared spectrum, one can identify the relevant molecule being linear, or quasi-linear, or bent.

Another molecule we consider here is FeCO. Many spectroscopic studies have been reported for  $\tilde{X}^3\Sigma^-$  FeCO (see ref. [15], for example), but none for  $a^5\Sigma^-$  FeCO. Our recent prediction at the MR-SDCI+ $Q+E_{rel}$ /[Roos ANO (Fe, C, O)] level for the  $a^5\Sigma^-$  FeCO is as follows. This is a linear molecule, with equilibrium structures  $r_e(\text{Fe-C}) = 1.843 \text{ \AA}$ ,  $r_e(\text{C-O}) = 1.153 \text{ \AA}$ ,  $\angle_e(\text{Fe-C-O}) = 180^\circ$ . The MORBID analysis gives ro-vibrationally averaged structures as  $r_0(\text{Fe-C}) = 1.845 \text{ \AA}$ ,  $r_0(\text{C-O}) = 1.157 \text{ \AA}$ , and  $\langle\bar{\rho}\rangle_0 = 9^\circ(4^\circ)$  with  $B_0 = 0.13422 \text{ cm}^{-1}$  (4023.7 MHz).  $\gamma_0 = -1.0$  as is expected for a *linear* molecule. We think that it would be worthwhile to characterize this molecule further spectroscopically and to search for it in interstellar space.

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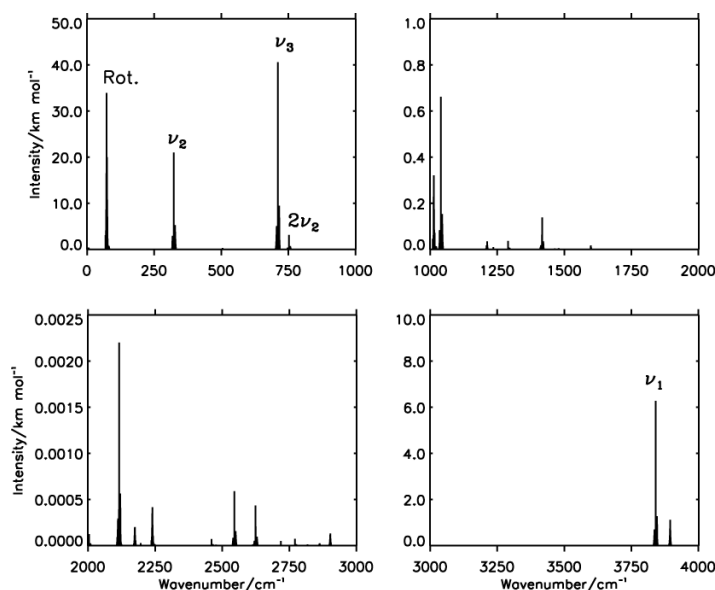


Fig. 2 Predicted spectra of the  ${}^6A'$  ( ${}^6\Delta$ ) FeOH Renner-degenerate states (at 10 K) [11].

## Far infrared imaging survey of the Chamaeleon region with AKARI: column density maps of molecular and atomic clouds resolving star forming cores

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Molecular clouds are the major form of interstellar matter in the Galaxy and are the birthplaces of stars. It is thought that molecular clouds are formed from atomic clouds, which have densities of  $\sim 1 - 10 \text{ cm}^{-3}$  and temperatures of  $\sim \text{several} \times 10 - 100 \text{ K}$ , through the phase transition process [1]. It is well known that the structures of molecular clouds are highly hierarchical. Especially, the scale of 0.1 pc “core”, in which gravitational collapse into a star occurs, is important for star formation. A recent study [2] reported that the core structures have been already determined in relatively tenuous ( $10^{+3} \text{ cm}^{-3}$ ) gas, strongly suggesting that the formation process of molecular cloud/core structures from atomic cloud is a key to understanding the origin of stars. Therefore, it is highly required to derive the column density distributions of molecular and atomic clouds with spatial resolutions high enough to resolve the cores. We carried out imaging observations toward the Chamaeleon star forming regions by Far-Infrared Surveyor (FIS) [3] onboard AKARI satellite. In the FIS bands of 60 - 160 microns we separate thermal radiation from cold ( $\sim 10 \text{ K}$ ) and warm (tens of kelvins) dust components associated with the molecular and atomic clouds, respectively. With the spatial resolutions in the FIS bands of 30 - 60 arcsec, we succeeded in the construction of the molecular/atomic column density maps, covering  $210 \text{ pc}^2$  with the linear resolution of 0.04 pc, which is enough to resolve the cores in the region (160 pc; [5]). There are five subregions named Cha I, II, III, Major Filament and Cha East [6]. Active star formations occur in Cha I and II, while little star formation is known in the other regions. We found a significant correlation between the star-formation activities and the ratio of the molecular to the atomic cloud mass among the subregions: the ratio is almost unity for Cha I and II, but is 0.5 for Cha III and 0.1 for the others. On the other hand, the column density histograms for the atomic components in the subregions are similar to each other and the upper end of the histograms are  $\sim 5-9 \times 10^{20} \text{ cm}^{-2}$ , corresponds to  $\sim 0.2-0.4 \text{ mag}$  for  $A_v$ . Considering that UV flux is responsible for molecular cloud formation, the observed low-extinction requires that the atomic component should be highly clumpy [6], and the core formation is probably related to the clumpiness of the atomic clouds.

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## Microwave spectroscopy of $^{13}\text{CH}_3\text{OH}$

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$\text{CH}_3\text{OH}$  is one of the most known interstellar molecules. As it is quite abundant, it is no doubt that its isotopologues are also good candidates as interstellar weeds. In this study, we carried out a microwave spectroscopic study of  $^{13}\text{CH}_3\text{OH}$ . Recommended rest frequencies based on the reviewed previous microwave results are compiled by Xu and Lovas. However, many experimental data are missing and the excited torsional state is limited up to the first excited state. We wish to supplement the experimental data and revise the analysis.

The microwave experiments below and above 40 GHz were carried out with conventional Stark- and source-modulation spectrometers, respectively at room temperature. Data up to 200 GHz and 215-225 GHz were accumulated without gaps. The bottom figure is an example of our spectrum in the 215 GHz region, showing assigned lines as well as unassigned lines.

Analysis has been done with RAM Hamiltonian. The detailed molecular constants will be reported.

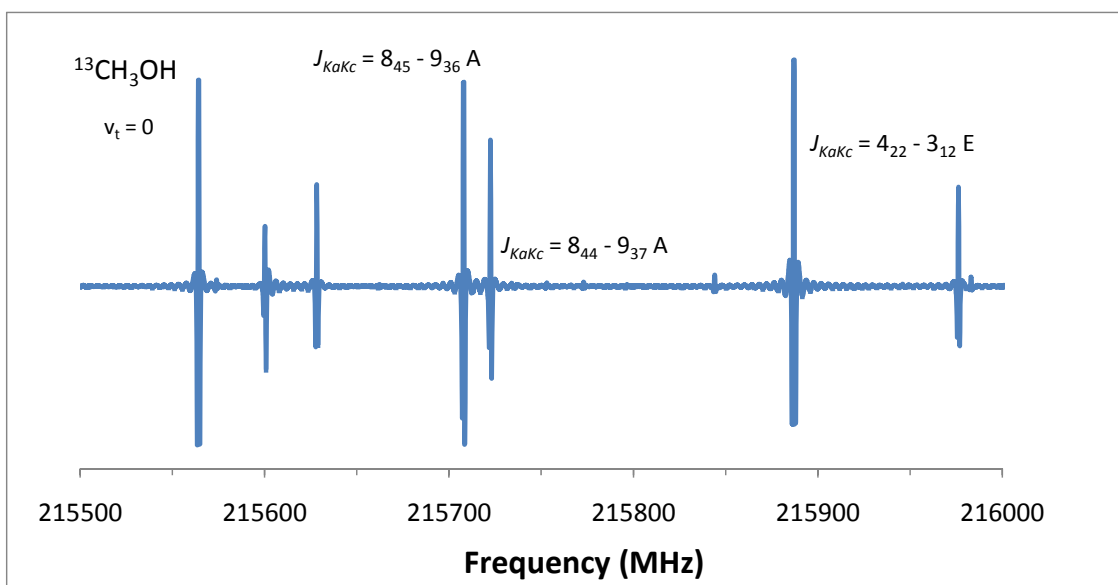


Figure 1: The spectrum of  $^{13}\text{CH}_3\text{OH}$  in the 215 GHz region.

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# Low temperature ion-molecule reactions with drift tube mass spectrometer

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Gas phase ion-molecule reactions are one of the important synthetic pathways for formation of complex molecules in the space. We have developed a new instrument to measure the mobility of gas phase ions. The drift tube technique is extensively used to investigate not only the transport properties of ions (mobility) but also the ion-molecule and charge transfer reactions in the low collision energy range. The temperature variation is achieved by a cryostat system in which the drift tube is integrated.

El-Shall et al.[1,2] studied about associative charge transfer (ACT) reactions in benzene<sup>+</sup>/propene and benzene<sup>+</sup>/acetylene systems and suggesting that ACT reactions initiates polymerization in cold astrochemical environments.

We have applied the drift tube mass spectrometer to investigation of ACT reactions and ternary molecular reactions. We show the details of the low temperature drift tube and some preliminary experimental results.

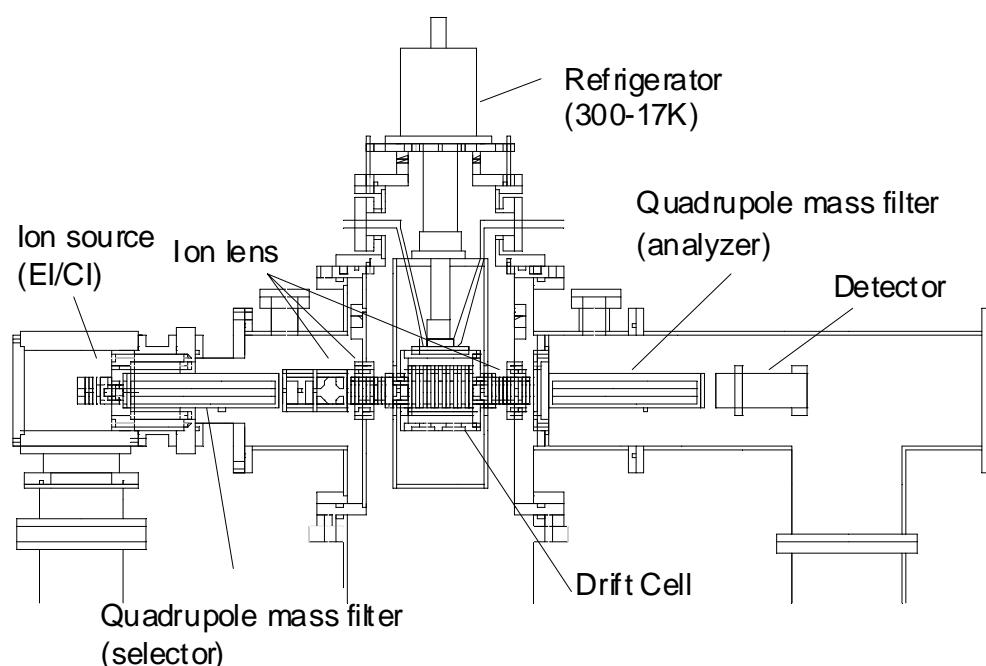


Figure 1: Schematic diagram of the low temperature ion drift tube mass spectrometer.

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## The irradiation of methyl cyanide (CH<sub>3</sub>CN) ice at 15 K with 200 keV protons

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Methyl cyanide (CH<sub>3</sub>CN) is the simplest of the organic nitriles found in the interstellar medium (ISM). It was first identified in the molecular clouds, Sagittarius Sgr A and Sgr B [1] through its emission lines in the vicinity of 2.7 mm from the  $J = 6 \rightarrow 5$  transition. In 1974 it was also reported in comet Kohoutek [2]. CH<sub>3</sub>CN, has since been detected in the Hale Bopp comet [3] and, as of 2009, there are no less than 58 hot molecular core objects in which CH<sub>3</sub>CN had been found [4]. Methyl cyanide has also been discovered beyond the Milky Way, in the NGC 253 galaxy [5], which lies in the local group of galaxies, some 10 million light-years from Earth. It has also been detected in the ISM where it is thought to be made on the grain mantles [6].

In the ISM any methyl cyanide produced on such ice grains may be exposed to a wide range of radiation which in turn may produce further chemical species. In order to determine the possible chemical products of such irradiation in the ISM we have prepared thin films of methyl cyanide at 15 K and exposed them to 200 keV protons using the ion beam facility at the Osservatorio Astrofisico di Catania.

The following species were found to be synthesized during such irradiation; methyl isocyanide (CH<sub>3</sub>NC), hydrogen cyanide (HCN/CN<sup>-</sup>), methylenimine (H<sub>2</sub>C=NH), ketenimine (H<sub>2</sub>C=C=NH), cyanoacetylene (HCCCN), and methane (CH<sub>4</sub>). These results and details of the possible production routes will be presented at the conference.

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## Experimental study of nucleation, coalescence and growth of nanoparticles

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Nucleation is a first step to form cosmic dust particles and is a beginning of their long evolutionary history accompanying with stellar lives. Nucleation determines number, morphology, polymorph, size and size distribution of nanoparticles, which strongly affect to the infrared spectra and also formation of molecules on their surface. Accordingly, nucleation is fundamental process on the cosmic dust formation. When nanoparticles are formed directly from gas phase in ejecta gas of evolved stars and possibly in a plume after energetic shock in primitive solar nebula, at least first nanoparticles must condense homogeneously. Then, they should be condensed under supercooling with nonequilibrium state. In this situation, we cannot apply general thermodynamic equilibrium to find formation sequence of mineral particles. In fact, however, there is no quantitative experimental data concerning a homogeneous condensation from a gas phase. Here, we will show a first achievement of in-situ visualization of the environments during homogeneous nucleation and subsequent growth of nanoparticles in smoke experiment using Mach-Zehnder interferometer and attempt to determine the homogeneous condensation temperature and supersaturation of several kinds of materials in gas phase.

Figure 1 shows an example of our first smoke produced in newly constructed smoke chamber. The smoke was produced by heating of a tungsten wire with 0.3 mm $\phi$  and 70 mm depth in a mixture gas of Ar ( $9\times 10^3$  Pa) and O<sub>2</sub> ( $1\times 10^3$  Pa). Tungsten has been evaporated as oxide at the source temperature  $\sim 1600$  K, which measured by pyrometer. Evaporated oxide molecules are subsequently cooled following the convection current produced by hot source and WO<sub>3</sub> particles have been condensed and formed the smoke. Since there is no heterogeneous nucleation site, solid grains were obtained homogeneously from the gas cloud. The evaporated tungsten oxide vapor is concentrated at the interface between interior WO<sub>3</sub> vapor rich atmosphere and outer mixture gas. Their condensation temperature can be determined from the interferogram. We observed the produced smoke particles using transmission electron microscope and recognized the formation of WO<sub>3</sub> single crystal nanoparticles with 20-200 nm in diameter.

We are trying to discuss using classical nucleation theory and calculated the growth velocity using Herz-Knudsen equation to this experimental result. As the result, we found that the theory no longer works in this nano-world and coalescence process, which is a process two different nanoparticles fused together and make larger nanoparticle, after nucleation is important to know the final product. In addition to the preliminary experiment using WO<sub>3</sub>, experimental results concerning astronomically important materials, such as alumina, silica and iron, will be shown in the presentation.

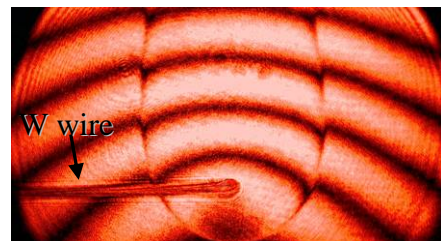


Figure 1: Typical interferometric image of smoke particles.

## THE SOFT X-RAY INDUCED CHEMISTRY OF CO AND CH<sub>3</sub>OH IN WATER ICE STUDIED BY NEXAFS

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The irradiation of organic molecules in condensed water is an important process in a wide variety of scientific areas, from the chemistry of the interstellar space medium[1] to radiobiology.[2] Aiming at characterizing these reactions at a molecular scale, we have recently developed the use of the Near-Edge X-ray Absorption Spectroscopy (NEXAFS) for studying irradiation of icy solutions. In this work, the soft X-ray induced chemistry of H<sub>2</sub>O, CO and CH<sub>3</sub>OH and the effects of the water and nitric acid hydrate (HNO<sub>3</sub>.1.65H<sub>2</sub>O) matrix on the photochemistry of CO and CH<sub>3</sub>OH have been investigated. For pure H<sub>2</sub>O, CO and CH<sub>3</sub>OH ices, the destruction rates are strongly limited by back reactions, leading to strikingly high survival rates of these molecules upon the harsh irradiation conditions to which they were submitted. We also evidence the interplay between the photochemical reactions of CO and CH<sub>3</sub>OH and those of the matrix. The OH and O radicals released by the photolysis of H<sub>2</sub>O and HNO<sub>3</sub> react with the CO and CH<sub>3</sub>OH and their fragments, considerably reducing the survival rates, especially in presence of nitric acid, and dramatically enhancing the formation of CO<sub>2</sub> at the expense of CO. Because NEXAFS spectroscopy allows identifying which reactions are important among those possible, it emerges a simple picture of the photochemical routes of CO and CH<sub>3</sub>OH in the H<sub>2</sub>O and HNO<sub>3</sub>/H<sub>2</sub>O environments.

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## SMA Observations toward the Massive Star-forming Core MM1 of W75N

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The massive star-forming core MM1 of W75N was observed using the Submillimeter Array (SMA) with  $\sim 1''$  and  $2''$  spatial resolutions at 230 and 340 GHz, respectively. From the 230 GHz continuum we found that the MM1 core consists of two sources, separated by about  $1''$ : MM1a ( $\sim 0.6 M_{\odot}$ ) and MM1b ( $\sim 1.4 M_{\odot}$ ), located near radio continuum sources VLA 2/VLA 3 and VLA 1, respectively. Within MM1, two gas clumps have been found to be expanding away from VLA 1 at about  $\pm 3$  km/s, resulting from the latest star formation of the region. Observed molecular lines show emission peaks at two positions, MM1a and MM1b: sulphur-bearing species have emission peaks toward MM1a, but methanol and saturated species at MM1b. We identified the high temperature ( $\sim 200$  K) gas towards MM1a and the hot core towards MM1b. The SiO molecule is unique in having an emission peak exactly towards VLA 2, probably tracing a shock powered by VLA 2. Observed sulphur-bearing species show similar abundances both in MM1a and MM1b, whereas the methanol and saturated species show significant abundance enhancement toward MM1b, by about an order of magnitude, compared to MM1a.

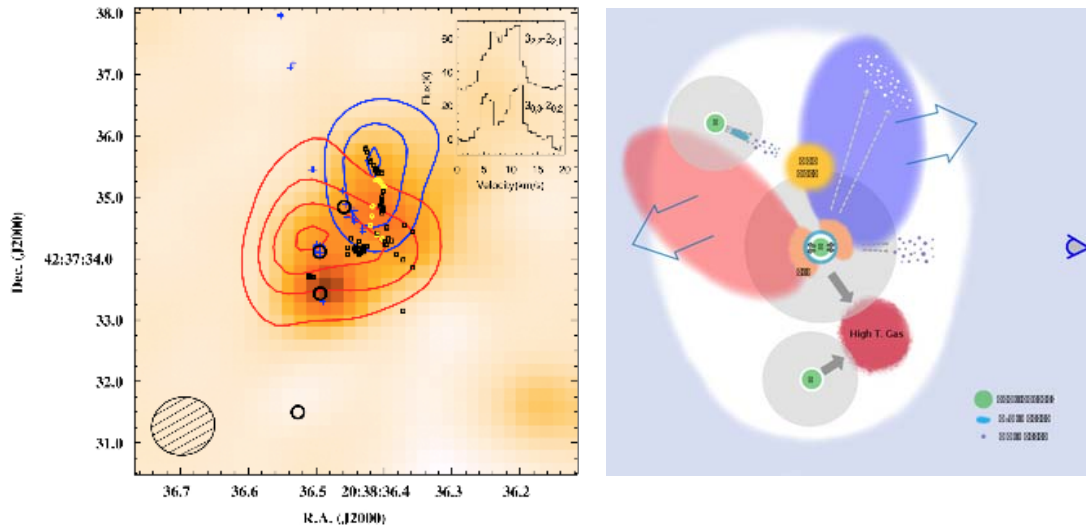


Figure 1: (Left) Integrated intensity map of the  $\text{H}_2\text{CO}$  3(0,3)-2(0,2) line. Blue contours are for  $v=2.0$ -8.5 km/s, and red contours for  $v=8.5$ -16.0 km/s. Both contour levels start from 1.2 Jy/beam km/s and increase by 1.5 Jy/beam km/s. (Right) A schematic diagram of the MM1 core.

**Line Survey Project of External Galaxies with NRO 45-m Telescope**  
 T. Nakajima,<sup>1</sup> S. Takano,<sup>1</sup> K. Kohno,<sup>2</sup> H. Inoue,<sup>2</sup> and the line survey team

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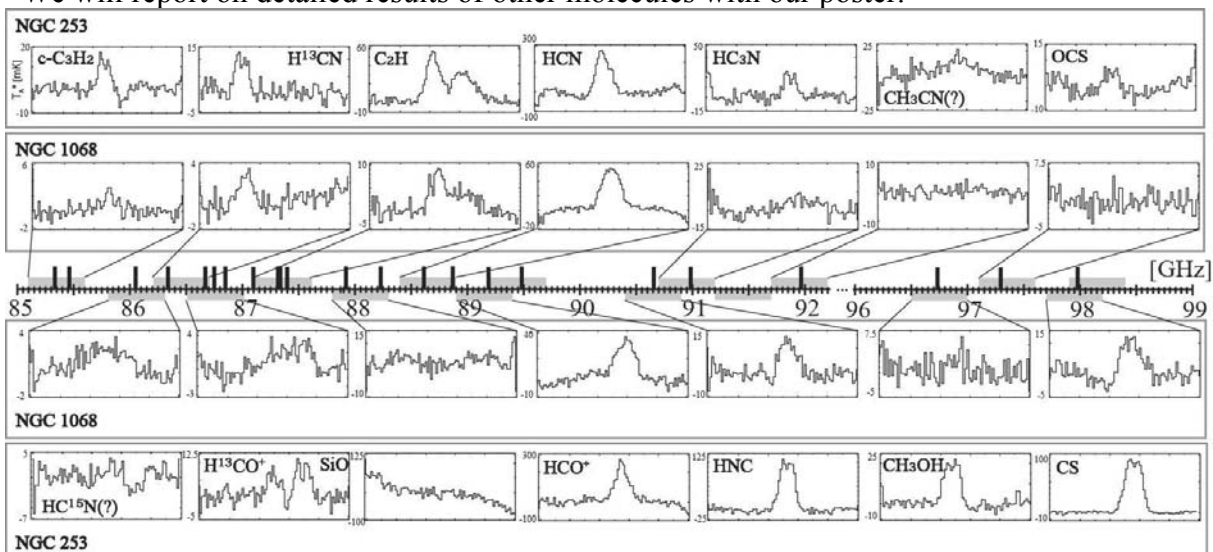
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So far about 37 molecules have been detected in external galaxies. Since various galaxies with different environments exist such as those with small or large amount of gas, with starburst and/or Active Galactic Nucleus (AGN), and with interaction, etc., we expect that various interesting phenomena could be observed in interstellar matter in galaxies. To study the effect of AGN on the circumnuclear molecular gas, further observations of molecular lines are indispensable. Therefore, we started a line survey in 3 mm band with the new receiver on the NRO 45-m telescope [1] toward NGC 1068, which is one of the nearest AGN where a presence of X-ray dominated regions (XDRs) has been suggested (e.g., [2][3]). We can make a selective study of the effect of AGN, because a beam size of the 45-m telescope ( $\sim 18''$  at 86 GHz) is smaller than the size of circumnuclear starburst ring in NGC 1068 ( $d \sim 30''$ ). This project is still continuing but we report some of the results from the initial observations.

The observations at the 3 mm region (85.1-92.2 GHz and 96.5-98.4 GHz) were carried out in February to May, 2009 and January to May, 2010. We successfully detected *cyclic*- $C_3H_2$  ( $J_{K_a, K_c} = 2_{1,2}-1_{0,1}$ ),  $C_2H$  ( $N = 1-0$ ) and  $H^{13}CN$  ( $J = 1-0$ ) for the first time in NGC 1068, and  $HC^{15}N$  ( $J = 1-0$ ) and  $CH_3OH$  ( $J_K = 2_K-1_K$ ) were tentatively detected. In addition, the detection of  $CS$  ( $J = 2-1$ ) has already been reported [4], but we detected for the first time with a single dish telescope in this galaxy. We are also observing NGC 253, which is the prototypical nearby starburst galaxy, as a comparison to study the effect of AGN on molecular abundance. The following results were obtained about the  $C_2H$  lines.

- (1) Using the fine structure, the optical depths toward NGC 1068 and NGC 253 were obtained to be less than 1. These molecular lines are optically thin in both galaxies.
- (2) The column densities are estimated to be  $0.9 \times 10^{14}$  and  $0.5 \times 10^{15} \text{ cm}^{-2}$ , respectively, assuming the excitation temperature of 30 K. The latter value is consistent with the value obtained toward NGC 253 from the previous study [5].

We will report on detailed results of other molecules with our poster.



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|---|--|
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# Formation of CO<sub>2</sub> and H<sub>2</sub>CO<sub>3</sub> through non-energetic surface reactions at low temperatures.

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## INTRODUCTION

Carbon dioxide (CO<sub>2</sub>) is one of the most abundant solid components in icy grain mantles of dense molecular clouds. It is well known that CO<sub>2</sub> can be synthesized from pure carbon monoxide (CO) or CO-containing ices through energetic processes such as UV irradiation, ion irradiation, and electron irradiation [e.g. 1]. However, recent detections of abundant CO<sub>2</sub> in dense clouds observed toward background stars, in which the UV field is relatively weak, suggest that some reactions without UV irradiation may also contribute to the CO<sub>2</sub> formation in these environments [2]

In contrast to CO<sub>2</sub>, carbonic acid (H<sub>2</sub>CO<sub>3</sub>) has never been detected either in the gas phase or solid phase in molecular clouds. However, it is considered that H<sub>2</sub>CO<sub>3</sub> may have a role in acid-base chemistry, such as in reactions with NH<sub>3</sub> to yield NH<sub>4</sub><sup>+</sup>, in astrophysical environments [3]. Therefore, elucidating the formation pathways of H<sub>2</sub>CO<sub>3</sub> and its astrophysical significance is necessary for understanding chemical reaction networks related to the presence of CO in molecular clouds.

In the present study, we demonstrate formation of CO<sub>2</sub> and H<sub>2</sub>CO<sub>3</sub> through surface reactions of CO with non-energetic OH radicals at low temperatures.

## EXPERIMENTAL

Experiments were performed using the Apparatus for SURface Reaction in Astrophysics (ASURA) system. ASURA consists of a main chamber, an atomic source, and a Fourier transform infrared (FTIR) spectrometer. Hydroxyl (OH) radicals, produced by dissociating water molecules in microwave-induced plasma, were cooled down to 100 K prior to react with CO. OH and CO were codeposited onto an Al substrate (10–40 K) and the reaction products were monitored *in-situ* by infrared reflection-absorption spectroscopy.

## RESULTS

When CO molecules were simultaneously introduced together with OH radicals onto the substrate, formation of CO<sub>2</sub> was clearly identified in the reaction product even at 40 K. In addition to CO<sub>2</sub>, several peaks were observed in the IR spectrum. It has been theoretically demonstrated that gas phase synthesis of CO<sub>2</sub> by CO + OH proceeds through the following pathways: CO + OH → *trans*-HOCO → *cis*-HOCO → CO<sub>2</sub> + H [4]. Detection of both HOCO radicals in the reaction product at 10 K further supports an assumption that CO<sub>2</sub> formed through the above reaction pathways in the present experiment.

After the sample was warmed up to 220 K, some peaks were still observed in the IR spectrum, which were attributable to carbonic acid (H<sub>2</sub>CO<sub>3</sub>). Formation of H<sub>2</sub>CO<sub>3</sub> was also demonstrated by the temperature-programmed desorption spectra of the reaction product. It is likely that H<sub>2</sub>CO<sub>3</sub> formed through reactions of *trans*- and *cis*-HOCO radicals with OH.

The present study demonstrated that CO<sub>2</sub> and H<sub>2</sub>CO<sub>3</sub> can form inside dense molecular clouds without external energy inputs from UV, ions, and electrons.

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# DISCS: A spatially and spectroscopically resolved survey of chemistry in protoplanetary disks

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Protoplanetary disks connect protostars and extra-solar systems chemically and physically, with implications for the composition of comets and planets both in our Solar System and in the increasing number of extrasolar systems. To address the chemical evolution of these disks, including their organic inventory, we are in the process of spatially resolving the abundances of eight key molecules and ions – CO, HCO<sup>+</sup>, DCO<sup>+</sup>, N<sub>2</sub>H<sup>+</sup>, HCN, DCN, CN, H<sub>2</sub>CO – in 14 protoplanetary disks using the Submillimeter Array (DISCS: the Disk Imaging Survey of Chemistry with the SMA, PI K. Öberg). The detection rates of minor species such as H<sub>2</sub>CO and N<sub>2</sub>H<sup>+</sup> are surprisingly high allowing us to directly compare the response of the chemistry – for example ionization rates, deuteration, signposts of photon dominated chemistry and ice evaporation – to the physical processes active in disks. A range of physical disk environments is ensured by including star+disk systems that span stellar spectral types from M1 to A0, orders of magnitude different accretion luminosities and X-ray fluxes, and exhibit the full range of grain evolution parameters found in disks. By combining the known physical structures of the disks with our survey of simple chemical systems, we aim both toward characterizing the main drivers of disk chemistry in the bulk of disk material and providing constraints on the physical processes active during planet formation.

# The evolving ice-gas interface during star- and planet-formation

Karin Öberg

Complex organic molecules (>6 atoms) have been detected toward low- and high-mass protostars, galactic center clouds, protostellar outflows and comets, demonstrating the existence of efficient astrophysical pathways to chemical complexity. The detected molecules all reside in the gas. Yet many probably form on interstellar grains, in ices that evolve with their environment and finally evaporate as the grains are heated by new-born stars or by shocks. I will explore this ice evolution during star formation by combining Spitzer spectra of the first, simple ices with laboratory simulations of UV induced ice photochemistry and with millimeter observations tracing complex ice evaporation. The experiments show that UV irradiation of protostellar ices is efficient enough to explain the complex molecule observations in so called protostellar 'hot cores'. Moreover, the experiments predict that before the onset of thermal evaporation close to the protostar, small fractions of the complex ice will continuously evaporate non-thermally due to photodesorption, resulting in gas-phase fingerprints of the ice composition as it evolves. To test this prediction and thus the ice origins of complex molecules in space, we searched for a number of gas-phase complex organic molecules –  $\text{HCOOCH}_3$ ,  $\text{CH}_3\text{CHO}$ ,  $\text{CH}_3\text{OCH}_3$ ,  $\text{C}_2\text{H}_5\text{OH}$  and  $\text{HCOCH}_2\text{OH}$  – toward an ice-rich cloud core irradiated by a nearby protostar. The observations have resulted in a modified scenario for complex ice formation and desorption during star formation. A key unknown is what happens to these molecules during planet formation and I will end with showing some exciting results on the chemistry in protoplanetary disks, acquired within the ongoing SMA legacy program DISCS.

## Observational evidence for the asymmetrical dust clouds around the peculiar SN impostor in the NGC 300.

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Development of the observational instruments have allowed us to discover such a interesting astronomical events as we have never seen. Among them, the supernova (SN) impostor, which is an optical transient with the maximum luminosity intermediate between that of classical nova and of supernova, is one of the most interesting objects. Although several studies have been made on SN impostors, the nature of them still remains to be discovered.

On 2008 May 14, an interesting optical transient was discovered around the nearby galaxy NGC 300 by B. Monard[1] (hereafter NGC300OT). NGC300OT is different from other SN impostors in that the progenitor of it was deeply dust-enshrouded[2] and it possibly produced a large amount of dust in its ejecta by comparing to its “twin” of SN 2008S[3]. We will present the result of near-infrared (NIR) multi-epoch observation of NGC300OT on day 398 and 582 with the Infrared Camera (IRC) on board AKARI. NIR spectra indicated that the NIR flux was mainly due to the thermal emission of hot dust, possibly newly-formed dust in the ejecta. Assuming the isothermal dust cloud, we derived the temperature and the optical depth of the dust cloud by SED fits. Although the result showed that the dust cloud should be highly optically thick at both epochs, no extinction in visible and UV had been observed in the former studies. In order to resolve the discrepancy, we propose the asymmetric distribution of the dust cloud. The asymmetric dust cloud also had been proposed by the former studies[4][5]. Our result strongly supports their conclusion in terms of NIR observation.

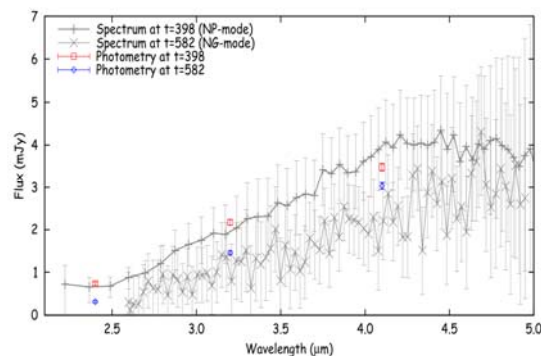


Figure 1: The NIR spectra and the results of photometry of NGC300OT

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# Quantum chemical study of water effect for hydrogen abstraction reactions in low temperature

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Hydrogen abstraction reactions and hydrogen transfer reactions are one of important processes of molecular formation and destruction processes of interstellar molecules. We have been studying the molecular processes of these reactions with small water clusters in order to model the chemical reactions on icy grain surfaces in terms of quantum chemical method. In this presentation, we show the differences of the molecular interactions between various chemical species and small water clusters and how water molecules affect the potential energy surfaces of the hydrogen abstraction reactions of hydrocarbons as well as hydrogen transfer reactions.

In order to obtain the interaction energies of various neutral radicals and small water clusters, we have calculated the molecular geometries of  $\text{CH}_3(\text{H}_2\text{O})_n$ ,  $\text{OH}(\text{H}_2\text{O})_n$ , and  $\text{H}(\text{H}_2\text{O})_n$  by using hybrid density functional B3LYP method with 6-311G(d,p) basis functions. Figure 1 shows the optimized structures of  $\text{CH}_3$  radical, OH radical and H atom interacting with two water molecules. The binding energies between radicals and water dimer are calculated to be 13, 52, and 2  $\text{kJ mol}^{-1}$  for  $\text{CH}_3$ , OH, and H species, respectively.

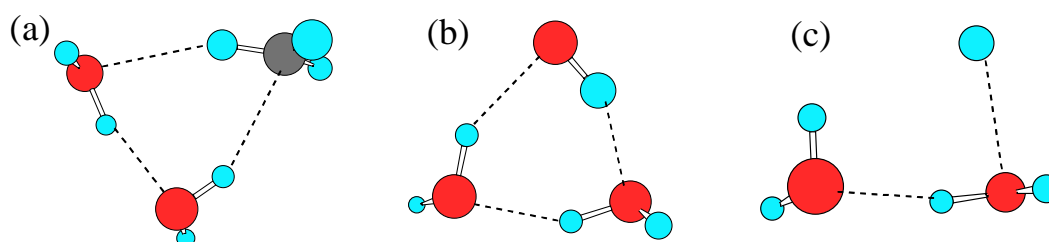


Figure 1. Optimized structures of (a)  $\text{CH}_3(\text{H}_2\text{O})_2$ , (b)  $\text{OH}(\text{H}_2\text{O})_2$ , and (c)  $\text{H}(\text{H}_2\text{O})_2$  radicals.

The calculated potential energy surface of the chemical reaction of  $\text{CH}_4 + \text{H} \rightarrow \text{CH}_3 + \text{H}_2$  shows the energy barrier of  $25 \text{ kJ mol}^{-1}$  and exothermic by  $6 \text{ kJ mol}^{-1}$ . When single  $\text{H}_2\text{O}$  molecule adds to this system, its energy barrier found to be lower by  $3 \text{ kJ mol}^{-1}$ . In the case of  $\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3 + \text{H}_2\text{O}$  reaction, the energy barrier  $4 \text{ kJ mol}^{-1}$  without  $\text{H}_2\text{O}$  molecule is calculated to become  $7 \text{ kJ mol}^{-1}$  with single  $\text{H}_2\text{O}$  molecule interacting in the  $\text{CH}_4 + \text{OH}$  system. The change of the energy barriers by interacting  $\text{H}_2\text{O}$  molecules depends on which reactant species has strong interaction with  $\text{H}_2\text{O}$  molecules. Figure 2 shows the structures of transition states of two reactions and indicates the difference of the interacting site of  $\text{H}_2\text{O}$  molecule with reacting species.

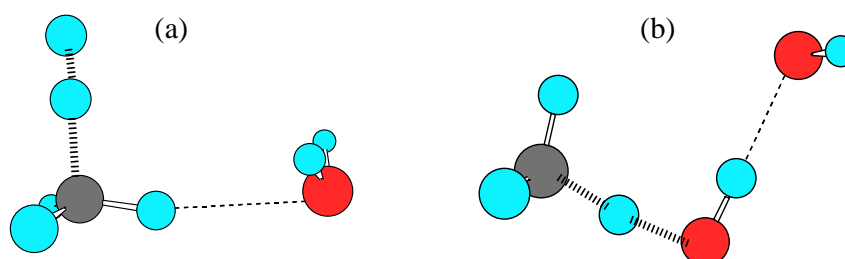


Figure 2: Transition state structures of (a)  $\text{CH}_4 + \text{H}$  and (b)  $\text{CH}_4 + \text{OH}$  interacting with  $\text{H}_2\text{O}$  molecule.

# THEORETICAL INVESTIGATION OF THE FORMATION OF H<sub>2</sub>CO IN THE INTERSTELLAR MEDIUM: A WATER ASSISTED REACTION

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It is believed that Formaldehyde is formed on dust grains coated with ice within Molecular Clouds.[1]With this in mind there have been several studies into the hydrogenation of CO to Formaldehyde (H<sub>2</sub>CO) reported within the literature.[2-5] These studies all consider the reaction scheme:



However, it is equally plausible that the second Hydrogen may add to the Oxygen of the Formyl radical to generate *trans*-HCOH. This is of importance in the interstellar medium as the gas phase barrier to isomerisation is large, and therefore will be unfavourable at low temperatures. Schreiner et al [6] showed that even with such a high activation barrier that HCOH does indeed isomerise at low temperatures to H<sub>2</sub>CO. They propose a tunneling mechanism for the reaction, as it is evident that at 10 K the barrier is insurmountable. They did not however look at the role that water may play within this isomerisation, our work, based on quantum chemistry calculations, focuses on the role that water may play in this reaction.

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## HYDROGEN/DEUTERIUM EXCHANGES IN INTERSTELLAR/COMETARY ICE ANALOGS

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Despite the low cosmic abundance of deuterium ( $D/H \sim 10^{-5}$ ), high degrees of deuterium enrichment in molecules are observed in star-forming regions with enhancements that can reach 13 orders of magnitude for multi-deuterated species [1]. High D/H ratios are also observed in planets and small bodies of the solar system. Quantitative modelling of the D/H ratios remains however hampered by the lack of appropriate chemical kinetics data. In particular, the detailed mechanisms responsible for the observed enrichment disparities between functional groups are currently poorly known. For example, there is significantly more  $CH_2DOH$  than  $CH_3OD$  ( $[CH_2DOH]/[CH_3OD] > 10$ ) in low-mass protostars [2]. Various hypotheses have been suggested to explain this anomaly, but none is fully convincing. In this work, we test a new hypothesis experimentally: the spontaneous exchange between hydrogen and deuterium atoms in  $H_2O:XD$  ice mixtures, where XD is either  $CD_3OD$  (methanol) or  $CD_3ND_2$  (methylamine).

To this aim, thin films of intimate  $H_2O:XD$  ice mixtures, condensed at low temperature ( $\leq 110K$ ), have been monitored by Fourier transform infrared (FTIR) spectroscopy up to the complete evaporation of XD molecules. Rapid hydrogen/deuterium (H/D) exchange has been observed, at 120K and above, through the growth of the  $\nu_{OD}$  stretching mode of HDO at  $2425\text{ cm}^{-1}$ . It has been also shown that H/D exchange occurs (i) on the hydroxyl and amino functional groups of XD molecules, i.e. through hydrogen bonds, and (ii) before the completion of crystallization. The present results suggest therefore that the much lower abundance of  $CH_3OD$  compared to  $CH_2DOH$  in low-mass protostars could simply reflect H/D exchanges in water ice either prior to or during the grain mantle sublimation [3]. This hypothesis will be further discussed in view of new millimeter observations of singly deuterated methanol towards high- and intermediate-mass protostars. Finally, new experimental data including the kinetics of H/D exchanges will be presented and the physical processes expected to promote or limit these exchanges in space will be emphasized.

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## ALMA for Interstellar Matter

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Atacama Large Millimeter-submillimeter Array (ALMA)[1] will start early science observation in 2011 and provide unprecedented power to address various issues on interstellar matter. The sensitivity of ALMA in spectral observations covering frequency ranges of 30-900 GHz (Fig. 1) is typically 10-30 times higher than that of the existing millimeter and submillimeter arrays. Its high spatial and spectral resolution will enable us to image detailed features of ISM and to reveal kinematics of ISM. Its high sensitivity enable us to detect very weak emission such as new molecular transitions toward star forming regions, protoplanetary disks, planetary nebulae, Galactic center and even galaxies. These ALMA data can be compared directly with theoretical studies enriching our understanding of the interstellar physics. ALMA can also diagnose molecular abundance, temperature, density and kinematics of many species with high precision.

The East-Asian ALMA Regional Center (EA-ARC) will provide user support in many aspects. We present the latest status and information for the observing proposal of ALMA.

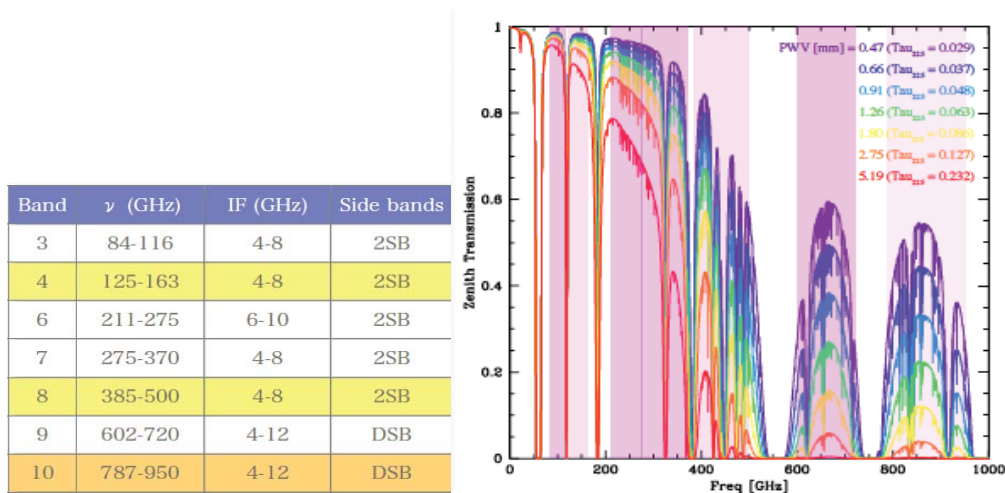


Figure 1: Left) Current frequency coverage of ALMA. Right) Atmospheric transmission in the ALMA frequency coverage given precipitable water vapor in atmosphere.

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# Recent Progress of Carbon-Chain Chemistry in Molecular Clouds

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In this talk, we will present two recent progresses of observational carbon-chain chemistry in molecular clouds. One is the understanding of formation processes of carbon-chain molecules. So far, the abundance ratio of the <sup>13</sup>C species relative to the normal species is assumed to be the same as the elemental abundance ratio of <sup>12</sup>C/<sup>13</sup>C (60). However, we have recently observed the <sup>13</sup>C species of CCS, and have found the CCS/C<sup>13</sup>CS and CCS/<sup>13</sup>CCS ratios are 54±5(3σ) and 230±130(3σ), respectively, in TMC-1. The abundance ratio of C<sup>13</sup>CS/<sup>13</sup>CCS is not unity and <sup>13</sup>CCS is heavily diluted. This indicates that the two carbon atoms are nonequivalent in the main formation pathway of CCS. Although the isotope exchange reaction between <sup>13</sup>CCS and C<sup>13</sup>CS may be responsible in part, these results will put strong constraints on the production pathways of CCS. For instance, non-equivalent processes like CH + CS is turned out to be important to produce CCS [1]. Similarly, the <sup>13</sup>C species of CCH is observed, and the C<sup>13</sup>CH/<sup>13</sup>CCH ratios are determined to be 1.6±0.4(3σ). Again, the two carbon atoms are nonequivalent. Furthermore, C<sup>13</sup>CH and <sup>13</sup>CCH are also found to be significantly diluted [2]. The heavy dilution of the <sup>13</sup>C species is now confirmed observationally, which will provide us with rich information on physical and chemical conditions of interstellar clouds.

Second is the discovery of new carbon-chain chemistry in a lukewarm region near the protostar triggered by the evaporation of the CH<sub>4</sub> ice. We have found low-mass star forming regions, L1527 and IRAS15398-3359, which show extremely high abundances of carbon-chain molecules [e.g. 3, 4]. In particular, we have confirmed the regeneration of carbon-chain molecules in the 20-30 K region near the protostar by interferometric observation toward L1527. The new chemistry is named as Warm Carbon-Chain Chemistry (WCCC) in contrast to the conventional one which has long been applied to cold starless cores. The understanding of the anion chemistry has been accelerated by the detection of C<sub>4</sub>H<sup>-</sup> and C<sub>6</sub>H<sup>-</sup> in L1527. The discovery of the WCCC sources demonstrates that the chemical composition of low-mass star-forming regions is not uniform, but has a significant variety. A remarkable contrast can be seen between WCCC and hot corino chemistry. A possible origin for this would be the time scale of the starless-core phase; a shorter contraction time would result in WCCC. If so, chemical compositions tell us the past history of the star formation processes, which would not be derived from the conventional observations.

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## Properties of PAH emission in Nova V1280 Sco

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We have carried out the near-infrared spectroscopy of dust forming nova V1280 Sco with Infrared Camera (IRC) onboard AKARI on 2009 Sep. 9, which corresponds to the epoch of ~940 days after outburst. The obtained near-infrared spectrum have shown distinct red continuum accompanied by 3.3 $\mu$ m “PAH” feature with extraordinary strong red wing in 3.4—3.6 $\mu$ m (see Figure 1). While the 3.3 $\mu$ m feature is assigned as the stretching mode of aromatic CH, the 3.4—3.6 $\mu$ m wing components are assigned as the stretching mode of aliphatic CH groups. Larger 3.4/3.3 ratio in V1280 Sco may indicate the higher aliphatic-to-aromatic ratio of the carriers than the case of general interstellar PAHs. Our results are consistent with the remark of Evans & Rawling (1994) that the observed ‘PAH’ features in nova are likely to be carried by HACs rather than free-flying PAHs. We also have carried out the follow-up mid-infrared observation of this nova with TRCS onboard Gemini South telescope on 2010 Aug. 2-3 (GS-2010B-C-7), which corresponds to the epoch of ~1260 days after the outburst. In this presentation, we will introduce the latest results of those observations and discuss the dust formation around an interesting nova V1280 Sco.

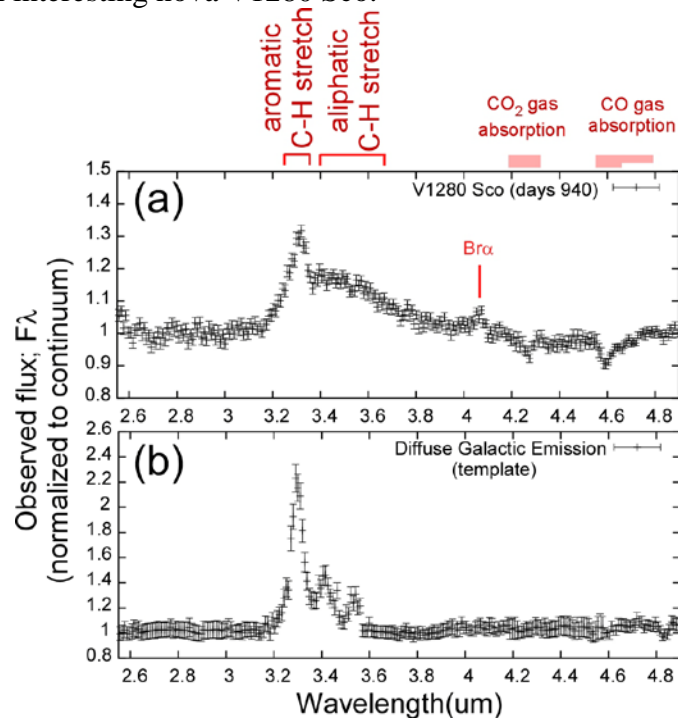


Figure 1: (a) Near-Infrared spectrum of V1280 Sco on the epoch 940 days after the discovery normalized to the continuum obtained with Infrared Camera (IRC) onboard AKARI. 3.3 $\mu$ m “PAH” feature with a strong red-wing components in 3.4-3.6 $\mu$ m was recognized in the obtained near spectrum (Sakon et al. 2010, in preparation). (b) An example of near-infrared spectrum of Galactic diffuse ISM obtained with AKARI/IRC for a comparison.

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# Infrared Observations of Ices around Young Stellar Objects in the Small and Large Magellanic Cloud

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Question of where molecules like water or carbon dioxide on the Earth's surface came from is one of the main topics of the current “astrochemistry”. One of the possible origins of these molecules is the “ices” around young stellar objects (YSOs). Observations of ices around extragalactic YSOs are one of the challenging topics in the recent ice studies. So far, infrared spectroscopic observations toward extragalactic embedded YSOs are few, and their circumstellar chemistry is still poorly understood. But it is highly probable that different galactic environments (e.g., metallicity, radiation field, etc.) could affect the properties of circumstellar material.

In this study, we first focused on YSOs in the Large Magellanic Cloud (LMC), which is the nearest metal-poor galaxy to our Galaxy. We investigated the chemical conditions of ices around high-mass YSOs in the LMC by near-infrared (2—5 micron) spectroscopic observations with the infrared satellite AKARI [1, 2]. As a result, we detected the absorption features of 3.05 micron H<sub>2</sub>O ice, 4.27 micron CO<sub>2</sub> ice, and 4.67 micron CO ice toward these extragalactic YSOs. We derived column densities of these ices and showed that YSOs in the LMC have higher abundance of CO<sub>2</sub> ice than similar Galactic counterparts. In addition, we investigated the correlation between the chemical abundance of ices and properties of each YSO. Next, we also performed the spectroscopic observations of YSOs in the Small Magellanic Cloud, whose metallicity is much lower than the LMC, and detected the absorption features of the above major ice species [3]. .

In this study, we present the latest results of our spectroscopic observations toward extragalactic YSOs, and discuss how the chemical properties of ices depend on the galactic metallicity and YSO properties.

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# **Properties of dust around Eta Carinae during the periastron event in 2009 based on near infrared multi-epoch photometric observations with the Wide Field Cryogenic Telescope 2 (WFCT 2)**

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Eta Carinae is known as one of the most massive binary system in a relatively old stage in its evolution. It has shown drastic variations in brightness, at least, during past few centuries. In recent several decades, it is known that this star has a periodic variation in brightness at various wavelengths occurring every 5.54 years, which corresponds to the orbital phase of the binary system, and it is termed as "spectroscopic event". Most believed that during this event dust is formed around Eta Carinae due to the wind-wind collision. The near-infrared observation was carried out during the 2009 spectroscopic event with the WFCT 2 in South Africa, which covered a period before and after the spectroscopic event. In this report we present the data from 10 to 29 January 2009. The light curve that we obtained from the data shows a steep decline in this period. Our interest is the properties of the dust grain around Eta Carinae in such a small time span near the spectroscopic event. Monitoring of the variation in near-infrared light curve is quite efficient to investigate the properties of the hot dust. The result shows that the dust temperature increases while the dust mass decreases. Our data lead to that there is some destruction of dust in a few weeks around the spectroscopic event.

## Separation and conversion dynamics of nuclear spin isomers of gaseous molecules

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Matter is composed of molecules and all molecules possessing identical nuclei with nonzero spin, in accordance with Pauli's principle, have distinct nuclear spin isomers [1]. Can one of nuclear spin isomers of the gaseous molecules be separated from others? Is it possible that nuclear spin conversions among the nuclear spin isomers occur and can be observed spectroscopically? How long can these isomers exist in real time? Addressing these questions leads to interesting scientific explorations. In astronomy and astrophysics, it is widely assumed that the conversion probabilities among nuclear spin isomers for the various molecules in the interstellar matter are zero, even over time spans of millions of years [1]. However, this assumption is quite questionable. The observed values obtained in our study are good tests for the validity of this assumption.

We are performing researches on separation of nuclear spin isomers of gaseous interstellar molecules by the most reliable and powerful light-induced-drift technique [1-3] and on the conversion observations of these enriched spin isomers in long time relaxation processes via precision measurements of the spectral line intensities. Our experimental results and detailed physical explanations of the nuclear spin conversion mechanisms will be reported in the Workshop on Interstellar Matter 2010.

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## Nobeyama 45 m telescope legacy project: Line survey (II)

Takano, S. (NRO), Aikawa, Y. (Kobe U.), Chen, V. (NTHU), Hirano, N. (ASIAA), Hirota, T. (NAOJ), Kamegai, K. (JAXA), Kobayashi K. (Toyama U.), Kohno, K. (U. Tokyo), Kuan, Y.-J. (NTNU), Liu, S.-Y. (ASIAA), Nakajima, T. (NRO), Ohashi, N. (ASIAA), Ohishi, M. (NAOJ), Ozeki, H. (Toho U.), Sakai, N. (U. Tokyo), Sakai, T. (U. Tokyo), Shiba, S. (U. Tokyo), Su, Y.-N. (ASIAA), Sugimura, M. (U. Tokyo), Takahashi, S. (ASIAA), Takakuwa, S. (ASIAA), Umemoto, T. (NAOJ), Wang, K.-S. (ASIAA), Yamada, M. (ASIAA), Yamamoto, S. (U. Tokyo), Zhang, Q.-Z. (CfA)

Line surveys are of fundamental importance in astronomy not only for complete understanding of chemical compositions in representative sources, but also for finding out new observing tools probing interstellar medium and star formation. We started the line surveys toward a few new types of sources with the Nobeyama 45 m telescope in December 2007. The target sources include the low-mass star forming region L1527, the shocked region of L1157, infrared dark clouds G28.34+0.06, and external galaxies Arp 220, NGC 1068 and NGC 253. Mainly with the new 3 mm receivers installed on the 45 m telescope [1], the frequency range of ~84-115 GHz will be surveyed with much higher sensitivity than the previous observations. The total observing time is expected to be about 1000 hours for four years. The results from the survey will be used for detailed studies on chemistry in each source, and will also provide us with useful templates for planning the observing strategy with ALMA. The third year of the line surveys was finished. We report the preliminary results.

L1527 is a very interesting object, because the abundances of carbon-chain molecules are high, though this source is a low-mass star-forming region [2]. We detected many lines including high excitation lines of HC<sub>5</sub>N (e.g. J=41-40, upper state energy of 110 K), isotopic species (D, <sup>13</sup>C) of some carbon-chain molecules, HCO, C<sub>3</sub>O, cyclic-C<sub>3</sub>H, etc. These data will be quite useful to understand chemistry in this warm environment.

In L1157, where interactions between an outflow and ambient clouds are prominent [3, 4], we detected many lines including C<sub>2</sub>H, C<sup>34</sup>S, CCS, HCNO, CH<sub>3</sub>CN, CH<sub>3</sub>CHO, HCOOCH<sub>3</sub>, and NH<sub>2</sub>CHO. To study shock chemistry and gas-grain interaction, these results are rather important information. After our observations, we noticed that HCOOCH<sub>3</sub> is independently detected with the IRAM 30 m telescope [5].

In G28.34+0.06 three interesting positions called mm1, mm4, and mm9 are selected. Toward mm1 and mm4 line wings were found in HCO<sup>+</sup>, HCN, SiO, CS, and CH<sub>3</sub>OH. These wings indicate outflow activities. In addition, CH<sub>3</sub>CHO is detected only in mm1 and mm4. This molecule is one of the probable grain related species. Therefore CH<sub>3</sub>CHO may be evaporated from grain. Based on these results, mm1 and mm4 are thought to be high-mass protostellar objects. Additional data supporting this view were obtained from DNC, DCO<sup>+</sup>, and N<sub>2</sub>D<sup>+</sup>.

About galaxies we are mainly observing NGC 1068, which is a nearby galaxy with Active Galactic Nucleus (AGN). Our motivation is to study the effect of AGN on molecular abundances (cf. [6]). In addition a prototypical starburst galaxy NGC 253 is observed for comparison. We detected C<sub>2</sub>H (*N*=1-0), H<sup>13</sup>CN (*J*=1-0), and cyclic-C<sub>3</sub>H<sub>2</sub> for the first time in NGC 1068. The details will be presented in this workshop by Nakajima et al.

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# Laboratory measurements of atomic hydrogen diffusion and the ortho-para conversion of nascent H<sub>2</sub> molecules on amorphous solid water

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We experimentally approach the two astronomically significant issues: diffusion of hydrogen atom on amorphous solid water (ASW) at a low temperature and the ortho/para ratio of nascent H<sub>2</sub> molecule formed by recombination on ASW. Atomic hydrogen on ASW was directly detected by the combination of a photostimulated desorption and a resonance enhanced multiphoton ionization techniques [1]. Using this method, attenuation in the number of hydrogen atoms on ASW due to recombination and/or desorption was first measured in temperature range 8—20 K at very low H atom coverage, relevant to H<sub>2</sub> formation on cosmic ice dust. The obtained attenuation curve at 8 K clearly consists of fast and very slow components. The fast component is mainly attributable to the loss by H-H recombination after H-atom diffusion on shallow potential sites, while the very slow component would reflect the hydrogen atoms trapped in deep potential sites of ASW. Activation energies of the H-atom diffusion on shallow and deep potential sites are determined to be ~20 and >50 meV, respectively. Our results cover the previously reported activation energies of both 22 [2] and 41-55 meV [3]. The ortho-para nuclear spin ratio of nascent H<sub>2</sub> formed by recombination on ASW has been obtained for the first time and is higher than approximately 200 K. After formation, H<sub>2</sub> molecules are trapped and their spin temperature decreases due to the conversion of spin states on ASW. The scenario for H<sub>2</sub> formation on cosmic ice dust is that the hydrogen atom encounters another atom strongly trapped in the deep site after traveling on the shallower potential sites and after formation, H<sub>2</sub> molecules are trapped and their spin temperature decreases due to the conversion of spin states on ASW.

## References

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## Line survey of RCrA IRAS7B in the 345GHz window with ASTE

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Recently it is established that chemical compositions of low mass star forming regions harboring the Class 0 protostar are different from source to source ([1], [2], [3] etc.). One extreme case is a hot corino, where various complex organic molecules like HCOOCH<sub>3</sub> are abundant. These complex molecules may be related to the pre-solar material found in meteorites. Therefore it is very important to characterize the chemical compositions of the hot corinos and its variation in detail. However, a line survey toward a hot corino source is carried out only toward IRAS 16293-2422, and it has not been published yet.

With these in mind, we have conducted a sensitive line survey in the 345 GHz band toward RCrA IRS7B with the ASTE 10 m telescope. RCrA IRS7B is a class 0 object in Corona Australis with the distance of about 170 pc [4]. Schoier et al. [5] detected the high excitation lines of H<sub>2</sub>CO and CH<sub>3</sub>OH toward this source, indicating that it is a good candidate of the hot corino source.

The RCrA IRS7B has been surveyed from 332 GHz to 352 GHz with frequency resolution of 0.5 MHz. The typical R.M.S. noise level is 10-15 mK in  $T_A^*$ . From the survey, we have identified 15 fundamental molecular species and 11 isotopomers. On the other hand, complex organic molecules, which consists of more than 4 heavy atoms, have not been detected definitively. In our poster, we will present the current results of our survey (fig.1 a) and discuss physical conditions of molecular gas (fig.1 b) and deuterium fractionation ratio in the source. This is a collaborative study with the University of Copenhagen group, which is conducting the line survey in the 230 GHz band toward the same source with APEX.

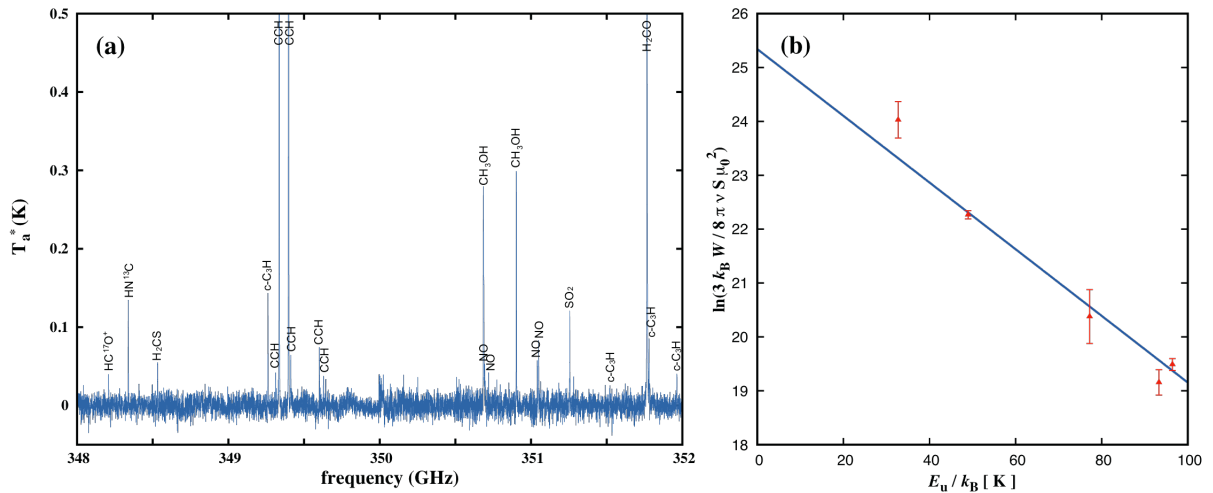


Figure 1: (a) A portion of obtained spectra from 348GHz to 352 GHz. (b) An example of the rotation-diagram analysis for c-C<sub>3</sub>H<sub>2</sub>. The estimated excitation temperature ( $T_{\text{rot}}$ ) and column density ( $N$ ) are  $16.2 \pm 1.2$  K and  $(4.0 \pm 1.3) \times 10^{12}$  cm<sup>-2</sup>, respectively.

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- [5] Schoier et al. 2006, 454, L67

# Translational and rotational energy measurements of vacuum-ultraviolet photodesorbed water molecules in their vibrational ground state from amorphous solid water

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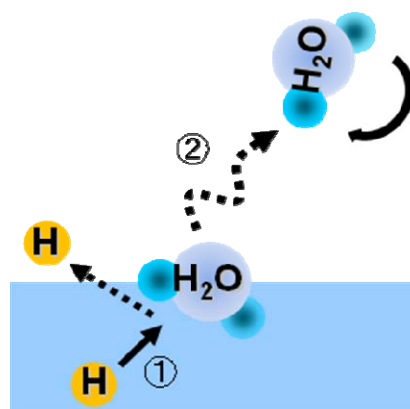
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For large grains in the cosmic space, the most important desorption mechanism at the edge of molecular clouds is photodesorption. To reveal the details of photodesorption mechanism, we have experimentally measured the average translational and rotational energies for photodesorbed H<sub>2</sub>O ( $v=0$ ) from amorphous solid water (ASW) and polycrystalline ice (PCI) at 90 K using 157 nm laser. The experimental findings are compared with the results of classical molecular dynamics (MD) calculations performed for photodesorption from ASW.

The rotational temperature  $T_{\text{rot}}(v=0)$  is estimated to be  $300 \pm 100$  K by spectral simulation. Time-of-flight spectrum of H<sub>2</sub>O ( $v=0$ ) measured for the (2<sub>02</sub>-3<sub>21</sub>) line of the REMPI spectrum was measured, which is well reproduced by a M-B distribution with  $T_{\text{trans}}(v=0) = 1800 \pm 500$  K. The main mechanisms for this photodesorption is a “kick-out” of an H<sub>2</sub>O molecule on the ice surface by the energetic H atom released from photodissociation of  $\text{H}_2\text{O} + h\nu \rightarrow \text{H} + \text{OH}$ . (Fig. 1) The experimentally observed average translational and rotational energies are in good accord with predictions by classical molecular dynamics calculations for the “kick-out” mechanism. H<sub>2</sub>O molecules desorbed from ASW might be expected to lose energy in interactions with cold ice surface. Hence, a slow TOF component might be expected. The absence of any such slow TOF component suggests that H<sub>2</sub>O only on the ice surface can desorb and not from bulk phase.



**Figure 1** Schematic illustrations of a “kick-out” of another H<sub>2</sub>O molecule in the ice by the energetic H atom released from VUV irradiation of amorphous water ice. The numbers dedicate for sequence of the reaction.

## References

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# THz high-resolution TuFIR spectroscopy of pure rotational transitions of molecular ions $\text{H}_2\text{D}^+$

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Light molecules or ions composed of small number of light atoms such as hydrogen play key roles in the history of chemical evolution of interstellar species. Precise frequency measurement of rotational lines of such light species is important to improve rotational constants of the species and to give precise prediction of the rotational lines for future search of the species.

So far, we have investigated rotational lines of molecules and ions in the far-infrared region (in the range from 0.8 to more than 5 THz) by using tunable far-infrared spectrometer (TuFIR) at University of Toyama. The spectrometer is based on the difference frequency generation from the selectable stabilized two  $\text{CO}_2$  laser lines. And He-liquid cooled Si-composite bolometer.

Fig.1 shows the  $2_{12} - 1_{11}$  line of  $\text{H}_2\text{D}^+$  observed at 2.363 THz with TuFIR spectrometer. This line was previously detected toward Sgr B2 by Cernicharo et al [1]. Four lines of  $\text{H}_2\text{D}^+$  were observed with our spectrometer.

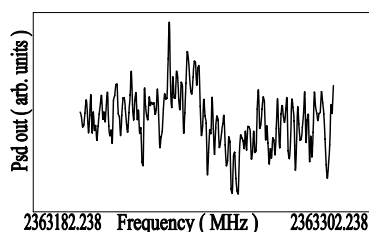


Figure 1:  $J = 2_{12} \leftarrow 1_{11}$  transition of  $\text{H}_2\text{D}^+$ .

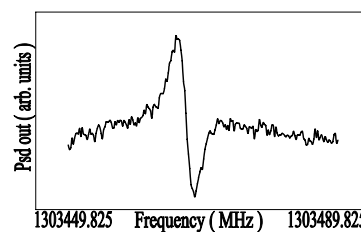


Figure 2:  $J = 14 \leftarrow 13$  transition of  $\text{N}_2\text{H}^+$ .

As for the lower frequency data, Asvany et al. [2] observed the  $1_{01} - 0_{00}$  line (1370085.3 MHz) by using laser induced chemical reaction detection method. Our observed THz lines ( $2_{11}-1_{10}$ ,  $3_{13}-2_{12}$ ,  $2_{02}-1_{01}$ ,  $2_{12}-1_{11}$ ) recorded in the shape of first derivative curve were analysed together with known millimeter- and sub-millimeter-wave lines, and the combination differences derived from the infrared lines to obtain the parameters in Watson's effective Hamiltonian. A set of improved molecular constants are obtained [3].

The spectrometer is now modified to introduce a discharge sample cell using extended negative glow discharge technique. Fig.2 shows the test data of  $\text{N}_2\text{H}^+$  observed by using the extended negative glow discharge. The spectral line was enhanced by one order of magnitude by using the new discharge cell.

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