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[P-CG19] Origin and evolution of materials in space

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Recent progress of astronomical observations, laboratory experiments, solar-system exploration, and theoretical work have enabled us to attempt to understand the origin and evolution of materials (dust and gas) in space. It is thus important to link further planetary material science and astronomy for a comprehensive understanding of dust and gas in space and their role in the evolution of galaxies, stars, and planetary systems. Infrared observations with future large satellites/telescopes, such as TMT, are suitable for the study of gas and dust, and are expected to bring a new frontier of gas/dust study. In this session, based on the latest results on astronomical observations (ALMA, etc.), experiments, and theoretical studies on materials in space, we discuss the next steps in science for materials in space to maximize the outcome of the observations with the future satellites/telescopes.

[PCG19-P01] Investigation of Dust-Surface Formation of Prebiotic Molecule CH₃NCO in Star-Forming Region Sagittarius B2(N)

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[PCG19-P02] Phyllosilicate minerals in comet P/2016 BA14 (PANSTARRS)

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[PCG19-P03] Test observations toward Orion-KL region using 2mm Band 4 Receiver onboard 50m Large Millimeter Telescope

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[PCG19-P04] **Modeling of Nitrogen Fractionation in the Protoplanetary Disk around TW Hya**

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[PCG19-P05] Effects of deposition temperature on structural changes of amorphous ice in heating process

*Yui Ono¹ (1.Meiji University)

[PCG19-P06] Phase transition of KOH-doped amorphous ice

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Investigation of Dust-Surface Formation of Prebiotic Molecule CH₃NCO in Star-Forming Region Sagittarius B2(N)

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Origin of organic molecules on Earth is thought to be interstellar clouds because comets carried molecules produced in clouds. Methyl isocyanate CH₃NCO is presumably one of delivered organic molecules at the primitive earth. However, observed abundance ratios of [CH₃NCO]/[HNCO] in molecular clouds [1] are clearly lower than that in the comet 67P [2]. Recently a theoretical study has suggested that this abundance anomaly can be explained by dust-surface formation of CH₃NCO in molecular clouds [3]. If that is the case, high-temperature CH₃NCO desorbed from dust surface makes a dense distribution in a central region of a star-forming core. To examine this condition, the spatial and spectral data of CH₃NCO toward the core of the high-mass star-forming region Sagittarius B2(N) in 94–113 GHz observed by the ALMA radio telescope were analyzed. Considering intensity maps and velocity structures, it was found that CH₃NCO shows a structure of a bipolar molecular flow and an accretion disk. Rotational temperatures are derived to be 20–50 and 50–60 K in the flow and the disk, respectively, and column densities of both the sources are $\sim 10^{15} \text{ cm}^{-2}$. These results suggest hot and dense conditions of this molecule in the central region of the core. Hence, CH₃NCO detected in the present data is likely to be produced on dust surface. [1] Halfen et al., 2015, ApJL, 812, L5. [2] Goesmann et al., 2015, Sci., 349, 6247. [3] Majumdar et al., 2018, MNRAS, 473, L59.

Keywords: ALMA, Prebiotic Molecule, Methyl isocyanate

Phyllosilicate minerals in comet P/2016 BA14 (PANSTARRS)

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Comets are thought to contain pristine materials formed in the early solar nebula. In periodic comets that have orbited the Sun many times, compared to dynamically new comets, with progressively smaller perihelion distances, the nucleus exhibits clues to investigate significant physical and chemical evolution, including the influence of solar heating on cometary nuclei. Thus, conducting observational and theoretical studies on evolved comets is essential. The evolutionary track of exceedingly weakly active comets is considered to lead up to their dormancy or extinction.

Here, we report on the mid-infrared imaging and spectroscopic observations of comet P/2016 BA14 (PANSTARRS). Its gas and dust production rates were notably low, even near the perihelion passage around 1 au from the Sun. We observed the comet P/2016 BA14 on UT 2016 March 21.3 at heliocentric and geocentric distances of 1.01 au and 0.026 au, respectively, approximately 30 hours before its closest approach to Earth (0.025 au). Low-resolution ($R \sim 250$) spectroscopic observations in the *N*-band and imaging observations centered at 8.8, 12.4, 17.7, and 18.8 microns were carried out using the Cooled Mid-Infrared Camera and Spectrometer (COMICS) mounted on the 8.2m Subaru telescope. The observed image of the comet has a spatial profile that is consistent with a point-spread function.

The normalized emissivity spectrum of the comet exhibits absorption-like features around 10 microns. The features are not reproduced by the anhydrous silicate minerals typically found in cometary coma dust, such as olivine and pyroxene. By comparing with the thermal emissivity spectra measured for various minerals in the laboratory, the shape and position of the observed ~ 10 -micron feature observed for P/2016 BA14 are more similar to those of phyllosilicates rather than anhydrous silicates, which are usually not observed in the mid-infrared comet spectra.

Keywords: comets, dust, phyllosilicate

Test observations toward Orion-KL region using 2mm Band 4 Receiver onboard 50m Large Millimeter Telescope

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We carried out test on-the-fly mapping observations toward the high mass star-forming region, Orion-KL located at a distance of about 414 pc from the Sun by using the Band 4 Receiver (B4R) employing 2-mm-band highly sensitive superconducting SIS receivers onboard the 50 m aperture Large Millimeter Telescope (LMT) operated at an altitude of 4600 m in Mexico. B4R allows us to observe both single sidebands for two orthogonal polarizations. The equivalent receive noise temperatures are less than 60 K. Observed areas were 10'x10' (Oct. 2018) and 5'x5' (Nov. 2019), and the observation frequency bands were 127.9-130.4, 131.9-134.4, 141.6-144.1, 145.6-148.1 GHz and 131.4-133.9, 136.2-138.7, 145.1-147.6, 149.9-152.4 GHz, respectively. The observed area includes the hot molecular core located close to a young protostar as an external heat source. This core is now well-known to contain a variety of complex carbon-chain molecules. On the other hand, the high-density and the comparatively low-temperature region called compact ridge in ~ 7 arcseconds southwest of the hot molecular core has various complex oxygen-bearing organic molecules. The chemical differentiation seen in these dense cores may have been driven by the difference in the physical conditions in their evolutionary/formation processes. Therefore, recently the chemistry in Orion-KL region is well studied by high spatial resolution interferometric observations with ALMA, SMA, etc to understand the formation mechanisms of high-mass stars. In this test observations with 50m-LMT/B4R extensive spread of oxygen-bearing molecules (CH_3OCHO , CH_3OCH_3 , etc.) centering on the compact ridge was confirmed. On the other hand, it was found that nitrogen-containing carbon chain molecules ($\text{C}_2\text{H}_5\text{CN}$, $\text{C}_2\text{H}_3\text{CN}$, HC_3N , etc.) and sulfur-containing molecules (SO_2 , OCS , etc.) widely distributed mainly in the hot core. Systematic changes in the distribution of chemical composition were clearly captured in this region. In addition, the high excitation lines of CH_3OCHO ($\nu_{18} = 1$) and the recombination lines of hydrogen were also detected for the first time in the 2 mm band. In this conference, we will report the results of the analysis of the spatial distributions of the molecular species and the temperature environment obtained toward Orion-KL at a spatial resolution of about 10 arcseconds (~ 0.02 pc) by the 50 m-LMT/B4R.

Keywords: ISM molecules, astrochemistry, star formation, radio lines, telescopes

Modeling of Nitrogen Fractionation in the Protoplanetary Disk around TW Hya

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Observations conducted using the Atacama Large Millimeter/submillimeter Array on the protoplanetary disk around TW Hya show the nitrogen fractionation of HCN molecules in $\text{HC}^{14}\text{N}/\text{HC}^{15}\text{N} \sim 120$ at a radius of ~ 20 AU. In this study, we investigated the physical and chemical conditions that control this nitrogen fractionation process. To this end, a new disk model was developed, in which the isotope-selective photodissociation of molecular nitrogen and isotope-exchange chemical reactions have been incorporated. Our model can successfully reproduce the observed HCN column density when the elemental abundances of the gas-phase carbon and oxygen are depleted by two orders of magnitude relative to those in the interstellar medium and carbon is more abundant than oxygen ($[\text{C}/\text{O}]_{\text{elem}} > 1$). The isotope-selective photodissociation of molecular nitrogen is the dominant nitrogen fractionation process in our models. The observed $\text{HC}^{14}\text{N}/\text{HC}^{15}\text{N}$ ratio, which increases outwards, can also be reproduced by the model by assuming that the small dust grains in the atmosphere of the outer disk are depleted more than those in the inner disk. This is consistent with grain evolution models, according to which small dust grains are continuously replenished in the inner disk due to fragmentation of the large dust grains that radially drift from the outer disk.

Keywords: Astrochemistry, Numerical, protoplanetary disk, isotope, TW Hya

Effects of deposition temperature on structural changes of amorphous ice in heating process

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In interstellar molecular clouds, various molecules such as H₂O, CO₂, NH₃, CH₄, H₂CO, and CH₃OH are formed from deposited elements such as hydrogen, oxygen, carbon, and nitrogen. The deposited H₂O exists as amorphous ice. The deposited molecules undergo chemical evolutions through various processes on amorphous ice. Amorphous ice formed from a vapor deposition is principally classified into two types: low-density amorphous (LDA) and high-density amorphous (HDA) ices. HDA ice is transformed into LDA ice with heating [1]. However, the mechanism of the phase transition is less conclusive, because the transition temperature depends on experiments [2]. To investigate the effects of deposition temperature on structural change in heating process, infrared spectra and temperature programmed desorption (TPD) curves of amorphous ice with heating were analyzed.

Amorphous ice was prepared with vapor deposition of distilled and degassed water on a substrate of oxygen-free copper at a temperature of 43.5–120.5 K. The total pressure in the vacuum chamber was kept at about 5.0×10^{-5} Pa during the deposition. After the deposition of amorphous ice, the substrate was cooled to 43.5 K at a rate of 2 K/min. Then, the sample was heated to 176 K at a rate of 1–4 K/min. The IR spectra were measured using Shimadzu IRPrestage-21 at every 15 seconds during deposition, and measured at 2 K intervals during cooling and heating. The TPD curves were measured using a quadrupole mass spectrometer. Q-mass (Pfeiffer QME220) during heating.

The wave number of the O–H stretching mode of the deposited amorphous ice changes in heating process due to a structural change. The result shows that the variation process of the wave number in heating process depends on the deposition temperature. The transition points can be analyzed from the variation in a changing rate of wave number with heating. For the ice deposited at temperatures below 82 K, three transition points exist in the temperature range of 43.5–160 K. The transitions observed at ~60 and ~100 K are attributed to the transition from HDA ice into LDA ice via an intermediate structure. The transition observed at around 150 K is crystallization to the cubic ice Ic from the LDA ice. For the ice deposited at temperatures above 85 K, only two transitions occur from the intermediate structure into LDA ice at ~100 K and the crystallization to Ic at ~150 K. The transition points depend on the deposition temperature before the heating. On the other hand, the beginning of the desorption of H₂O analyzed from TPD curves are ~50, ~90 and ~140 K. These values are approximately independent of the deposition temperature. This suggests that the transition of amorphous ice is induced by the desorption of H₂O due to a rearrangement of H₂O.

Keywords: Amorphous ice, Infrared spectroscopy

Phase transition of KOH-doped amorphous ice

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In interstellar molecular clouds, dust grains from a silicate mineral surrounded by amorphous ice exist [1]. The elements such as H, O, C, and N are adsorbed on the dust grains and form various molecules such as H₂O, CO₂, NH₃, CH₄, H₂CO, and CH₃OH. The molecules undergo chemical evolutions to organic molecules through various reaction processes. A photochemical reaction caused by ultraviolet (UV) irradiation is one of the dominant reaction processes [2]. Since amorphous ice is a reaction field in interstellar molecular clouds, it is important to understand the mechanism of structural change of amorphous ice due to the UV irradiation. Recently, Tachibana et al. [3] found that the viscosity of the UV-irradiated amorphous ice decreases at around 50 K.

The OH⁻ defects formed by UV irradiation are expected as a cause of the decrease in viscosity. To investigate the effect of OH⁻ on the structural changes during heating, the infrared (IR) spectra of KOH-doped amorphous ice were analyzed. KOH, has an effect to introduce the OH⁻ defect on ice and to promote the rotational motion of water molecules in ice [4].

Amorphous ice was prepared with vapor deposition of a solution of KOH on a substrate of oxygen-free copper at a temperature of 43.5 K. The concentrations of KOH were 0.0049–0.1 M. The total pressure in the vacuum chamber was kept at about 5.0×10^{-5} Pa during the deposition. After the deposition of amorphous ice, the substrate was heated to 176 K at a rate of 1–4 K/min. The IR spectra were measured using Shimadzu IRPrestage-21 at every 15 seconds during the deposition, and measured at 2 K intervals during the heating.

The structural transitions during the heating in the temperature range of 43.5–176 K are classified into the following four processes (i) transition from high density amorphous (HDA) ice to an intermediate structure at around 60 K, (ii) transition from the intermediate structure to low density amorphous (LDA) ice at around 100–120 K via the glass transition, (iii) crystallization to cubic ice (Ic) at around 145 K, and (iv) phase transition from Ic to hexagonal ice (Ih) at around 175 K. These transition temperature can be analyzed from the variation in a changing rate of wave number of the O–H stretching mode in IR spectrum with heating. The result shows that the transition temperatures of the transition (ii) depends on KOH concentration. The doped KOH has effect to promote the rotational motion of H₂O, because the decomposed OH⁻ from KOH is introduced in the hydrogen-bonding network and acts as a defect. This indicates that the rotational motion is a dominant mechanism for the transition (ii). Furthermore, it was found that the transition temperature of the transition (iii) depends on the wave number of the O–H stretching mode at the deposited temperature (i.e., 43.5 K), whereas no dependence was observed for the transition (i). This suggests that the surface structure is a dominant factor for the crystallization, and a rearrangement of water molecules due to the translational motion of oxygen is a cause for the formation of the intermediate structure.

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