Preliminary results on spectral line survey of Uranus at the millimeter/sub-millimeter wavelength using ALMA data

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Abstract. Previous studies and spectroscopy observations concluded that Uranus has the fewest spectral line features among other giant planets. It is challenging yet very possible to conduct the line survey with the abundance of available Uranus observation data, particularly in millimeter/sub-millimeter. As a sensitive radio interferometer, Atacama Large Millimeter/submillimeter Array (ALMA) frequently observes Uranus from wide viewing windows and the narrow spectral resolution which is very suitable for spectral survey study. In this paper, we report the preliminary results of Uranus’ spectral line survey over various ranges of ALMA spectral windows at bands 3 to 9, taken from 2012 – 2018. With CASA data processing tools, the survey results from 451 spectral windows (spw), 216 line candidates from 98 spw were suspected as the first step to examine molecule’s existence in Uranus. Although most of them had SNR below 3, some prominent spectral line features were detected tentatively such as the line profiles at the frequency of carbon monoxide (CO) and methanol (CH\textsubscript{3}OH). The inconsistent results on CO confirmed the previous theory that this molecule might be originally from external. Although this CO detection is an important finding as it might be the first time to be discovered in Uranus from ALMA, to declare as a real detection, it is necessary to confirm with more observations and correction with some relevant factors.

1. Introduction
In our Solar System, Uranus is an enigmatic body with its extreme rotational axis, very low internal heat source, and poorly constrained interior structure as well as its magnetic fields, magnetosphere, and ring-moon system [2]. The knowledge of this ice giant is limited by the only spacecraft to visit was flyby mission of Voyager 2 in 1986. Meanwhile, Uranus has become more essential to look after since the recent exoplanet finding state that ice giants turn out to be the most common type [10]. This body indeed occupies a special place in the formation and evolution of the Solar System as our local laboratory [1, 11, 9].

Along with the development of technology, it is widely possible that new observations can simply revise prior theories or discoveries. Despite the unknown detail from the closer look over spacecraft, many Uranus’ observation has been carried out with cutting-edge instruments both on space and ground-based. From multi-wavelength observation, many surprising results were obtained. Features like cloud-storm during the equinox period when the equator comes towards Earth have been observed in visible light and infrared (e.g. [12, 7, 21, 22]). With spectroscopy at infrared, some molecular spectra especially the hydrocarbon (e.g. [4, 19]) as
well as hydrogen sulfide (HS) [13] were observed. At radio wavelength, Marten et al. (1993) searched carbon monoxide (CO) and hydrogen cyanide (HCN), resulting in the non-detection on Uranus but successfully detected on Neptune [16]. There was also new finding of CS in Neptune using Atacama Large Millimeter/submillimeter Array (ALMA) by Moreno et al. (2017) [18]. CO on Uranus finally was first discovered at infrared wavelengths with ESO-VLT [8]. Then, at the mm/sub-mm, CO was also searched with IRAM and JCMT, but only resulting in the new upper limit value [5]. They continued to look for CO at sub-mm in 2012 with Heschel-HIFI, then finally obtained the glory results of the first CO detection in sub-mm using the space telescope [6]. The observation from Cavalie et al. (2014) also concluded that CO abundance in Uranus decreases with altitude, very convincing that it is sourced externally [6].

Compared to other giant planets, Uranus atmospheric dynamics, enrichment, including hydrocarbon specimens is quite distinguish [14]. As the twin of Neptune, which is supposed to has similar inner atmospheres, the compositions and thermal structures is different [16]. It is probably due to very low internal heat regarding the slower internal circulation in the ice mantle [10]. The vertical convection pressure on Uranus inner atmosphere is more likely to hold molecules out of the interior, causing some molecules are disequilibrium before emerging to its surface [16]. It can also be the reason for fewer features and spectra found in the Uranus atmosphere. Meanwhile, Neptune possesses internal heat flux and high air content which can trigger turbulence and storms. The very weak internal heat source on Uranus also indicates that most of the dynamics are influenced by the Sun [24, 7].

With the understanding of the near absence of internal heat, as well as less dynamic atmospheric condition on Uranus, the search for new spectral line is somewhat challenging. However, some of those previous findings motivate us to conduct the line survey, especially to the related molecules such as CO and HCN. It could be difficult yet widely open the possibilities to find feature by spectral line survey with the abundance of available Uranus data. In mm/sub-mm, ALMA frequently observes Uranus from time to time, mostly as the calibrator target. With the narrow spectral resolution and a wide window of ALMA, this research aims to conduct the spectral line survey on Uranus over various spectral windows. In this paper, we report the preliminary results of this line survey study.

2. Data and method

Uranus is a relatively close and bright object to be observed with the sensitive radio telescope antennas, making it one of the most widely used calibrators for observing major scientific targets. Therefore, the available Uranus’ observation data are quite abundant, particularly the early cycle data from bands 3, 6, 7, and 9. In this section, the Uranus observation data at the millimeter/sub-millimeter of ALMA as well as the processing tools to find the desired spectra will be explained.

2.1. ALMA data

The Atacama Large Millimeter/submillimeter Array (ALMA) consists of 66 antennas with the longest baseline up to 16 km. It is located in a dry climate and very high altitude around 5000 m at Chajnantour Plateau, Chile. The telescope’s resolution can reach arcseconds to milliarcseconds, while its pointing accuracy reaches less than 0.6 arcseconds [3]. ALMA interferometer covers a large frequency range divided into several bands which operate in several cycles. With the wide window but narrow channel width, ALMA data are very appropriate and widely potential to achieve the objectives of this study.

In this survey study, the more data used the wider opportunity to find features. However, the data selection is important to confine a large amount of Uranus data available from the ALMA archive. Since Uranus was often observed on several projects in ALMA, we listed selections criteria in table 1. All the Uranus data used for the survey were calibrator
observations of ALMA from 2012 to 2017 at band 3 (35-50 GHz), 4 (125-163 GHz), 6 (211-275 GHz), 7 (275-373 GHz), 8 (385-500 GHz), 9 (602-720 GHz). The relatively large Uranus data were downloaded from the ALMA archive, which can be accessed through its website (https://almascience.nrao.edu/aq/?resultview=observation).

| Table 1. ALMA Data Selection. |
|-------------------------------|
| Parameter | Option                  |
| Spectral resolution | <1000 kHz             |
| Integration time    | >300 seconds           |
| Option             | public data only       |
| Selected Bands     | 3, 4, 6, 7, 8, 9       |

A completed data package should contain all of the ALMA data structure such as several directories of product, calibration, and raw data which are compiled in one main project directory. More about ALMA and its data archive can be seen at ALMA Technical Handbook [20] and Data Archive Manual [23].

2.2. CASA data processing
After careful data selection, we used the Common Astronomy Software Application (CASA) with a python interface by McMullin et al. (2007) [15]. In this work, data processing was carried out with CASA version 4.5.3, 4.7.2, 5.1.0, and 5.4.0, because we used data from the early cycle until 2018. The difference between versions 4 and 5, generally is the use of pipeline for the upgrade version, in which each version can be downloaded at the CASA website (https://casa.nrao.edu/casaobtaining.shtml).

To begin with, ALMA data as input will experience a flagging process to eliminate unnecessary signals and generate a flagging table. ALMA provides raw data, named Alma Science Data Models (ASDM). After being successfully calibrated, the raw data will have output extension as measurement set (.ms). This file is a dataset consisting of several tables of visibility data from observations and their supporting files. As an important step, the calibration itself was time-consuming, depending on the amount and size of the raw data. At the CASA logger, we can see some important information such as the time and duration of the observation, all observation objects both scientific targets and calibrators, the number of spectral windows (spw), the number of channels in each spw, spectral resolution or channel width in kHz.

All calibrated data were analyzed using calibratorLines to detect possible lines in the ALMA calibrator. The program extracts each spectral window from the calibrator object, analyzes the spectrum with wavelet filtering, then assigns values and labels to the detected lines. The final result of the calibratorLines is a frequency table file against flux and plots of each object in each spectral window in two polarization. Then, some data containing prominent features were also plotted at each spw with task CASA plotms.

2.3. Molecular line identification
Each surveyed spectral window containing both emission and absorption features was assigned a molecular name that coincides with the particular frequency. In this work, we used the ALMA catalog, called Splatalogue database for astronomical spectroscopy (https://splatalogue.online/). Especially, for all spectral windows that span at some rotational line frequencies of CO and HCN, were directly matched with molecule catalogs.
Then, we used NASA Planetary Spectrum Generator (PSG) (https://psg.gsfc.nasa.gov) as an initial analysis of the radiative transfer of several line profiles detected. PSG is a tool for synthesizing the spectrum of planets and other objects with a very wide wavelength range from various observation instruments, developed by NASA [25]. Radiative transfer modeling was carried out using a hydrostatic equilibrium atmosphere with a vertical profile of 50 layers adopted from Marten et al. (2005) [17].

Before investigating the molecule candidate from survey result, it is important to distinguish a line source other than Uranus. The absorption lines that appear very deep are highly possible originate from the Earth’s atmosphere, known as the telluric contamination line. This can be confirmed from the other calibrator objects with similar profile at the same frequency. So it can be ascertained that it is telluric line contamination, not from Uranus. Examples of telluric lines detection are given in figure 1.

![Figure 1](https://example.com/figure1.png)

**Figure 1.** Telluric contamination of the Earth’s atmosphere on Uranus (left) and the bandpass J2333-237 calibrator (right) from project 2011.0.00172 spw 2.

Telluric features are clearly visible from both Uranus (left) and from other calibrator (right). It was observed on August 11, 2012 from project 2011.0.00061.S at spw 3. The figure shows two distinct absorption features marked in red rectangular dots. At 109.5619 GHz it coincides with the vinyl cyanide (CH$_2$13CHCN) band, while at 110.8328 GHz it coincides with the ethyl cyanide (13CH$_3$CH$_2$13CN) band. Telluric confirmation was answered by the spectrum of J2258-279 as a bandpass calibrator which also showed an absorption profile at exact frequency.

3. Result and analysis

Over 451 spectral windows from 94 observational data, the appearance of the suspected line was only obtained from 98 spectral windows. We suspected 216 lines from 50 observational data within 21 different projects. In other words, 44 spectral data which have been successfully calibrated did not provide line features. Most of the detected lines coincide with the frequency of organic compounds containing C and H atoms, such as methanol, methyl format, acetone, vinyl cyanide, ethyl cyanide, and others. Some of them belong to the alcohol group containing the -OH hydroxyl group. Nevertheless, in the catalog, such molecules have many rotational lines, so that the validation is rather difficult. The result also shows that almost all of the lines have SNR value of <3, which is too weak as a radio signal. Because the strong lines candidate with appropriate SNR value are limited, our results on the acquisition of 216 lines are still a tentative detection. However, this work is also an important step as the initial study to determine molecules candidate on Uranus, making use of many ALMA data.

This kind of statistic results briefly proves that Uranus is indeed different from other planets because it contains very few particular molecules in its atmosphere. In the subsections below,
some tentative detection spectra will be presented both from Plotms CASA (left images) and the wavelet filtering with calibratorLines (right images). Each horizontal axis explains frequency in GHz, while the vertical axis explains amplitude in Jansky.

3.1. Prominent lines spectra
After being distinguished from the telluric line profile, there are several detection lines with a fairly prominent profile. Some of these lines shown in figure 2 are coincide with organic compounds. Two spectra above were observed at band 6, while a spectrum below was observed in band 7. Last image also contains telluric line as it was also detected on the other calibrator which is shown on square box inside spectrum. The following spectra are the line identification results at the frequency of acetone ((CH$_3$)$_2$CO) at 249.96 GHz, methyl formate (CH$_3$O$_{13}$CHO) at 221.53 GHz, and ethylene glycol ((CH$_2$OH)$_2$) at 352.863 GHz.

![Some prominent detection at the frequency of organic molecules: acetone (top left), methyl formate (top right), and ethylene glycol containing telluric (bottom).](image)

Despite having a high amplitude relative to the other profiles obtained, the prominent line at the frequencies of these three molecules was not found in other observational data. These groups of organic compounds also have many rotational lines in the molecular catalog because of their non-linear nature. Thus, these spectra in figure 2 need to be reviewed more, especially with other observational data as confirmation and comparison.

3.2. Line detection at the frequency of methanol
The four-panel images in figure 3 are the most prominent profile obtained from the survey results in the observation of band 8 project 2015.1.00384.S spw 22. It is quite surprising that the lines were found outside the criteria because it has a wide channel width of 15 625 kHz. Band 8 data was limited, so we used the existing Uranus observation data. The emission profile of the line on the methanol frequency in figure 3 comes from 4 observations of Uranus as a flux calibrator conducted on 16 July 2016/09:08:55.3 (X293), 29 July 2016/08:58:38.4 (X1019), 10 August 2016
/ 07:12:35.5 (Xa728), and 12 August 2016/06:35:18.1 (X8e84). In each image two emission lines are seen, the shorter amplitude falling at the frequency of 481.601 GHz coincides with CH3OH vt = 0-2 (10(0) - 9(0)) while the higher feature at the frequency of 481.220 GHz coincides with CH3OH vt = 1 (10(8.3) - 9(8.2)).

Figure 3. Detected lines at the frequency of methanol (CH3OH) from 4 observation data at band 8/project 2015.1.00384.S.

Methanol itself is a complex chemical compound derived from methane. As a building block for more complex compounds, such as amino acids, methanol plays an important role in the formation of the rich organic chemicals for life. Even though the detection of several lines at these bands is interesting as it also has never been found on Uranus, further observations and confirmations are certainly important. Thus, the initial studies of the radiative transfer model have been carried out to confirm these methanol line detection in figure 3. We used PSG NASA by entering several observation parameters such as instruments, wavelength, resolution, antenna diameter, and others in the model.

Figure 4. Spectrum Model of related methanol frequency on Uranus with the Planetary Spectrum Generator. The left panel shows all noise components in which the line color descriptions are given at the top right. The right panel describes telluric transmission as the absorption line at the related frequencies.
The left panel of figure 4 illustrates all noise components which are represented in different color lines. It turns out the profile with two precise peaks at the detected frequency is shown as the contribution of the source itself (Uranus), detector, telescope, background, Earth, and the total. Unfortunately, there is a high possibility that the sharp lines detected in figure 3 coincides with methanol bands are not only from Uranus. This analysis is also reinforced by the right panel of telluric transmission from Earth’s atmosphere which clearly shows the presence of two absorption line profiles at the exact same frequencies.

3.3. Line detection at the frequency of carbon monoxide
There are a number of spectral windows containing rotational frequencies of CO and HCN bands as well as their isotopes. But unfortunately, most of the data do not contain their spectral profiles. Particularly in the HCN bands, non-detection was confirmed after examining all data. In the following discussion, several candidates of CO lines obtained from the survey results is shown in figure 5. The first two images are spectra from the same data but different spw, while the following two images were observed at different periods. At the panel above, it appears that there are many emission and absorption lines which the boundaries and noise floor are somewhat unclear. But after wavelet filtering, several profiles that coincide with some molecular lines appear (below). Even so, in this section, we focus on the detection only at the CO frequency.

![Figure 5](image.png)

**Figure 5.** Some features were found at several CO rotational lines and isotopes, presented from Plotms CASA (above) and the wavelet filtering (below). The 2 images on the left were from project 2016.1.01305.S in spw 1 and 5, while the other last 2 images were from two observation data of project 2012.1.00097.S spw 0.

The first and second spectra were originated from the same data project 2016.1.01305.S at spw 1 (345.678 - 345.928 GHz) and 5 (330.720 - 330.470 GHz). The observation on band 7 was carried out on 7 July 2017, with a 7-meter array. Each has a channel number of 2,048, a channel width of 122 kHz, and a total bandwidth of 250,000 kHz. On the first image, at a frequency of 345.796 GHz, there is a spectral profile that coincides with the (3-2) line of CO. While in the second image, a more prominent emission line profile is found at the isotope frequency 13CO (3-2) at 330.588 GHz. The value of noise of the observation data is estimated at 0.683 Jy. Both third and fourth images, from project 2012.1.00097.S spw 0 (345.107 - 346.045 GHz), show an absorption line that coincides with the the (3-2) line of CO at 345.796 GHz. The data
observed at band 7 was taken with 7 meters array at two different observation times, 26 April 2014 at 12:27:52.4 UT (third) and 08 October 2013 at 05:12:08.9 UT (fourth). Each data has total of channel 3,840, a width of channel 244 kHz, and a total of bandwidth of 937,500 kHz. Nevertheless, all the SNR are very low, and there are too many undulations to the noise floor, so that it is doubtful whether these spectra are real CO lines.

Finally, the remarkable profiles at the CO frequency were found, as the most prominent feature among all line survey result. The data were carried out with a 7 meter mosaic array, resolution of 488 kHz, and integration time of around 300 seconds. The image in figure 6 above was observed on 3 October 2016 and below was on 4 October 2016, both from band 6 project 2016.1.00007.S. The scientific target of the observations was the variable star Mira LL Pegasi (AFGL3068), while the flux calibrators other than Uranus were Neptune and QSO J2253+1608 as the phase calibrator. Observations of Uranus were made with 7-meters array for 302.400 seconds with a resolution of 488.278 kHz. The two fairly strong CO emission line profiles in figure 6 were detected at spw 16.

Figure 6. Strong line detection at (2-1) line frequency of CO from band 6 with noise of around 0.12 Jansky.

Both observation data in figure 6 show emission lines at a frequency of 230.540 GHz which almost coincides with the (2-1) line of CO frequency at 230.538 GHz. A slight shift may be due to the absence of a correction factor. The left panel shows that the amplitude values around 9 Jansky (above) and 8 Jansky (bottom), but the results on the right show the value reduced by half. These appropriate values were caused by further processing including wavelet filtering analysis.

As on the previous confirmation of methanol, a preliminary radiative transfer analysis was also performed on CO finding parameters. Yet much different from methanol, the CO analysis result is actually quite appropriate, despite of the fairly high frequency shift and appearance of the absorption continuum. In figure 6 it can be seen the spectrum coincides with frequency of 230.540 GHz, while in the model (see figure 7) the spectrum peaks at 230.516 GHz, which shifts
quite far even from the rest frequency of CO(2-1) line at 230.538 GHz. Nevertheless, in the noise component spectra as seen in figure 7 left, the CO contribution only comes from Uranus. Meanwhile, the telluric spectra show no absorption indicating the line is not contaminated. Therefore, if there is a line at that particular frequency, it means it really comes from Uranus.

**Figure 7.** Spectrum Model of noise components (left) and telluric transmission (right) in the related CO frequency on Uranus with the Planetary Spectrum Generator.

The finding of candidate CO(2-1) lines, especially those shown in figure 6 among hundreds of lines surveyed in this study, is a satisfactory result. As it is explained in section 1, the original aim of this work was to conduct a line survey making use of the abundance of available ALMA data without targeting many new discoveries due to Uranus internal and atmospheric condition. If the line is indeed the CO(2-1) band, this discovery can be said to be the first discovery made at millimeter/sub-millimeter wavelengths on the Earth’s surface with the ALMA interferometer data. The high sensitivity of ALMA has proven that the interferometer can detect the sharp profile coincide with the CO(2-1) line of Uranus at band 6.

However, such a line profile hasn’t been found in the other spectral windows data, even though the same observation parameter was used. Thus, the inconsistency of the appearance of CO in this finding needs to be scrutinized. Generally, in the atmosphere of a planet, there are equilibrium reactions in the inner atmosphere, cooling reactions in the middle atmosphere, and photochemistry in the upper atmosphere. Since its presence is not always consistent, it is possible that the CO on Uranus is not in equilibrium. As it was explained in section 1, due to the low internal heat and the vertical convection pressure in the inner atmosphere, the molecules may disequilibrium before they emerge to the surface. Various literature discussing CO intake on Uranus most likely come from external sources such as comets. As comparison, CO in Neptune is quite balanced because apart from external sources, it also sources from its internal. This is also as expected as the observation that the abundance of CO decreases with altitude from the stratosphere to the troposphere [6].

4. Summary

(i) ALMA frequently observes Uranus as calibrator target with the narrow spectral resolution and wide observation window, making it very suitable for spectral line survey studies. Of all the data downloaded, 83.3% were successfully calibrated. We obtained 451 spectral windows from 95 observation data of 37 ALMA projects, yet only 18% contains detectable spectra, resulting in 216 tentative line detection. Using Splatalogue molecular database, it is known that most of them roughly coincide with the frequency of organic compounds which have many rotational lines. Meanwhile, the result shows a very low average SNR of 3. It can be concluded that detection of lines on Uranus is not simple despite the use of sensitive instruments and large survey data. Uranus barely undergo such phenomena in the atmosphere due to almost no internal heat sources to trigger chemical reactions to form molecules.
(ii) The most intriguing finding were probably on the line detection at methanol and CO(2-1) bands as the spectra look fairly sharp and found in some data. However, the spectral irradiance model of methanol indicates the line features were contributed not only from Uranus but also other sources. Meanwhile, the strong line on CO(2-1) was confirmed from Uranus, in spite of the frequency shift. Yet, the inconsistency of CO line candidate finding is in line with the previous research that CO molecules on Uranus might decrease with altitude [6], and is not in equilibrium [16]. This result may reinforce preceding finding that CO in Uranus most likely come from an external source.

(iii) Detection line at CO(2-1) band on Uranus can be a new notable finding because previously this molecule rotation line has never been found with ground-based telescopes in millimeter/sub-millimeter, especially ALMA. However, to declare it as real detection, more findings in various frequency bands, such as 7, and 9, are needed as complementary data as well as the deeper radiative transfer analysis to investigate the spectra. It is also necessary to add correction factors such as rotation effects and other relevant factors.

Acknowledgments
This project makes use of some ALMA data: ADS/JAO.ALMA2011.0.00061.S, ADS/JAO.ALMA2011.0.00172.S, ADS/JAO.ALMA2016.1.00193.S, ADS/JAO.ALMA2012.1.00720.S, ADS/JAO.ALMA2016.1.00911.S, ADS/JAO.ALMA2016.1.01123.S, ADS/JAO.ALMA2016.1.01533.S, ADS/JAO.ALMA2016.2.00006.S, ADS/JAO.ALMA2016.2.00042.S, ADS/JAO.ALMA2016.2.00171.S, ADS/JAO.ALMA2016.1.00007.S, ADS/JAO.ALMA2016.1.00803.S, ADS/JAO.ALMA2015.1.01008.S, ADS/JAO.ALMA2016.2.00147.S, ADS/JAO.ALMA2016.1.00121.S, ADS/JAO.ALMA2012.1.00097.S, ADS/JAO.ALMA2016.1.01206.S, ADS/JAO.ALMA2016.1.01305.S, ADS/JAO.ALMA2016.1.01533.S, ADS/JAO.ALMA2016.2.00117.S, ADS/JAO.ALMA2015.1.00997.S, ADS/JAO.ALMA2015.1.00384.S, ADS/JAO.ALMA2011.0.00083.S. ALMA is a partnership of ESO (representing its member states), NSF (USA) and NINS (Japan), together with NRC (Canada), MOST and ASIAA (Taiwan), and KASI (Republic of Korea), in cooperation with the Republic of Chile. The Joint ALMA Observatory is operated by ESO, AUI/NRAO and NAOJ.

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