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研究課題名（和文）Icy Origins of Organic Molecules Unveiled by JWST

研究課題名（英文）Icy Origins of Organic Molecules Unveiled by JWST

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研究成果の概要（和文）：太陽系の形成と進化の理解は、天文学研究の重要な課題です。新たに形成された原始星における複雑な分子の発見は、初期段階で広範な化学進化が進行していることを示しています。本研究では、これらの複雑な分子の生成に至る化学進化を解明することを目指しています。私はジェームズ・ウェッブ宇宙望遠鏡を用いて、若い原始星の氷の化学組成を調査し、水や二酸化炭素などの一般的な氷種、およびメタノールなどの複雑な分子を検出することに成功しました。また、その観測データから氷にどのような分子種が存在するかを調べました。さらに、氷の化学組成が形成され進化するシステムの物理的特性を解明するために気相分子に関する研究を進めました。

研究成果の学術的意義や社会的意義
The chemical evolution during star formation directly relates to the origin of solar system. At the same time, JWST has been revolutionizing our understanding of the universe. This program not only expand the view of our origin but also increase the public interests in astronomy.

研究成果の概要（英文）：Understanding how do we get here and how does our Solar system form and evolved have been a major pursue of astronomy research. Recent observations in the newly formed stars (protostars) found relatively complex molecules, indicating an extensive chemical evolution already taken place at such an early stage. In this research program, we aim to understand the chemical evolution that leads to the production of these complex molecules. To do so, we use the James Webb Space Telescope to probe the ice compositions in these young protostars, where complex molecules are thought to be formed. Using the data from the CORINOS program, we successfully detect common ice species, including water and CO2, as well as complex species, such as methanol and other complex molecules. In this program, we constructed the ice inventory in IRAS 15398-3359 and present comprehensive studies on the gas-phase molecules to constrain the physical properties of the system where these ices are formed and evolved.

研究分野：Astronomy

キーワード：Interstellar ice　Astrochemistry　Star formation

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１．研究開始当初の背景

Protostellar chemistry, while may appear distant from life on Earth, has substantial implications to planet formation as well as the chemical environment in the early stage of Solar system. Comets, which are thought to be a major reservoir of Earth's oceans, likely inherit heavy water (deuterated water) from the formation stage of our Sun because of their similar abundance to that in young protostars, classified as Class 0 and I protostars (Cleeves et al. 2014; Tobin et al. 2023; Nomura et al. 2023). For more complex molecules, recent observations start to routinely detect gaseous organic molecules in protostars, some of which also have similar compositions as that in comet 67P/Churyumov–Gerasimenko, which is the most well-studied comet (Drozdovskaya et al. 2019), further emphasizing the need of understanding protostellar chemistry to realize the formation and evolution of our solar system.

Protostellar environments are cold (~10-20 K; ~250°C below zero) and low-density (10^6-10^8 cm^{-3} compared to ~10^{19} cm^{-3} in Earth's atmosphere at surface), making them uniquely different from terrestrial chemistry. In such environments, substantial amount of gas freezes out onto dust grains, forming ice mantles where molecules have greater opportunities to react. Thus, the reactions take place on the ice mantles and between gas and ice drives the chemical evolution at the protostellar stage. In the last decade, interferometric observations at sub-millimeter wavelengths enable a leap of discovery in the gas-phase protostellar chemistry, detecting rare isotopologues and complex organic molecules (so-called COMs; Jørgensen et al. 2020 and the references therein). Using the gas-phase measurements, we can infer the chemical reactions on ice mantles if the gas simply sublimates from ice at high temperate without any additional gas-phase reactions. However, this assumption greatly simplifies the reality and must be tested by direct observations of ice.

Measuring the absorption spectral features at infrared wavelengths is the most accessible way to characterize the ice compositions. Radiation coming from the central protostar penetrates the icy molecules in the cold dense gas around the protostar (so-called the envelope). In this process, parts of radiation could be absorbed due to the vibration of the icy molecules, leaving distinct absorption patterns on the observed IR spectra, which allow us to identify the species as well as quantify their abundances. Detecting ice absorption requires high sensitivity IR observations, especially toward young protostars where the dusty envelope. Prior to the arrival of the James Webb Space Telescope (JWST), ice measurements relied on the Infrared Space Observatory (ISO), and the AKARI Space Telescope, and the Spitzer Space Telescope (e.g., Whittet et al. 2001; Öberg et al. 2011; Kim et al. 2022). Because of the limited sensitivity, these observations detect mostly simple ice species, including H_2O, CO, CO_2, CH_4, and CH_3OH, toward the sources with sufficiently bright continuum. Thus, while we obtained a general picture of ice compositions and their evolution in protostars, further studies on ice mixtures in various environments and the search for rare isotopologues and complex organic ice species were on hold until JWST.

２．研究の目的

JWST enables a leap in our capability to measure and search for absorption features of distinct molecular ices. The aims of this program are leveraging the Cycle 1 JWST observational program, CORINOS, to achieve the following goals.

- Characterize the ice composition in embedded protostars
- Search for complex organic molecule ice
- Determine the origin of the apparent gas-phase chemical diversity in protostars
- Impact of protostellar structure on ice composition

These goals are set to start from basic characterization of ice composition in IRAS 15398-3359 (hereafter IRAS 15398) using JWST spectra to plot a roadmap for the analyses of three other sources. The sensitivity and instrumental properties of JWST are substantially different than that of previous facilities, which requires substantial investigation with a single source. Beside ice absorption features, we also aimed to investigate the emission lines in the spectra, which trace the inner disks and/or outflows. Both structures play major roles in regulating the thermal history and chemical evolution of the source, complementing the interpretation of detected ice features.

３．研究の方法

The main goal of this program is to develop a roadmap for analyzing ice composition in embedded protostars. To achieve this goal, we initiated several projects covering both the ice- and gas-phase chemistry in IRAS 15398. The ice projects adopt two different methods to derive the ice optical depth spectra, local baseline and global baseline subtraction, which is where ice absorption features are further identified and measured. A local baseline is useful to extract isolated absorption features, which greatly simplifies the measurements. However, the JWST spectra, as we will show in the results section, have various broad absorption features that are very likely blended, hindering simple isolated studies of individual species. Thus, a global baseline with a global inventory of ice species provides another perspective to understand the ice composition.

The gas-phase emission lines are analyzed using slab models with Monte-Carlo Markov-chain fitting to simplify the physical structures while characterizing the uncertainties statistically. We also compare the outflow morphology detected in infrared wavelengths by JWST with the colder molecular gas detected in sub-millimeter wavelengths by ALMA, obtaining a complete picture of hot and cold gas in the outflows.

４．研究成果

As mentioned in above section, most of the results achieved in this KAKENHI program focus on IRAS 15398. As the PI of the observing program, I either lead the studies or serve as the primary collaborator or supervisor of the projects. Below sections highlight the results of individual projects related to this source.

First analysis of the MIRI MRS spectrum of IRAS 15398

We present detections of previously identified ice species and provide evidence for the possible presence of organic ice species (Figure 1). We also show gaseous emission of warm water and CO, which is often found in warm disks. Other detected emission lines, including H_2, [Fe II], [Ne II] and [S I], appear extended along the outflow direction, tracing a wide-angle outflow cavity and a collimated jet. The MIRI imaging serendipitously captured the south-western outflow of IRAS 15398, providing us an exquisite view of the outflow structure in the infrared.

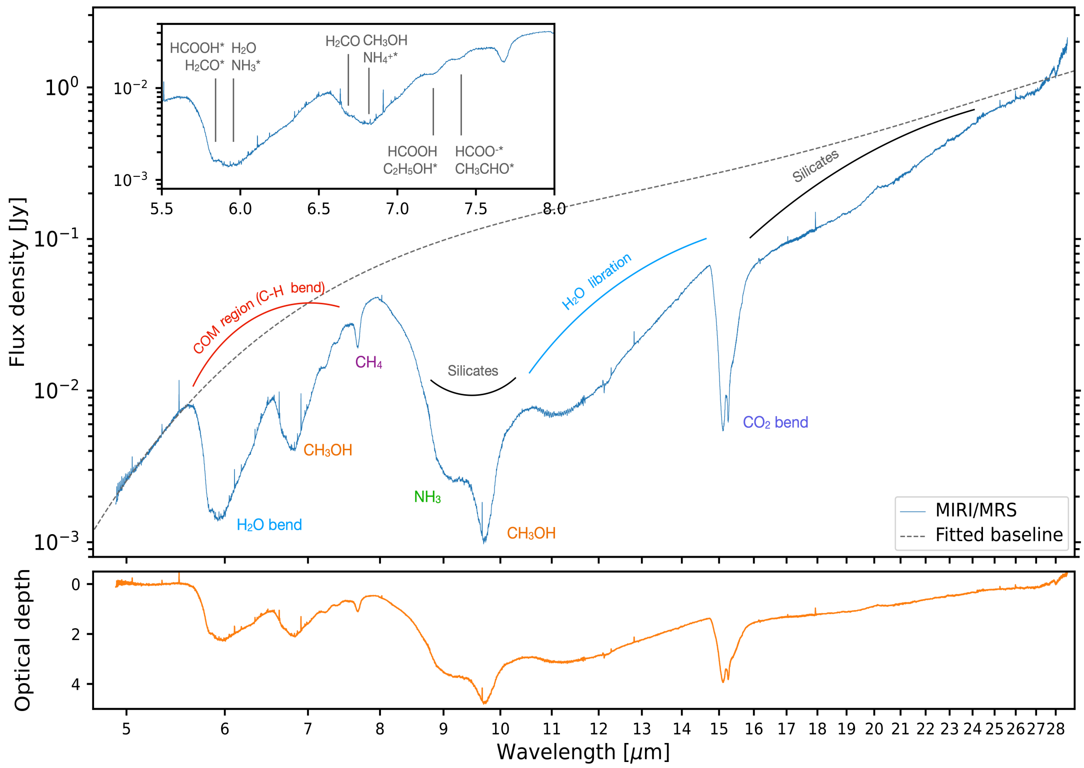

Figure 1. JWST MIRI/MRS spectrum of IRAS 15398-3359 with ice features labelled (top panel; Fig. 1 in Yang et al. 2022). The inset figure shows a zoom-in view of the 5.5-8.0 μm range. The bottom panel shows the optical depth spectrum derived with the estimated continuum in the dashed line.

The main conclusions of this first analysis of the JWST/MIRI observations of IRAS 15398 are summarized below.

- A MIRI MRS spectrum of a Class 0 protostar, IRAS 15398, is reported for the first time. The protostar appears as a point source over the full wavelength range at 5-28 μm.
- The MRS data show rich ice absorption features. Particularly, the ice features between 5 and 8 μm are detected with high S/N, allowing us to search for organic ice species. We robustly identify ice species including H_2O, CO2, CH_4, NH_3, CH_3OH, H_2CO, and HCOOH. Furthermore, we detect ice absorption features that could imply the presence of NH_4^+, $HCOO^-$, C_2H_5OH, CH_3CHO, and CH_3OCHO. The CH_4 and pure CO_2 ice features appear stronger in the MIRI MRS spectra compared to previous Spitzer studies. Significantly improved spectral resolution could result in deeper absorption, providing

accurate constraints on the ice compositions. Stronger absorption could also imply variability in ice column densities.

- The spectra between 5 and 8 µm have many weaker emission lines. The continuum-subtracted spectra present similar features to those from the synthetic spectra of warm water vapor and CO gas. These emission lines only appear toward the protostar, hinting at warm water vapor and CO gas on small scales possibly on the disk surface.
- The MIRI imaging captures the blue-shifted outflow of IRAS 15398, showing multiple shell-like structures consistent with the molecular outflows seen at sub-mm wavelengths. The infrared outflow has similar length as the sub-mm outflow. The proper motion of the compact shock knot indicates a dynamical time of ~150 year for that ejection.
- Multiple emission lines are detected in the MRS spectra, including [Fe II], [Ne II], [S I], and H_2. The H_2 S(8) line is the first detection in young protostars
- The [Fe II] and [Ne II] emission show a collimated bipolar jet-like structure along the known outflow direction. The emission also highlights a bright knot ~2.5" away from the protostar toward southwest. The emission of H_2 appears more extended, tracing a wide-angle outflow cavity.

Ice inventory of IRAS 15398

For the absorption features within the wavelength range of 8-22 µm, we conducted a continuum determination employing a method to subtract the absorption caused by silicate dust. Additionally, we isolated the ice component of H_2O, which predominates over other ice species in the spectrum, facilitating a comprehensive analysis of the present absorption features. Under the comprehensive fitting process to the absorption features in the H_2O-subtracted optical depth spectrum, we initially decomposed pure and mixed components comprising NH_3-, CH_3OH-, and CO2-containing absorption features. We derived the ice column densities from their prominent vibrational modes at each corresponding band. Furthermore, we discriminated other organic ice species such as H_2CO, HCOOH, CH_3COOH, CH3CHO, CH_3CH_2OH, NH_4^+, $HCOO^-$, CH_4, and SO2 from the absorption features superimposed on those major ice components. A tentative detection of NH_2CHO ice was suggested to contribute to the absorption at 5.88, 7.2, and 7.53 µm, corresponding to their respective vibrational modes. The presence of crystalline H_2O, pure CO_2, and NH_4^+ ice components indicates a hot phase history during the past mass accretion to IRAS 15398. The composite ice model is shown in Figure 2.

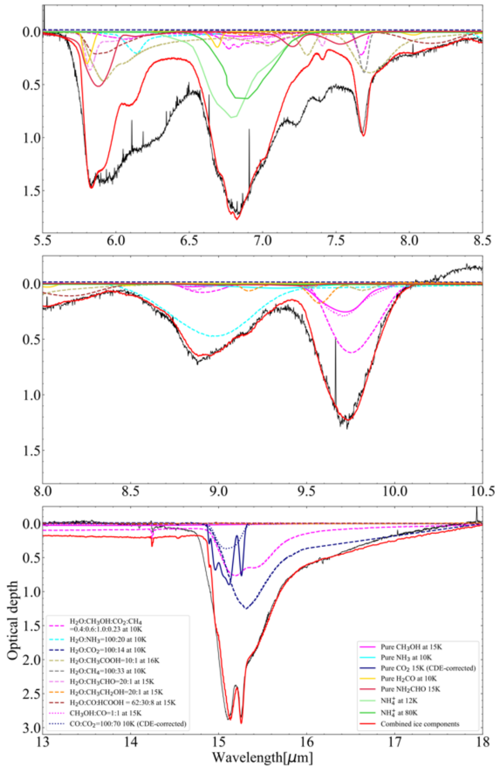

Figure 2. The composite ice model of IRAS 15398. The overall synthetic model is shown in red, while each ice species is indicated with colored lines.

COM ice modeling

The 7-9 µm spectrum contains the absorption features of several complex molecule ices (e.g., Terwisscha van Scheltinga et al. 2018), making it a particular interest to study and compare with the detection of their gas-phase counterparts using ALMA. Rocha et al. (2024) demonstrate that complex molecule ices can be identified and constrained in this wavelength range using

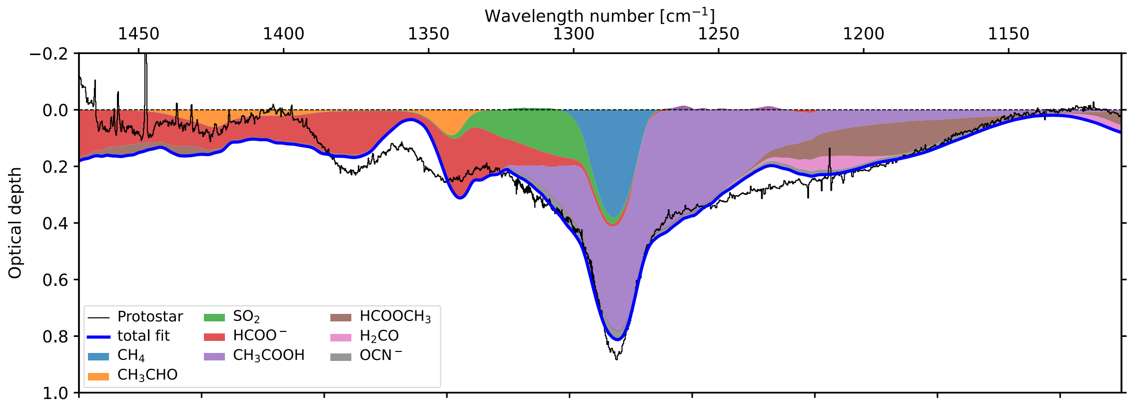

Figure 3. Optical depth spectra obtained with local baseline subtraction along with the best-fitting composite model of complex molecular ices.

JWST. In the spectrum of IRAS 15398, we detect potential absorption features of C_2H_5OH and CH_3CHO in the first analysis study of this source (Yang et al. 2023). In this research program, we further modeled these features with careful local baseline subtraction and optimizations with various laboratory data of complex ice species. Figure 3 shows the optical depth spectra after the removal of a local baseline as well as the best-fitting model of composite complex ice species. This model suggests the presence of several complex molecules in ice phase, including C_2H_5OH, CH_3CHO, CH_3COOH, $HCOOCH_3$, as well as simple species, such as SO_2 and CH_4. Most interestingly, the model also indicates the presence of $HCOO^-$, which has a specific interest for chemical evolution in ice mantles as it can indicate various salts formation in ice.

CO and water emission lines

In this work, we analyze newly-discovered mid-IR molecular gas-phase emission from the protostar IRAS 15398 - a discovery only made possible with the exquisite sensitivity of JWST's MIRI-MRS instrument. The MIRI-MRS line images constrain the observed CO and H_2O emission to $R \lesssim 40$ au, consistent with the size of the SO disk (Okoda et al. 2018), and in contrast to the much larger outflow cavity traced by HDO (Bjerkeli et al. 2016) in ALMA images. However, the CO and H_2O emission observed from IRAS 15398 do not have exactly the same characteristics as emission observed from Class II disks.

The CO emission temperature of > 1500 K is similar to CO observed from Class II T Tauri disks, in which the emission arises at or near the dust sublimation radius (Salyk et al. 2011b; Banzatti et al. 2015). However, the emission observed from Class II disks is consistent with $N \gtrsim 10^{18}$ cm^{-2} (Salyk et al. 2011b), at least a factor of a few higher than would be consistent with our observation of optically thin CO. The CO mass we derive here is also a factor 10^2-10^4 lower than total CO masses derived for the emitting column of T Tauri disks (Salyk et al. 2011b). If the CO we observe here arises from the inner circumstellar disk, perhaps this young disk atmosphere is less settled than in Class II disks, revealing a smaller CO gas column above the dust $\tau_{5\mu m} = 1$ layer. This is qualitatively consistent with first results from the ALMA eDisk program, which finds evidence that dust in protostellar disks is less vertically settled than in Class II disks (Ohashi et al. 2023). The CO emission from IRAS 15398 shows a ~7 km s^{-1} blueshift, similar in magnitude to CO emission line blueshifts attributed to disk winds in Class II disks (Bast et al. 2011; Pontoppidan et al. 2011). Therefore, the CO emission may also be associated with a slow molecular wind originating from the disk surface.

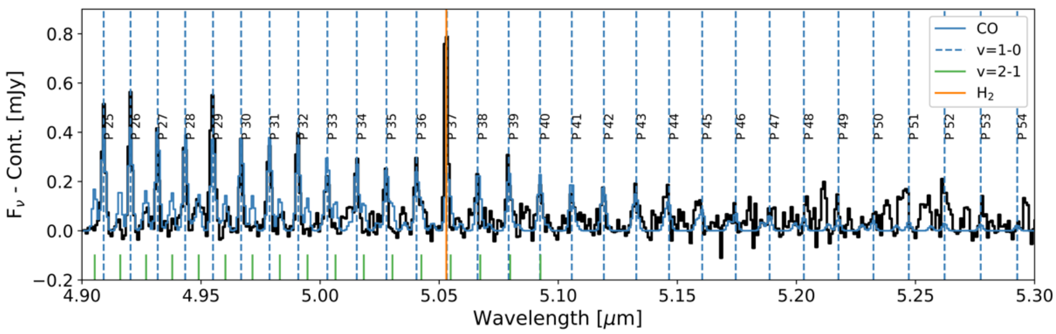

Figure 4. Identified CO v=1-0 lines along with the best-fitting model.

The H_2O emission from IRAS 15398 has different properties from the H_2O emission reported for Class II disks. We derive a water temperature of ~200 K, in contrast to typical ~500 K temperatures observed from Class II disk atmospheres (e.g., Salyk et al. 2011a). However, the improved spectral resolution of JWST as compared to Spitzer-IRS is now revealing multiple temperature components in water emission spectra from Class II disks, with cooler components as low as ~ 200 K (Banzatti et al. 2023b; Gasman et al. 2023). Banzatti et al. (2023b) suggest that the cooler water component might arise near the water snowline.

Summary

The projects enabled by this KAKENHI program cover a wide range of investigations on the composition of interstellar ice and their origins. This program supports the data analysis and modeling of the JWST CORINOS program, which is one of the first chemical characterization of young protostars with JWST. While the unprecedented sensitivity and resolution of JWST unveils signatures that have never been seen, the analysis of these data faced substantial challenges to produce robust and impactful results. In this report, we show the results ranging from broad characterization of ice absorption features to detailed modeling of specific ice species. We also show the physical properties of gas-phase emission related to the disk and outflow structure close to the protostar, unveiling a new region which cannot be probed by other facilities. These results serve as the roadmap to facilitate the analysis of other sources in the CORINOS program as well as other JWST programs with similar scientific goals.

5．主な発表論文等

〔雑誌論文〕　計3件（うち査読付論文　3件／うち国際共著　3件／うちオープンアクセス　3件）

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掲載論文のDOI（デジタルオブジェクト識別子） 10.3847/2041-8213/aca289	査読の有無 有
オープンアクセス オープンアクセスとしている（また、その予定である）	国際共著 該当する

1．著者名 Evans II Neal J.、Yang Yao-Lun、Green Joel D.、Zhao Bo、Di Francesco James、Lee Jeong-Eun、Jorgensen Jes K.、Choi Minho、Myers Philip C.、Mardones Diego	4．巻 943
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オープンアクセス オープンアクセスとしている（また、その予定である）	国際共著 該当する

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オープンアクセス オープンアクセスとしている（また、その予定である）	国際共著 該当する

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2．発表標題 Complex Chemistry in a Class 0 Protostars IRAS 15398-3359
3．学会等名 First Science Results from JWST（国際学会）
4．発表年 2022年

１．発表者名 Yao-Lun Yang
２．発表標題 Evolution of Organic Chemistry from Ice to Gas: The Synergy between ALMA and JWST
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１．発表者名 Yao-Lun Yang
２．発表標題 Ice Chemistry in the Era of JWST
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1．発表者名 Yao-Lun Yang
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〔図書〕　計0件

〔産業財産権〕

〔その他〕

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6．研究組織

	氏名 （ローマ字氏名） （研究者番号）	所属研究機関・部局・職 （機関番号）	備考

7．科研費を使用して開催した国際研究集会

〔国際研究集会〕　計0件

8．本研究に関連して実施した国際共同研究の実施状況

共同研究相手国	相手方研究機関			
韓国	KASI	Seoul National University		
米国	University of California Berkeley	University of Virginia	Vasser College	他3機関
オランダ	Leiden Observatory			