Preliminary study of CH_3CN as a chemical thermometer of molecular cores

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Received: 09 February 2024 / Accepted: 01 June 2024

Resumen / Se sabe que las estrellas de gran masa se forman como resultado de la fragmentación de grumos moleculares de alta masa. Esto da origen a los núcleos que son las estructuras más pequeñas del medio interestelar que pueden dar lugar al nacimiento de estrellas. Caracterizar sus parámetros físicos y químicos es fundamental para comprender los procesos de formación estelar. En particular, una correcta determinación de la temperatura de los núcleos moleculares es de vital importancia para la estimación de su masa en el contexto de los distintos escenarios de formación de las estrellas masivas. En este trabajo, se presentan resultados preliminares de un estudio estadístico de la molécula CH_3CN como trazadora de temperatura hacia una muestra de grumos moleculares de alta masa. El estudio fue llevado a cabo a partir de observaciones en Banda 6 obtenidas del ALMA Science Archive.

Abstract / High-mass stars are known to form as a result of the fragmentation of high-mass molecular clumps. This gives rise to cores, which are the smallest structures in the interstellar medium that can lead to the birth of stars. Characterizing their physical and chemical parameters is essential to understanding star formation processes. In particular, accurately determining the temperature of molecular cores is crucial for estimating their mass in the context of different scenarios of massive star formation. In this work, preliminary results of a statistical study of the CH_3CN molecule as a temperature tracer toward a sample of high-mass molecular clumps are presented. The study was carried out from observations in Band 6 taken from the ALMA Science Archive.

Keywords / ISM: clouds — ISM: molecules — stars: formation

1. Introduction

The formation of a high-mass star begins with the fragmentation of a massive clump into smaller structures known as molecular cores. There are two models under debate for high-mass star formation: monolithic collapse (Palau et al., 2018; Moscadelli et al., 2021) and competitive accretion (Motte et al., 2018; Schwörer et al., 2019). For the study and validation of these models, it is essential to determine the masses of the cores involved in the fragmentation of molecular clouds. For this, the correct estimation of the temperature of the molecular cores is of crucial importance since it is directly related to the calculation of their masses.

One of the most used tools in temperature estimation is the Rotational Diagram (Goldsmith & Langer, 1999) applied to top-symmetric molecules. In particular, the top-symmetric molecule methyl cyanide (CH_3CN) is a good temperature tracer. CH_3CN is formed in interstellar grains by recombination of radicals such as CN- and CH_3- (Hernández-Hernández et al., 2014) and it is generally detected in hot molecular cores (Brouillet et al., 2022). In this work, we present preliminary results of a statistical study of the CH_3CN molecule as a temperature tracer toward a sample of high-mass molecular clumps with cores in its interior.

2. Data

Data cubes were obtained from the ALMA Science Archive. We used data from the project 2015.1.01312.S (P.I. Gary Fuller). The telescope configuration used baselines L5BL/L80BL of 39.84/215.91m, respectively, in the 12 m array. The observed frequency range of the spectral window used in this work goes from 238.81 to 240.69 GHz (Band 6). The angular and spectral resolutions are $0\farcs7$ and 1.4 MHz, respectively. The velocity resolution is about 1.4 km s^{-1}. The rms noise level is 4.2 mJy $beam^{-1}$ for the emission line (averaged each 10 km s^{-1}) and 0.14 mJy $beam^{-1}$ for the continuum emission. The maximum recoverable spatial scale is $6\farcs53$.

3. Results

Using data from the APEX Telescope Large Area Survey of the Galaxy (ATLASGAL; Schuller et al. 2009), we studied 19 sources representing condensations of cold dust (molecular clumps) of a few (between 2 to 10) parsecs in size. For each molecular clump, we analyze the 1.2 mm continuum emission to identify possible fragmentation. The typical size of these fragments (molecular cores) is on the order of the subparsec. Figure 1 displays the continuum emission from the ALMA data toward each analyzed source. The spectrum of each core

✉ *Contact* / amarinelli@iafe.uba.ar Research article

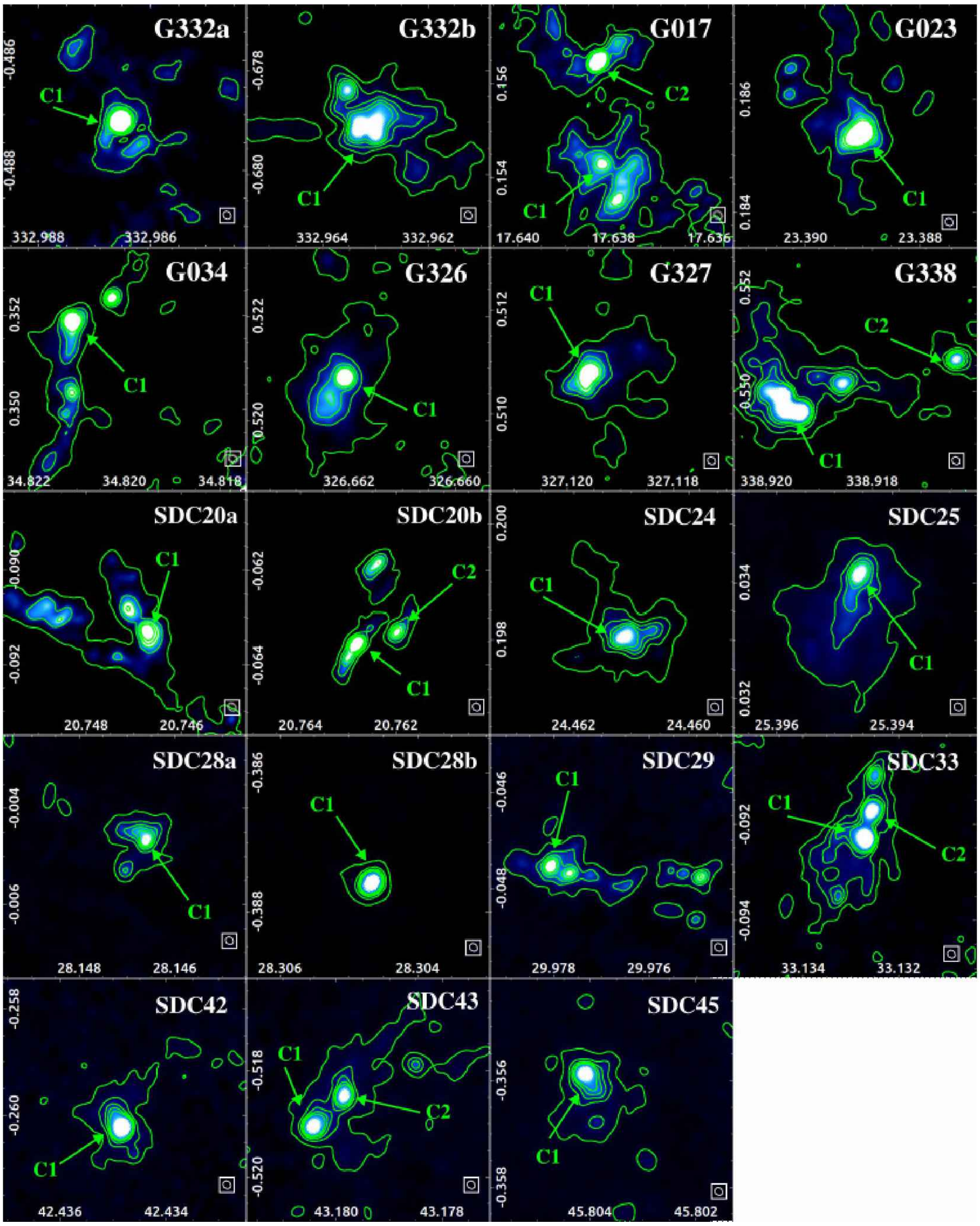

Fig. 1. ALMA continuum emission at 1.2 mm toward the 19 ATLASGAL sources analyzed in this work, represented by colors and contours (at levels 0.001 Jy beam^{-1} to 0.01 Jy beam^{-1}). The active cores (C#) are indicated for each source. The maps are in Galactic coordinates. The beam of the continuum emission at 250 GHz is shown in the bottom right corner of each panel.

was inspected to detect the presence or not of CH_3CN emission, and in the case of a positive detection, we calculated the temperatures of the core.

In Table 1, we present the main physical parameters of the studied ATLASGAL sources (Cols. 1 to 6). The systemic velocity (V_{LSR}) of most of the sources were obtained from Wienen et al. (2015), while for those sources not studied in that work, the systemic velocity was estimated using the intense and ubiquitous transition J=5−4 of the methanol at 239.746 GHz. For these last sources, the kinematic distances were obtained using the Galactic rotation model of Brand & Blitz (1993) based on their estimated systemic velocities.

The study of the possible fragmentation of each ATLASGAL clump in multiple molecular cores was carried out by analyzing the high resolution and sensitivity ALMA continuum emission at 1.2 mm (see Fig. 1). From a careful inspection of the spectrum toward each core, we determined the presence or not of methyl cyanide emission. For the purposes of this work, active cores (labeled as C# in Fig. 1) are defined as those that exhibit CH_3CN emission strong enough to allow us for a reliable estimation of the core temperature. Therefore, it is possible that a source is fragmented into several cores, but only some of them are active cores as defined here. If the clump is fragmented, the number of active cores within it is indicated in Cols. 3 and 4 of Table 1.

3.1. Rotational diagrams and rotational temperature.

The primary objective of this work is to conduct a statistical study of the CH_3CN molecule as a chemical thermometer for hot molecular cores. To achieve this, we first estimate the rotational temperature (T_{rot}) of each active core using the CH_3CN emission through the rotational diagram method. Under the assumption of LTE conditions and that the lines are optically thin, with a beam filling factor equal to unity, we derive the T_{rot} for each core. This analysis is based on a derivation of the Boltzmann equation:

$$\ln\left(\frac{N_u}{g_u}\right) = \ln\left(\frac{N_{\rm tot}}{Q_{\rm rot}}\right) - \frac{E_u}{kT_{\rm rot}}, \quad (1)$$

where N_u represents the molecular column density of the upper level of the transition, g_u the total degeneracy of the upper level, E_u the energy of the upper level, N_{tot} the total column density of the molecule, $Q_{\rm rot}$ the rotational partition function, and k the Boltzmann constant.

Following Miao et al. (1995), for interferometric observations, the left-hand side of Eq. 1 can also be estimated by,

$$\ln\left(\frac{N_u^{obs}}{g_u}\right) = \ln\left(\frac{2.04\times10^{20}\,W}{\theta_a\theta_b\,g_k g_l \nu_0^3\,S_{ul}\mu_0^2}\right), \quad (2)$$

where N_u^{obs} (in cm^{-2}) is the observed column density of the molecule under the conditions mentioned above, θ_a and θ_b (in arcsec) are the major and minor axes of the clean beam, respectively, W (in Jy $beam^{-1}$ km s^{-1}) is the integrated intensity of each K-projection, g_k is the K-ladder degeneracy, g_l is the degeneracy due to the nuclear spin, ν_0 (in GHz) is the rest frequency of the transition, S_{ul} is the line strength of the transition, and μ_0 (in Debye) is the permanent dipole moment of the molecule. The free parameters, $(N_{\rm tot}/Q_{\rm rot})$ and T_{rot} (see Table 1) were determined by a linear fitting of Eq. 1. The typical errors in T_{rot} are about 10%.

3.2. Correlation between CH_3CN and CH_3CCH

Methyl Acetylene (CH_3CCH) is also a top-symmetric molecule that can serve as a good temperature indicator. CH_3CCH is probably produced in interstellar ices by radical combination and by successive hydrogenation of physisorbed C_3 (Kalenskii et al., 2022; Hickson et al., 2016; Wong & An, 2018).

However, as different authors pointed out (e.g., Tychoniec et al. 2021), CH_3CN would trace more internal regions of the core, because this molecule requires higher temperatures to be sublimated from the surface of the dust grains, while the emission of CH_3CCH is preferentially found mapping the coldest envelopes. Interestingly, the transitions of CH_3CN (J=13-12) and CH_3CCH (14-13), which exhibit a K-ladder form, are very close in frequency in the ALMA Band 6 (see Fig. 2), which allow us to simultaneously characterize both emissions in the context of our statistical study of chemical thermometers.

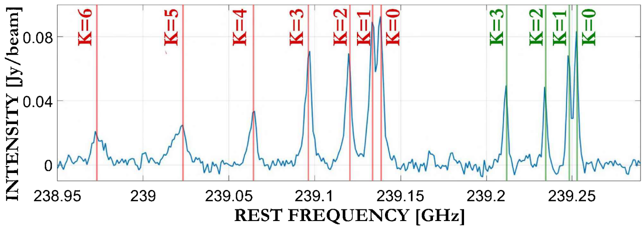

Fig. 2. Example of a spectrum taken toward the molecular core C1 of the SDC24 source. The K projections (K-ladders) of the CH_3CN and CH_3CCH molecules are indicated with vertical red and green lines, respectively.

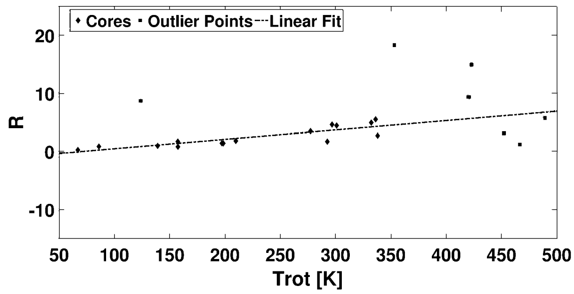

Fig. 3. Linear fitting of the ratio I_{CH_3CN}/I_{CH_3CCH} vs. T_{rot}. The peak intensities of the K=2 projections of each molecule were used. Cores with $T_{rot} > 350$ K or cores that presented atypically high values of R were not taken into account (outlier points). The linear fitting obtained is $R = 0.016\,T_{\rm rot} - 1.1$

The possible correlation between the ratio of the peak intensities of CH_3CN and CH_3CCH (R=I_{CH_3CN}/I_{CH_3CCH}) and the temperature of the cores was studied. We used the K=2 projection for both molecules because it is an intense component not blended with others lines, and thus it can be used to reliably determine its peak intensity, in this way we limit the error of R to 5%. Figure 3 shows the linear fitting between R and the rotational temperature of the cores. The fitting was carried out on cores with temperatures lower than 350 K. This cutoff is attributed to the high dispersion observed in the ratios above such a temperature, an issue that will be studied in a future work.

Some cores present an atypical behavior in R and were not considered for the fitting. These atypical points (outlier points) will also be studied individually in a future work, seeking to determine their evolutionary stages and the reason for their discrepancy with the most common cases.

Taking into account the limitations previously stated, we performed a linear fit on the data, obtaining a relationship of $R = 0.016\,T_{\rm rot} - 1.1$, with a ρ^2

Table 1. Main physical parameters of the sources

Source	Gal. Coord.	Frag.	Active Cores	V_{LSR} (km s^{-1})	Dist.(kpc)	T_{rot}(K)		R	
						C1	C2	C1	C2
G332a	332.987 −0.487	no	1	−55.2	3.7	177	-	76.6‡	-
G332b	332.963 −0.680	yes	1	−48.4	3.3	489*	-	5.7	-
G017	017.638 0.156	yes	2	22.5	2.2	124	67	8.6†	0.3
G023	023.389 0.185	no	1	75.7	4.8	451*	-	3.1	-
G034	034.821 0.352	yes	1	56.9	3.7	335	-	5.5	-
G326	326.669 0.520	yes	1	−39.5	2.6	420*	-	9.3	-
G327	327.119 0.510	no	1	−82.9	5.2	423*	-	14.9	-
G338	338.919 0.549	yes	2	−64.0	4.4	752	139	9.7	1.0
SDC20a	020.747 −0.092	yes	1	59.0	4.5	86	-	0.9	-
SDC20b	020.775 −0.076	yes	2	57.0	4.1	337	157	2.7	1.7
SDC24	024.462 0.219	no	1	119.0	6.8	197	-	1.4	-
SDC25	025.426 −0.175	no	1	−13.7	17.1	198	-	1.4	-
SDC28a	028.147 −0.006	yes	1	98.0	5.8	210	-	1.83	-
SDC28b	028.227 −0.352	no	1	84.2	5.1	353	-	18.3†	-
SDC29	029.844 −0.009	yes	1	101.3	6.3	332	-	4.9	-
SDC33	033.107 −0.065	yes	2	76.9	9.3	296	300	4.6	4.4
SDC42	042.401 −0.309	no	1	65.0	4.8	292	-	1.7	-
G043a	043.186 −0.549	yes	2	59.6	4.8	466	157	1.2	0.8
SDC45	045.787 −0.355	no	1	58.4	7.1	277	-	3.5	-

* In this preliminary study, cores that have a T_{rot} > 350 K are not taken into account for the linear fitting (see Fig. 2).
† These cores have an unusually high value of R, so they are not taken into account for the linear fitting.
‡ Part of the spectrum of this core falls outside the spectral window, resulting in an off-scale R. This value is not used.

(Pearson's correlation coefficient) around 0.7. Figure 3 shows a clear linear correlation between R and the temperature of the cores, which suggests that the ratio R could be useful, under certain conditions, to estimate the temperature of a core in a simpler way than using the rotational diagram method.

4. Summary

We characterized 19 ATLASGAL sources/clumps using high resolution and sensitivity ALMA data in Band 6. The continuum emission at 1.2 mm revealed fragmentation in most of the clumps. We classified 24 molecular cores as active.

We estimated the cores temperatures using the rotational diagram method applied to the emission of the CH_3CN. In addition, we built the ratio R=I_{CH_3CN}/I_{CH_3CCH} (K=2) as a first exploration of the study of the CH_3CN and CH_3CCH molecules as a chemical thermometer for the active cores. We found a linear correlation between the ratio R and the rotational temperature of the cores in the range of temperatures going from 50 to 350 K. Active cores whose rotational temperature exceeds 350 K and those that present R values that deviate from the behavior of the majority are not considered for the linear fitting. These cores were called 'outlier points' and the interpretation of what is occurring with such cores will be studied in a future work. The open and important question that arises from this study is what are the underlying factors contributing to the observed linear correlation between R and the rotational temperature, as well as its dependence on the evolutionary stage of the source, are yet to be determined.

Finally, once we are able to determine the accuracy in the calculation of the temperature through these methods, we will estimate the active core masses in the context of the two main models of massive star formation.

Acknowledgements: We thank the anonymous referee for her/his useful comments pointing to improve our work. This work was partially supported by the Argentina grants PIP 2021 11220200100012 and PICT 2021-GRF-TII-00061 awarded by CONICET and ANPCYT.

References

Brand J., Blitz L., 1993, A&A, 275, 67
Brouillet N., et al., 2022, A&A, 665, A140
Goldsmith P.F., Langer W.D., 1999, ApJ, 517, 209
Hernández-Hernández V., et al., 2014, ApJ, 786, 38
Hickson K.M., Wakelam V., Loison J.C., 2016, Molecular Astrophysics, 3, 1
Kalenskii S.V., et al., 2022, ApJ, 932, 5
Miao Y., et al., 1995, ApJL, 445, L59
Moscadelli L., et al., 2021, A&A, 647, A114
Motte F., Bontemps S., Louvet F., 2018, ARA&A, 56, 41
Palau A., et al., 2018, ApJ, 855, 24
Schuller F., et al., 2009, A&A, 504, 415
Schwörer A., et al., 2019, A&A, 628, A6
Tychoniec Ł., et al., 2021, A&A, 655, A65
Wienen M., et al., 2015, A&A, 579, A91
Wong W.H., An T., 2018, Research in Astronomy and Astrophysics, 18, 134