Spectroscopic detection of $^{13}$CH$_3$CH$_2$CN, CH$_3$COCH$_3$ and H$_2$O in the atmosphere of Jupiter using ALMA

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ABSTRACT

Various trace species were detected for the first time in the atmosphere of Jupiter with the collision of comet Shoemaker-Levy 9 in July 1994 near 44° S. These trace species can be used to understand the dynamics and chemical mystery in the atmosphere of Jupiter. We present the spectroscopic detection of the emission lines of ethyl cyanide ($^{13}$CH$_3$CH$_2$CN) ($\sim$12σ) with transition J = 52(5,48)–51(6,45) at frequency $\nu$ = 195.430 GHz and acetone (CH$_3$COCH$_3$) ($\sim$3σ) with transition J = 50(38,12)–50(37,13)EE at frequency $\nu$=195.721 GHz in the atmosphere of Jupiter using Atacama Large Millimeter/Submillimeter Array (ALMA) with column density $N(^{13}$CH$_3$CH$_2$CN) = 3.52 x 10$^{14}$ cm$^{-2}$ and $N$(CH$_3$COCH$_3$) = 5.31 x 10$^{10}$ cm$^{-2}$. We also confirm the presence of water vapour in the atmosphere of Jupiter with the detection of absorption line of water (H$_2$O) at frequency $\nu$ = 183.310 GHz with transition J = 3(1,3)–2(2,2) with column density $N$(H$_2$O) = 9.25 x 10$^{14}$ cm$^{-2}$ ($\sim$4.3σ statistical significance). We discussed possible photochemical pathways to produce detected organic molecules in the atmosphere of Jupiter.

Subject headings: Jupiter; Jupiter, atmosphere; Millimeter; Planetary systems; Spectroscopy; Astrochemistry
1. Introduction

In 1994, the fragments of comet Shoemaker-Levy 9 collided with the stratosphere of Jupiter (known as SL9 event) and formed many volatile gases like CS, HCN, CO, $\text{H}_2\text{S}$, CS$_2$, S$_2$, and OCS (Lellouch et al. 1995; Nol et al. 1995; Moreno et al. 2003). Jupiter atmosphere consists of 71% hydrogen, 24% helium, and 5% other dense elements (Gautier et al. 1981). The atmosphere of Jupiter also contains a large number of trace gases like methane, ammonia, carbon, ethane, hydrogen sulfide, phosphine, sulfur, and silicon-based compounds (Kunde et al. 2004). The outer layer of the atmosphere contains frozen ammonia in crystal form (Mason 1980). In the Jupiter atmosphere, a big amount of benzene and other hydrocarbons are found using infrared and ultraviolet measurements (Friedson et al. 2002). Jupiter is permanently covered with a composed cloud of ammonia crystals and possibly ammonium hydrosulfide (Loeffler et al. 2017).

In the interstellar medium, the CN compounds (which is also known as propionitrile) are quite abundant. It is a simple aliphatic nitrile and water-soluble liquid. We detected ethyl cyanide (CH$_3$CH$_2$CN) from the atmosphere of Jupiter. Earlier, ethyl cyanide was also found in Saturn’s largest moon Titan (Cordiner et al. 2015) and recently ethyl cyanide was found in Venus atmosphere at $\nu$=259.869 GHz with transition J = 29(12,17)–28(12,16) with 9.8$\sigma$ statistical significance (Manna et al. 2020) using Atacama Large Millimeter/Submillimeter Array (ALMA).

We also detected acetone (CH$_3$COCH$_3$, also known as propanone) from the atmosphere of Jupiter. In the solar system, acetone is the second detected molecule with ten atoms after glycine. Glycine is the first ten atoms molecule detected in solar system which is observed in Venus atmosphere with transition J=13(13,1)–12(12,0) at $\nu$=261.87 GHz (16.7$\sigma$ statistical significance) with column density N(glycine) = 7.8×10$^{12}$ cm$^{-2}$, using the ALMA (Manna et al. 2020). Acetone was first detected in the hot molecular core of Sgr B2 (Combes et al. 1987; Snyder et al. 2002).

Infrared spectra of the Short-Wavelength Spectrometer (SWS) of ISO detected the water vapour (between 39.48–44.19 $\mu$m) in the upper atmosphere of four giant planets and Saturn moon Titan in order of (1–30)$\times$10$^{14}$ molecules cm$^{-2}$ which provided the evidence with an external source of oxygen (Feuchtgruber et al. 1999). In the atmosphere of Jupiter, the Juno microwave radiometer detected the abundance of water vapour (with J = 5–6 transition) at 1.25–22 GHz with approximate pressure 0.7 to 30 bar (Li et al. 2020). The detection of water vapour using Juno spacecraft microwave instrument indicated the Jupiter is enhanced in oxygen by roughly three times the solar abundance at the equator which is very important to understand the formation of Jupiter cloud and weather (Bjoraker 2020). The atmospheric cloud layer is 50 km deep and consists of two decks of clouds with a thick lower deck and a
thin cloudy region. In the thin cloudy region, a layer of water clouds is present under the layer of ammonia (Benard et al. 1967). In the atmosphere of Jupiter, the water clouds make flashes of lighting, and these electrical discharges are a thousand times more powerful than the lightning on Earth (Dyudine et al. 2002).

In this paper, we present the detections of ethyl cyanide and acetone in the atmosphere of Jupiter using ALMA with TP (Total power)+7m ACA (Atacama Compact Array) data. We also confirmed the presence of water in the atmosphere of Jupiter with detection of transition $J = 3(1,3)\rightarrow 2(2,2)$. In Sect. 2, we briefly describe the observations and data reductions. The result of detection and photochemical reaction is presented in Sect. 3 and 4. The discussion is presented in Sect. 5.

2. Observations and data reduction

The giant solar planet Jupiter was observed with ALMA\(^1\) in the cycle 4 using combining Atacama Compact Array (7m diameter with short baseline) and total power (TP) 12m single-dish. The ACA observation was done on 27 August 2018, and TP observation was done on 20 September 2018. The data set initially included four spectral windows with bandwidth 125 MHz for TP data and 200 MHz for ACA data with ALMA Band 5 which centred at 195.940, 183.297, 183.297, and 195.940 GHz, respectively. A total of 14 antennas were used during ACA and TP observations. The spectral setup included the $\text{H}_2\text{O}$ ($J=3(1,3)\rightarrow 2(2,2)$) line at $\nu=183.310$ GHz which was part of spectral window 18 in single-dish data. The spectral peaks were identified using the online Splatalogue database for astronomical molecular spectroscopy and also using Cologne Database for Molecular Spectroscopy\(^2\) (CDMS) (Müller et al. 2001) and the JPL catalogue. The line corresponding to the atmospheric gas $^{13}\text{CH}_3\text{CH}_2\text{CN}$ and $\text{CH}_3\text{COCH}_3$ were also covered within the frequency range (see detail in Table. 2). During the observation, J1256–0547 was used as a phase calibrator, and J1507–1652 was used as a bandpass calibrator. We used standard calibration using the Common Astronomy Software Application\(^3\) (CASA) with ALMA data for initial data reduction and imaging for both ACA and TP data sets. For an improved amplitude calibration, we scaled the datasets to a single reference Jupiter’s angular diameter of 34.45” and 32.56”. The spectrum was created for $\text{H}_2\text{O}$ and $\text{CH}_3\text{CH}_2\text{CN}$ by ALMA data cubes from the centre of Jupiter (139,822 km at Jupiter distance) with 12” diameter circular region. The continuum flux density for each baseline

\(^1\)https://almascience.nao.ac.jp/asax/
\(^2\)https://cdms.astro.uni-koeln.de/cgi-bin/cdmssearch
\(^3\)https://casaguides.nrao.edu/
was scaled and matched with Butler-JPL-Horizons 2012 (Butler 2012) for Jupiter model flux for both ACA and TP data which is accurate to within 5%. The background continuum-subtraction of the visibility amplitudes was performed using task UVCONTSUB in CASA and imaging was carried out using TCLEAN task with 500 number of iterations with Hogbom algorithm and natural visibility weighting. The self-calibration process was used for Jupiter continuum which is also used as a perfect flux reference with 5% accuracy. The resulting spatial resolution (FWHM of the gaussian restoring beam), after combining both ACA and TP data using task CONCAT, was 8.78″×6.33″. The final spectrum of Jupiter was converted from equatorial coordinates to linear distances with respect to the centre of Jupiter. The spectrum was corrected for Doppler-shift to Jupiter’s rest frame using NASA JPL Horizons Topocentric radial velocity using geocentric outframe due to TCLEAN operation.

3. Result

3.1. Emission line of ethyl cyanide and acetone

We detected the absorption line of $^{13}$CH$_3$CH$_2$CN which is also known as propionitrile at frequency $\nu$=195.430 GHz with molecular transition J=52(5,48)–51(6,45) in the atmosphere of Jupiter. The corresponding spectrum is shown in Fig. 1. In this spectrum, there is also exitance of another emission line of CH$_3$COCH$_3$ on the right side of CH$_3$CH$_2$CN emission peak at frequency $\nu$ = 195.721 GHz with transition J = 50(38,12)–50(37,13)EE. The illumination factor of Jupiter during the observation was 10.31% which means 89.69% of the mapped planet was in dayside at the time of observation. Two emission lines were detected with $\sim$12σ and $\sim$3σ statistical significance. The area of ethyl cyanide emission spectra = 0.126±0.001 Jy/Beam GHz with a large value of FWHM = 0.0905±0.002 GHz. In the atmosphere of Jupiter, column density of ethyl cyanide is $N$(13CH$_3$CH$_2$CN) = 3.52×10$^{14}$ cm$^{-2}$ but in case of acetone, the column density is $N$(CH$_3$COCH$_3$) = 5.31×10$^{10}$ cm$^{-2}$.

Earlier, CH$_3$CH$_2$CN was detected in the atmosphere of Saturn’s largest moon Titan with vertical column density in the range (1–5)×10$^{14}$ cm$^{-2}$ (Cordiner et al. 2015). Ethyl cyanide was also found in the atmosphere of Venus at frequency $\nu$ = 259.586 GHz with transition

| UT start date | Array | Geocentric distance (AU) | Integration time (s) | Species | Frequency (GHz) | Transition | $E_u$ (K) |
|---------------|-------|--------------------------|----------------------|---------|----------------|-----------|---------|
| yyyy-mm-dd    |       |                          |                      |         |                |           |         |
| 2018-08-27    | ACA   | 5.5966                   | 1387.459             | CH$_3$CH$_2$CN \ CH$_3$COCH$_3$ | 195.430 \ 195.721 | J=52(5,48)-51(6,45) \ J=50(38,12)-50(37,13)EE | 607 \ 1091 |
| 2018-09-20    | TP    | 5.9215                   | 3775.104             | H$_2$O  | 183.310        | J=3(1,3)-2(2,2) | 204.7 |
J = 29(12,17)–28(12,16) with column density $5.21 \times 10^{14}$ cm$^{-2}$ which detected with 9.8$\sigma$ statistical significance (Manna et al. 2020).

The present detection of CH$_3$COCH$_3$ in the atmosphere of Jupiter is the first detection of the molecule in the solar system. Earlier, acetone was detected in the hot molecular core of Sgr B2 (Combes et al. 1987; Snyder et al. 2002).

### 3.2. Absorption line of water

We confirmed the presence of water vapour in the atmosphere of Jupiter with the detection of the absorption line of H$_2$O at $\nu = 183.310$ GHz with transition $J = 3(1,3)–2(2,2)$ with $\sim 4.3\sigma$ statistical significance level. The column density corresponding to the H$_2$O line is $N(\text{H}_2\text{O}) = 9.25 \times 10^{14}$ cm$^{-2}$. In Fig. 2, we have shown the ALMA individual detection of H$_2$O at $\nu = 183.310$ GHz with transition $J = 3(1,3)–2(2,2)$. The observation was done on 20th Sept 2020 with ALMA 12m single dish (TP) aperture. In this spectrum, both vertical and horizontal polarizations are fully averaged. The continuum value of the absorption spectrum is 0.0097 Jy/Beam. The water is most probably created due to the collision of comet Shoemaker-Levy 9 in July 1994 near 44$^\circ$S (Lellouch et al. 1995; Nol et al. 1995; Moreno et al. 2003). The area of H$_2$O absorption spectra is $-0.068 \pm 0.001$ Jy/Beam GHz with FWHM $= 0.134 \pm 0.003$ GHz. The illumination factor of Jupiter, during the observation, is 8.58% which means 91.42% of the mapped planet was in dayside at the time of observation.

Earlier space mission, using Juno microwave radiometer, also detected abundance of water in the equatorial zone of Jupiter (Li et al. 2020). The present paper reported the first radio interferometric detection of the water absorption line in Jupiter.

### 4. Photochemical reaction in the atmosphere of Jupiter

In the atmosphere of Jupiter, the water molecules are split in the presence of sunlight, electron, and oxygen during non-cyclic photo-phosphorylation with the artificial photolysis method (Kudo 2014). The carbon dioxide can be converted to various organic compounds by the reaction with hydrogen. Using hydrogen, artificial photosynthesis is achieved by the hydrogenation of carbon dioxide.

$$h\nu + \text{H}_2\text{O} \longrightarrow \text{OH} + \text{H}$$

$$h\nu + \text{H}_2\text{O} \longrightarrow \text{H}_2 + \text{O} \quad (1)$$

The production of CO could be done by reactions such as
Fig. 1.— ALMA individual detection of $^{13}$CH$_3$CH$_2$CN ($J = 52(5,48)–51(6,45)$) and CH$_3$COCH$_3$ ($J = 50(38,12)–50(37,13)$EE) at $\nu=195.430$ GHz and $\nu = 195.721$ with 7m ACA data. In this spectrum, both polarizations are fully averaged. The continuum value of emission spectrum is 0.115 Jy/Beam.

Fig. 2.— ALMA individual detection of H$_2$O at $\nu = 183.310$ GHz with transition $J = 3(1,3)–2(2,2)$ on Jupiter at 2018-09-20 with ALMA 12m single dish (TP) data. In this spectrum, both vertical and horizontal polarizations are fully averaged. The continuum value of the absorption spectrum is 0.0097 Jy/Beam.
\[
\text{OH} + \text{C}_2\text{H}_2 \rightarrow \text{C}_2\text{H}_2\text{O} + \text{H} \quad (2) \\
\text{and,} \quad \text{OH} + \text{C}_2\text{H}_4 + \text{M} \rightarrow \text{C}_2\text{H}_4\text{OH} + \text{M} \quad (3)
\]

In reaction (2) and (3), the primary output products are observed in Jupiter by mass spectroscopy (Kanofsky et al. 1974; Morris et al. 1974) where M is any reactants but the details of subsequent chemistry and structure are unknown. We assumed that they rapidly isomerize to the stable forms in terms of CH$_2$CO and CH$_3$CHOH which may be removed by the reaction sequence later.

\[
\text{CH}_2\text{CO} + h\nu \rightarrow ^1\text{CH}_2 + \text{CO} \quad (4) \\
\text{CH}_3\text{CHOH} + \text{H} \rightarrow \text{CH}_3\text{CHO} + \text{H}_2 \quad (5) \\
\text{CH}_3\text{CHOH} + \text{CH}_3 \rightarrow \text{CH}_3\text{CHO} + \text{CH}_4 \quad (6)
\]

A lot of different formation mechanisms have been proposed for the compounds detected in the present paper. For acetone, Herbst et al. (1990) showed that the ion-molecule radiative association reaction proposed by Combes et al. (1987) is not efficient enough to produce the observed values. Garrod et al. (2008) proposed a model where acetone can be formed on grains by the combination of CH$_3$ and CH$_3$CO.

\[
\text{CH}_3 + \text{CH}_3\text{CHO} \rightarrow (\text{CH}_3)_2\text{CHO}^+ + h\nu \quad (7) \\
(\text{CH}_3)_2\text{CHO}^+ + e^- \rightarrow \text{CH}_3\text{COCH}_3 + \text{H} \quad (8)
\]

Equation (8) indicated possible reaction pathway of the formation of CH$_3$COCH$_3$ in the atmosphere of Jupiter with complex chemical reactions.

The mechanisms of ethyl cyanide (C$_2$H$_5$CN) is based on ion-molecule reactions with the simplest ions of gas in the Jupiter atmosphere and cosmic ray-induced photo-dissociation method. In the Jupiter atmosphere, the HCN is also present. So, ethyl cyanide and additional oxygen will be produced in Jupiter atmosphere with reaction of HCN and CH$_3$CHO.

\[
\text{HCN} + \text{CH}_3\text{CHO} \rightarrow \text{CH}_3\text{CH}_2\text{CN} + \text{O} \quad (9)
\]

The above chemical pathways indicate that the ethyl cyanide and acetone are both produced with the help of CH$_3$CHO.
5. Discussion

In this paper, we discuss the spectroscopic detection of $^{13}$CH$_3$CH$_2$CN, CH$_3$COCH$_3$ and confirm the presence of H$_2$O vapour (with transition J = 3(1,3)–2(2,2)) in the atmosphere of Jupiter. These molecular species are very important to understand the chemical dynamics in the atmosphere of the planet. The CN radical is a symmetry-breaking identifier of $^{13}$CH$_3$CH$_2$CN compound. The $^{13}$CH$_3$CH$_2$CN emission spectrum shows characteristically broad feature due to its high dipole moment. Here we point out that CH$_3$CHO may be responsible for the production of CH$_3$CH$_2$CN and CH$_3$COCH$_3$.

The detection of water on Jupiter fills a critical space to understand the molecular chemistry in the solar system. Earlier, water vapour was found in the atmosphere of solar planet Mars (Fouchet et al. 2011), Venus (Belton & Hunten 1996), Jupiter’s moon Europa (Roth et al. 2014) and Saturn’s moon Titan (Hueso & Sánchez-Lavega 2002). Recently the water molecular emission line was also detected from the thin atmosphere of Moon at 6$\mu$m using the NASA/DLR Stratospheric Observatory for Infrared Astronomy (SOFIA) (Honniball et al. 2020). The detection of an absorption line of water in Jupiter may be critical in the formation of some complex bio compounds as well as the formation of life. The formation and evolution of life with carbon-based metabolism are difficult without the presence of water.

The presence of water and other carbon-based molecules gives confidence to the possibility of the formation of amino acids in the atmosphere of Jupiter. The first laboratory simulation demonstrated by Miller and Urey’s (Miller 1953) experiment indicated the formation of prebiotic molecules in the Earth and other planets. Recently, Miller and Urey’s experiment is used to explain the formation of glycine in the atmosphere of Venus which may be an indicator of the presence of life in the planet (Manna et al. 2020). More spectroscopic study of other transition lines of CH$_3$CH$_2$CN and CH$_3$COCH$_3$ will help to confirm the nature of these gases in the atmosphere of Jupiter and may help to study other complex and prebiotic organic molecules in the atmosphere of solar system’s largest planet Jupiter.

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