Detection of hydroxyacetone in protostar IRAS 16293–2422 B *

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Abstract Hydroxyacetone (CH$_3$COCH$_2$OH) is one of the smallest molecules that contain both hydroxyl and carbonyl group on neighboring carbon atoms. This steric configuration is characteristic of saccharides and determines their biochemical activity. The attempt to search for hydroxyacetone toward the massive star formation region Sagittarius B2(N) was unsuccessful. Here we report the first detection of CH$_3$COCH$_2$OH in the solar–type protostar IRAS 16293–2422 B, using the Atacama Large Millimeter Array science verification data at Band 4. In a total of 11 unblended transitions of CH$_3$COCH$_2$OH with upper level energies ranging from 86 to 246 K are identified. From our Local Thermodynamic Equilibrium analysis, we derived that the rotational temperature of CH$_3$COCH$_2$OH is 160 ± 21 K and the column density is $(1.2 ± 1.0) \times 10^{16}$ cm$^{-2}$, which results in a fractional abundance of $7 \times 10^{-10}$ with respect to molecular hydrogen. In this work, we present the identification of CH$_3$COCH$_2$OH in IRAS 16293–2422 B and propose a simple formation mechanism. The unambiguous identification of hydroxyacetone may provide the basis for future study of the origin and evolution of saccharides in the interstellar medium.

Key words: ISM: abundances — ISM: individual objects IRAS 16293–2422 B — ISM: molecules

1 INTRODUCTION

The carbohydrates have caused increasing interests of astrophysical studies in recent years since these molecules can serve as energy storage1, can participate in the building of DNA and RNA, and are structural elements in cellular molecular organization (e.g., cell membranes) (Moháček–Groše 2005). They can also form sophisticated extracellular matrices throughout the organism (Iozzo 1998). Therefore, carbohydrates are vital to all known lifeforms (Cooper et al. 2001). All monosaccharides show common structural feature that carbonyl group occurs next to hydroxyl group in the chain conformation of sugar molecule (Moháček–Groše 2005). Examples of the smallest sugar molecules are glycolaldehyde HCOCH$_2$OH and hydroxyacetone CH$_3$COCH$_2$OH. Searching for the monosaccharides in interstellar medium (ISM) has caused considerable interests as the existence and the process to form these molecules in ISM may help with answering the question of the origin and evolution of life in the universe (Bossa et al. 2014).

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1 The energy discussed here is the energy sustaining the vital activities of body, such as blood circulation, digestion and absorption of the stomach and so on.
Glycolaldehyde HCOCH$_2$OH has been studied intensively in various sources. The glycolaldehyde was firstly detected toward the Galactic Center (Hollis et al. (2000); Hollis et al. (2001, 2004a); Halfen et al. (2006); Requena–Torres et al. (2008)). Then it was detected in a number of other places in ISM, associated with the star formation regions of high (Beltrán et al. 2009; Calcutt et al. 2014), intermediate (Fuente et al. 2014) and low mass (Jørgensen et al. 2012; Coutens et al. 2015; Taquet et al. 2015; Jørgensen et al. 2016). It was also detected in comet C/2014 Q2 (Lovejoy) (Biver et al. 2015).

Hydroxyacetone CH$_3$COCH$_2$OH, compared with glycolaldehyde HCOCH$_2$OH, exhibits the next level of molecular complexity among the smallest sugar molecules (Apponi et al. 2006a). And in laboratory, this molecule is an important starting material in the synthesis of aldehydes and ketones (see, e.g., Solomons (1984)). Therefore, the assumption that such molecule could lead to the production of complex prebiotic species in ISM should be plausible (Apponi et al. 2006b). Two searches for hydroxyacetone toward Sagittarius B2(N) (hereafter Sgr B2(N)) were conducted with non-detection of the molecule. The first attempt was at 1.3 mm using the Caltech Submillimeter Observatory (CSO), with no detected transitions of hydroxyacetone (Braakman et al. 2005). The second attempt was at 3 mm using the Arizona Radio Observatory (ARO) 12 m telescope. Although there are several coincidental transitions matching CH$_3$COCH$_2$OH lines, the absence of several favorable transitions indicates that the result is not enough for claiming a detection (Apponi et al. 2006b). The aim of our study is to present a reliable identification of CH$_3$COCH$_2$OH with the highly sensitive Atacama Large Millimeter Array (ALMA) at Band 4, toward a typical young solar–type protostar IRAS 16293–2422 B (hereafter I16293B).

The class 0 protostar IRAS 16293–2422 (hereafter I16293) contains at least two sources A and B with a separation of 5′′ (~ 700 AU) (Calcutt et al. 2018). Many line surveys have been carried out towards I16293 by using single dish telescopes and interferometers (Cazaux et al. 2003; Bisschop et al. 2008; Caux et al. 2011; Jørgensen et al. 2016; Lykke et al. 2017; Martín-Doménech et al. 2017). The results show that I16293 exhibits a rich chemistry and chemical complexity of COMs. There are many oxygen–bearing COMs that have been detected in I16293. Examples are glycolaldehyde, ethanol, ethylene glycol, acetic acid, propanal and others, which are reported by the Protostellar Interferometric Line Survey (PILS) studies, (e.g., Jørgensen et al. (2012, 2016); Lykke et al. (2017); Jørgensen et al. (2018)). Since the hydroxyacetone closely resembles glycolaldehyde, I16293 is very likely to be a source to search for hydroxyacetone.

In this work, we report the identification of hydroxyacetone at the 2 mm waveband toward I16293B. We describe the observations in Sect. 2, and present the results and analyze the data in Sect. 3 and 4, respectively. We draw a few conclusions in Sect. 5.

2 OBSERVATIONS

We took the uncalibrated data from the ALMA science verification (SV) program toward I16293 at Band 4 $^2$. We downloaded and re-calibrated the data using the standard ALMA calibration scripts. These data were obtained by observations that were carried out with 23 × 12 m antennas in July 14th, 2014. The primary beam size at Band 4 is about 30′′. The phase–tracking center is at R.A.(J2000) = 16°32′22.73 and decl.(J2000) = −24°28′32″.50. There are four spectral windows with 3840 channels each. These four spectral windows cover frequency ranging from 145.1 to 159.2 GHz, with spectral resolutions from 0.06 to 0.49 MHz. We did the follow–up calibration and imaging employing the CASA software $^3$. We have flagged the first and last 20 channels to avoid edge problem. We processed the continuum–subtraction with STATCONT software (Sánchez–Monge et al. 2018).

The continuum image is constructed from line–free channel as shown in color scale in Figure 2. The peak intensity of I16293B is 0.35 ± 0.006 Jy beam$^{-1}$, and the synthesized beam size is 1″.04 × 0″.59. Therefore, the beam averaged H$_2$ column density is derived to be 1.7 × 10$^{25}$ cm$^{-2}$ for I16293B (Lis et al. 1991). The result is similar to the H$_2$ column density calculated by Martín-Doménech et al. (2017) and Jørgensen et al. (2016) toward I16293B.

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$^2$ Obtaining ALMA data and calibration scripts: https://almascience.nrao.edu/almadata/sciver/IRAS16293Band4/

$^3$ CASA homepage: http://casa.nrao.edu
Detection of hydroxyacetone in IRAS 16293–2422 B

![Graphs showing spectral lines of hydroxyacetone](image)

**Fig. 1** The unblended and partially blended (denoted with “PB”) lines of hydroxyacetone detected in these four spectral windows at Band 4 toward 116293B overlaid with an LTE spectral model of the emission.
3 RESULTS

In IRAS 16293–2422 A, the lines are quite broad, leading to significant line confusion that prevents the search for complex species (e.g., Jørgensen et al. (2012)). This report is therefore focusing on source B only. Full band spectra\(^4\) are extracted at the continuum peak position of source B. The extended CASA Line Analysis Software Suite (XCLASS) (Möller et al. 2017) package\(^5\) is employed for identifying line transitions under the assumption of Local Thermodynamical Equilibrium (LTE)\(^6\), and is used to access database Cologne Database for Molecular Spectroscopy (CDMS) (Müller et al. 2001, 2005; http://cdms.de) as well as Jet Propulsion Laboratory (JPL) database (Pickett et al. 1998; http://spec.jpl.nasa.gov). For hydroxyacetone, the JPL database is used to access the XCLASS package. The spectroscopic data of CH\(_3\)COCH\(_3\)OH with the A and E torsional states, has been studied by Kattija–Ari & Harmony (1980) (from 4 to 180 GHz), and more recently by Apponi et al. (2006b) (from 4 to 180 GHz) and Braakman et al. (2010) (near 300 GHz). Since the spectra of I16293B are really rich, a careful check should be done to avoid blended or overlapped line problems. To achieve this, we have made a full source model (coded in solid green color in Figure A-1 of Appendix) including as many as species to model the observed spectra toward I16293B. The species which were observed in I16293B up to now (from Table 1 by Drozdovskaya et al. (2019)) are all included in the full source model.

3.1 Detection of the hydroxyacetone

We identified a total of 11 unblended emission lines of CH\(_3\)COCH\(_3\)OH with upper–level energies ranging from 86 to 246 K, among which 10 transitions have line–strength higher than 5 \(\sigma\). The \(\sigma\) is the rms noise level of the specific lines. We determined the rms noise level from emission free regions of the channel maps. The unblended or partially blended synthetic spectra for CH\(_3\)COCH\(_3\)OH toward I16293B are generated and showed in Figure 1, and the corresponding parameters for these individual detected lines are listed in Table A.1. The full spectra of CH\(_3\)COCH\(_3\)OH at Band 4 are presented in Figure A-1 in Appendix. The transitions which are higher than 3\(\sigma\) and totally blended with other molecules are denoted with “B” in Figure A-1. The frequencies of CH\(_3\)COCH\(_3\)OH totally blended transitions with peak intensities lower than 3\(\sigma\) are listed in Table A.1 and presented in Figure A-1 denoted with “w” in the Appendix. We made the Gaussian fitting to unblended transitions and obtained the parameters \(V_{LSR}\) and \(\Delta V\) for each individual unblended transitions and showed in column 7–8 in Table 2. The averaged \(V_{LSR}\) value is 2.65 \(\pm\) 0.045 km s\(^{-1}\). The averaged line width obtained from the eleven unblended transitions is 2.51 \(\pm\) 0.058 km s\(^{-1}\). Our results of \(V_{LSR}\) and \(\Delta V\) are consistent with previous results of other molecules in I16293 B (Caux et al. 2011; Jørgensen et al. 2011). The spatial distribution of CH\(_3\)COCH\(_3\)OH is shown in Figure 2 and it is coincident well with the continuum emission of source B. The source size is derived by performing two–dimensional Gaussian fitting to the line images. The source size of CH\(_3\)COCH\(_3\)OH is unresolved. The compact source size of CH\(_3\)COCH\(_3\)OH is consistent with the other COMs detected in previous studies (e.g., Martin-Doménech et al. (2017) or PILS papers (e.g., Jørgensen et al. (2016); Calcutt et al. (2018); Coutens et al. (2019)) toward I16293B.

The detected transitions of CH\(_3\)COCH\(_3\)OH are well reproduced by a rotational temperature of \(T_{rot} = 160 \pm 21\) K. The derived \(T_{rot}\) agrees with the reported rotational temperature of other COMs detected in PILS studies, such as methyl isocyanide in I16293B (Calcutt et al. 2018). We derived that the column density is \((1.2 \pm 1.0) \times 10^{16}\) cm\(^{-2}\) for CH\(_3\)COCH\(_3\)OH. The fractional abundance of CH\(_3\)COCH\(_3\)OH relative to H\(_2\) is \(7 \times 10^{-10}\). The column density \((1.2 \times 10^{16}\) cm\(^{-2}\)) of CH\(_3\)COCH\(_3\)OH is lower than that of glycolaldehyde \((3.2 \times 10^{16}\) cm\(^{-2}\)) detected in I16293B by PILS data Jørgensen et al. (2012).

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\(^4\) Figure 1 shows the unblended or partially blended emission lines of hydroxyacetone toward I16293B. Full band spectral are presented in Figure A-1, which are populated by many molecular lines.

\(^5\) The spectroscopic database contained in XCLASS is interfacing with Virtual Atomic and Molecular Data Centre (VAMDC): http://www.vamdc.org/activities/research/

\(^6\) LTE is a good assumption in this case, because the densities are high at the chosen position and thus the molecules are expected to be thermalised.
Our result is consistent with the previous report discussed by Apponi et al. (2006b) – column densities roughly follow a monotonic decrease from glycolaldehyde to hydroxyacetone.

To verify the calculated results from the XCLASS, we have made rotational temperature diagram (RTD) based on the 11 unblended transitions. Under the LTE assumption, the population of a certain energy level will follow the Boltzmann distribution. Assuming the line emissions in question are optically thin, we fitted the 11 unblended transitions by using the least-squares method as done by Qin et al. (2010). The RTD for these unblended CH$_3$COCH$_2$OH lines from I16293B is shown in Figure 3. The

The Table 1 Observed Spectral Line Parameters of Detected Species CH$_3$COCH$_2$OH Toward I16293B

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<th>Rest Frequency (MHz)</th>
<th>Uncertainty (MHz)</th>
<th>Einstein A (10$^{-5}$ s$^{-1}$)</th>
<th>$E_u$ (K)</th>
<th>$g_{sp}$</th>
<th>Quantum numbers</th>
<th>$V_{16293}$ (km s$^{-1}$)</th>
<th>$\Delta V$ (km s$^{-1}$)</th>
<th>I$_{P}$ (K)</th>
<th>$\sigma$ (K)</th>
<th>Detection Level</th>
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example, acetic acid (CH$_3$COOH). Acetic acid shares the C–C
O(OH) backbone with the simplest

4 DISCUSSION
There are a number of compact organic molecules are considered to be the potential precursors of biological molecules. And the most well studied among these molecules are [C$_2$H$_4$O$_2$] family, for example, acetic acid (CH$_3$COOH). Acetic acid shares the C–C=O(OH) backbone with the simplest
amino acid glycine (NH₂CH₂COOH), from which acetic acid differs only by an amino group (–NH₂) (Bergantini et al. 2018). Another example is glycolaldehyde (HCOCH₂(OH)), a diose and the simplest sugar–related specie (Hollis et al. 2000). The more complex molecules in the [C₃H₁₀O₃] family have not been detected in ISM, which include the simplest three–carbon aldehyde sugar glycaldehyde (CH₂(O)(CH(OH)CH₂(OH)), Hollis et al. (2004b)) and ketose sugar dihydroxyacetone (CH₂(OH)COCH₂OH; hereafter DHA; Apponi et al. (2006a)). Therefore, searches for species in the [C₃H₁₀O₃] family with complexity in between [C₂H₄O₂] and [C₃H₁₀O₃] families might prove significant in understanding the lack of detection of the latter in the ISM. The detection and analysis of [C₃H₁₀O₃] family species may serve as a probe for the next step to understand the formation mechanism of biological molecules in ISM.

Glycolaldehyde (HCOCH₂OH), which belongs to [C₂H₄O₂] family, can be produced by the recombination of two free radicals HCO and CH₃OH on the grain surface in ISM (Öberg et al. (2009); Butscher et al. (2015); Fedoseev et al. (2015); Chuang et al. (2016); Fedoseev et al. (2017)). The reactive intermediates CH₂O and HCO are formed through irradiation of CH₃OH–rich ices by various energetic particles (including protons, electrons, X–rays, UV photons, etc.) on the grain surface (Öberg et al. 2009). In addition, the intermediate radical CH₂OH was proposed to be formed by the H₂CO to CH₃OH hydrogenation processes (H₂CO + H → CH₂OH, CH₃OH + H → CH₃OHH (Butscher et al. 2015; Chuang et al. 2016), possibly at 15 K. Among the six of the lowest–energy members in the [C₃H₁₀O₃] family (species including propionic acid, methyl acetate, ethyl formate, hydroxyacetone, lactaldehyde, and methoxyacetaldehyde; reported in Kolesnikova et al. (2018) and Alonso et al. (2019)), the hydroxyacetone (CH₃COCH₂OH), which belongs to [C₂H₄O₂] family, is a structural intermediate between glycolaldehyde (HCOCH₂OH) and the DHA (CH₃(OH)COCH₂OH) (Braakman et al. 2010). And the hydroxyacetone (CH₃[COCH₂OH]) shares the O=C–(CH₂OH) backbone with the simplest sugar–related species glycaldehyde (H[COCH₂OH]), from which hydroxyacetone dihydroxyacetone (CH₂(OH)COCH₂OH), that hydroxyacetone (CH₃OHOCC₂H₂) might be formed upon recombination of two free radicals on the grain surface at low temperature as the following:

\[
CH₂CO + CH₂OH → CH₃COCH₂OH. \tag{1}
\]
The intermediate radical CH$_3$OH might be induced through UV-irradiation of CH$_3$OH–rich ices (CH$_3$OH + UV → CH$_3$OH + H), or hydrogenation process of H$_2$CO to CH$_3$OH (H$_2$CO + H → CH$_3$OH) as mentioned before. The other intermediate radical CH$_3$CO are formed through the hydrogenation process of ketene (H$_2$CCO + H → CH$_3$CO) on the grain surface as reported by Michael et al. (1979) and Ruaud et al. (2015). This reaction suggests an effective chemical formation pathway of the hydroxyaceton. Thus, we propose that the hydroxyaceton can be formed upon the recombination of CH$_3$OH and CH$_3$CO on the grain surface for the first time.

At low temperature, the COMs are considered to be formed through free radicals’ recombination on grain surface as discussed above (Fedoseev et al. 2015; Chuang et al. 2016; Fedoseev et al. 2017). As the temperature increases when the source evolves, the species with lower binding energies formed on the dust grains can be evaporated into the gas phase thus complex molecules with relatively low binding energies are observable. In the gas phase, the complex molecules can also be produced by the reactions between cations and the complex molecules precursors that are evaporated from dust grains, followed by recombination with electrons, as proposed in Remijan et al. (2002); Garrod (2013); Redondo et al. (2017). Thus, we propose a novel gas phase production route of CH$_3$COCH$_2$OH as the other COMs:

$$\text{CH}_3\text{COOH}^+ + \text{CH}_3\text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH}^+ + \text{H}_2\text{O},$$

(2)
Detection of hydroxyacetone in IRAS 16293–2422 B

Fig. 3 Rotation temperature diagram for CH$_3$COCH$_2$OH. The filled circles are for the observed transitions. The vertical bars indicate the 3σ errors. A linear least-squares fit is shown as the red solid line.

$$\text{CH}_3\text{COCH}_2\text{OH}_2^+ + e^- \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + H,$$

where the intermediate ion CH$_3$COOH$_2^+$ can be formed through two ion–molecule reactions CH$_3$CO$^+$ + H$_2$O $\rightarrow$ CH$_3$COOH$_2^+$, and CH$_3$OH$_2^+$ + HCOOH $\rightarrow$ CH$_3$COOH$_2^+$ + H$_2$O, as proposed in Remijan et al. (2002).

5 CONCLUSIONS

We present ALMA Band 4 observations of hydroxyacetone (CH$_3$COCH$_2$OH) toward IRAS 16293–2422 B. We have identified the molecular transitions and calculated physical parameters under LTE assumption. Main findings in this work are summarized below:

1. Totally 11 unblended transitions of CH$_3$COCH$_2$OH with upper level energies ranging from 86 to 246 K are identified in I16293B. It can be claimed the first unambiguous detection of this molecule in interstellar space.

2. A rotational temperature of 160 ± 21 K and a column density of (1.2 ± 1.0)×10$^{16}$ cm$^{-2}$ have been obtained for CH$_3$COCH$_2$OH by using the LTE model. The compact gas distribution of CH$_3$COCH$_2$OH is coincident with the continuum emission of source B, which shows that this molecule is probably originated from the inner region near the hot corino of I16293B.

3. As a structural analogy of glycolaldehyde (HCOCH$_2$OH), we propose a similar reaction route to produce hydroxyacetone that it might be formed upon recombination of two free radicals CH$_2$OH and CH$_3$CO on the grain surface at low temperature. In the gas phase, the CH$_3$COOH$_2^+$ and CH$_3$OH reaction, followed by an electron recombination to produce hydroxyacetone are proposed in our work.
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Table A.1  Transitions of Hydroxyacetone with Weak Intensities (< 3σ) at Band 4 Toward 116293B

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Appendix A: LINES OF HYDROXYACETONE

For a proper identification, all transitions presented in the JPL catalog of molecule CH₃COCH₂OH at Band 4 were contained in our LTE synthetic spectrum. The frequencies of transitions with lower peak intensities than 3σ are presented in Table A.1.

Appendix B: FULL BAND SPECTRA

To make sure that the spectral models are reliable, we added full source model fitting. All published species in source B which are explicitly listed in recently work by Drozdovskaya et al. (2019) have been included. The full source model is shown with solid green line in Figure A-1.
Figure A1: Full band spectra and line identification. The black curve is the observed data.
Fig. A-1 continued