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Abstract

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Full Text

Preamble

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Early Phases of Star Formation: Testing Chemical Tools
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Abstract

Star-forming processes strongly influence the ISM chemistry. Nowadays, many high-quality databases are available at millimeter wavelengths. Using them, it is possible to carry out studies that review and deepen previous results. If these studies involve large samples of sources, it is preferred to use direct tools to study the molecular gas. With the aim of testing these tools such as the use of the HCN/HNC ratio as a thermometer, and the use of H¹³CO⁺, HC₃N, N₂H⁺ and C₂H as “chemical clocks,” we present a molecular line study toward 55 sources representing massive young stellar objects at different evolutionary stages: infrared dark clouds (IRDCs), high-mass protostellar objects (HMPOs), hot molecular cores (HMCs) and ultracompact H II regions. We found that the use of the HCN/HNC ratio as a universal thermometer in the ISM should be taken with care because the HCN optical depth is a big issue that can affect the method. Hence, this tool should be utilized only after a careful analysis of the HCN spectrum, checking that no line, neither the main nor the hyperfine ones, presents absorption features. We point out that the analysis of the emission of H¹³CO⁺, HC₃N, N₂H⁺ and C₂H could be useful to trace and distinguish regions among IRDCs, HMPOs and HMCs. The molecular line widths of these four species increase from the IRDC to the HMC stage, which can be a consequence of the gas dynamics related to the star-forming processes taking place in the molecular clumps. Our results not only contribute with more statistics, acting as a probe of such chemical tools, useful to obtain information in large samples of sources, but also complement previous works through the analysis of other types of sources.

Key words: stars: formation -ISM: molecules -ISM: clouds

1. Introduction

The sites in which the stars form are characterized by a rich and complex chemistry. The smallest gaseous fragments within a molecular cloud, known as hot molecular cores (HMCs), which are related to the formation of massive stars, are the chemically richest regions in the interstellar medium (ISM) (e.g., Herbst & van Dishoeck 2009; Bonfand et al. 2019).

Molecules and chemistry are ubiquitous along all the stages that a forming star goes through, and moreover, forming processes strongly influence the chemistry of such environments (Jørgensen et al. 2020). For instance, as material collapses and becomes ionized by the young massive stars and shocked by jets and outflows, temperature and density can change drastically, leading to the formation and destruction of molecular species. Thus, observing molecular lines and studying their emission and chemistry are important to shed light on the different stages of star formation and to characterize physical and chemical conditions.

To explore the star-forming processes in different environments, one should work with accurate values of the physical properties, such as the kinetic temperature (TK). For example, calculating the excitation temperature (T_{ex}) of carbon monoxide $^{12}\text{C}^{16}\text{O}$, the TK of a molecular cloud can be roughly estimated if it is assumed that there is a complete thermalization of the lines ($T_{\text{ex}} = \text{TK}$). Ammonia (NH_3) has been found in different interstellar environments: from dark quiescent clouds, circumstellar envelopes, and early stages of high and low luminosity star formation to planetary atmospheres and external galaxies (Betz et al. 1979; Martin & Ho 1979; Ho & Barrett 1980; Rathborne et al. 2008; Takano et al. 2013; Bógner et al. 2022). Estimating the NH_3 rotational temperature usually results in a reliable indicator of the kinetic temperature.

Hydrogen cyanide (HCN) and hydrogen isocyanide (HNC) are two of the most simple molecules in the ISM, first detected almost fifty years ago (Snyder & Buhl 1971, 1972). These isomers have a linked chemistry, and differences in the spatial distributions in which they lie within a cloud can reflect the gas chemical conditions and the evolution of the star-forming regions (Schilke et al. 1992). Recently, Hacar et al. (2020) proposed the HCN-to-HNC integrated intensity ratio as a direct and efficient thermometer of the ISM with an optimal working range $15 \text{ K} \leq \text{TK} \leq 40 \text{ K}$. The authors performed an analysis of such isomers throughout the Integral Shape Filament in Orion, deriving an empirical correlation between the HCN/HNC ratio and the kinetic temperature TK. Based on the analysis of such correlation toward many dense molecular clumps from the MALT90 survey, they proposed that the HCN/HNC thermometer can be extrapolated for the analysis of the ISM in general, particularly in star-forming sites, aiming to explore it toward different regions and sources along the ISM.

Molecular species that emerge and are destroyed during the birth of stars can be used to track the star-forming processes within molecular clumps and cores (Stephens et al. 2015; Urquhart et al. 2019). Comparisons between column densities and molecular abundance ratios that can be used to estimate the age and mark the evolutionary stages of star-forming regions are known as “chemical clocks.” As Sanhueza et al. (2012) pointed out, only molecules that exhibit differential abundances with time can be used to evaluate the evolutionary status of a star-forming region. In general, chemical clocks have been studied in depth in low-mass star-forming regions, but this effort has been less developed in the context of high-mass star-forming regions.

As shown by Yu & Wang (2015), in the context of an analysis of chemical

clocks it is important to not only study abundance ratios of such molecules, but also the integrated line intensities, the line widths, among other parameters. For instance, line widths (Δv_{FWHM}) are related to the gas molecular kinematics of the molecular clump interior, regarding turbulence, outflows and shocks among other processes (Sanhueza et al. 2012) which can give information about the evolutionary stage of a massive young stellar object (MYSO).

Some interesting molecular species for probing physical and chemical properties of star-forming regions are diazenylium (N_2H^+) and ethynyl radical (C_2H). Both molecules seem to be good tracers of dense gas in the early stages of the star-forming evolution (Beuther et al. 2008; Sanhueza et al. 2012, 2013). N_2H^+ traces cold gas due to its resistance to depletion at low temperatures (Li et al. 2019), and the latter, additionally, can indicate the presence of a photodissociation region (PDR), where ultraviolet (UV) photons from young and hot massive stars irradiate acetylene to produce C_2H (Fuente et al. 1993; Nagy et al. 2015; García-Burillo et al. 2017). HCO^+ and H_13CO^+ (formylium species) are usually employed to investigate infall motions and outflow activity (Rawlings et al. 2004; Veena et al. 2018), and HC_3N is helpful to explore gas associated with HMCs (Bergin et al. 1996; Taniguchi et al. 2016; Duronea et al. 2019).

The mentioned molecules are among the brightest lines, and they were called molecular fingerprints in a study of a large sample of molecular clumps (Urquhart et al. 2019). As the authors pointed out, such molecules are able to trace a large range of physical conditions including cold and dense gas (HNC , H_13CO^+ , HCN , HN_13C , H_13CN), outflows (HCO^+), early chemistry (C_2H), and gas associated with protostars and young stellar objects (YSOs) (HC_3N , and cyclic molecules).

Thus, the analysis of such molecules gives us a significant amount of scope to search for differences in the chemistry as a function of the evolutionary stage of the star formation taking place within molecular clumps. For instance, Yu & Wang (2015) studied 31 extended green object (EGO) clumps with data from the MALT90 aiming to better understand the chemical processes that take place in the evolution of massive formation. They classified the sources and made a molecular line study over 20 MYSOs and 11 H II regions.

Through the comparison of integrated intensities, line widths and column densities, derived from the emission of N_2H^+ and C_2H with those of the formylium (H_13CO^+) and cyanoacetylene (HC_3N), they suggested that N_2H^+ and C_2H could act as efficient chemical clocks. They found that the N_2H^+ and C_2H column densities decrease from MYSOs to H II regions, and the $[\text{N}_2\text{H}^+]/[\text{H}_13\text{CO}^+]$ and $[\text{C}_2\text{H}]/[\text{H}_13\text{CO}^+]$ abundance ratios also decrease with the evolutionary stage of the EGO clumps.

In addition they ascertained that the velocity widths of N_2H^+ , C_2H , H_13CO^+ and HC_3N are comparable to each other in MYSOs, while in H II regions the velocity widths of N_2H^+ and C_2H tend to be narrower than those of H_13CO^+ and HC_3N .

Nowadays, many high-quality databases are available that were generated from observations obtained with the most important (sub)millimeter telescopes such as the IRAM 30 m Telescope and the Atacama Large Millimeter/submillimeter Array (ALMA), among others. For instance, using this kind of data, it is possible to carry out new chemical studies that, in turn, review and deepen previous results. If these studies involve large samples of sources, it is preferred to use direct tools to study and probe the molecular gas like what presented in Hacar et al. (2020) and Yu & Wang (2015).

Infrared dark clouds (IRDCs) are massive, dense and cold clumps that may harbor budding stars, while high mass protostellar objects (HMPOs) are already protostars accreting material from their surroundings; at this stage, both temperature and density increase, but it is thought that at the beginning, they are chemically poor from an evolutionary point of view. HMCs are considered hotter sources where the chemistry is prolific as a consequence of embedded and evolved HMPOs (Giannetti et al. 2017) until they eventually reach the last stage here considered: ultracompact H II (UCHII) regions. The stars responsible for the UCHII regions have generally finished their accretion process and have begun to ionize the gas around them. All the processes involved in this evolutionary path impact the molecular gas that eventually can be investigated through the emission of molecular lines. It is important to highlight that the mentioned phases in the massive star formation may not have well-defined limits, and sometimes one determined source may have some physical conditions overlapping with those of another kind of source (e.g., Beuther et al. 2007; Gerner et al. 2014). Moreover, different kinds of sources may be embedded within the same molecular clump. Given this complex scenario, comparative studies with many sources are needed to analyze the involved physics and chemistry.

With the aim of testing the presented tools concerning the use of the HCN/HNC ratio as a thermometer (following the methodology published in Hacar et al. 2020), and the analysis of H₁₃CO⁺, HC₃N, N₂H⁺ and C₂H (following the methodology reported in Yu & Wang 2015), we present this study toward 55 sources representing MYSOs at different evolutionary stages as described above. After the presentation of the data and the analyzed sources (Section 2), the paper is structured as follows: a reporting of the results regarding each tested tool (Section 3), their respective discussion (Section 4) and a summary of the main results (Section 5).

2. Data and Analyzed Sources

We made use of the catalog “IRAM 30 m reduced spectra of 59 sources” J/A+A/563/A97 in the VizieR database^[1] (Gerner et al. 2014), from which the molecular data were obtained and the sources were selected to perform our study. The particular molecular lines analyzed in our work are presented in Table 1.

These data, obtained by Gerner et al. (2014), with the 30 m IRAM telescope,

are single pointing spectra observed toward each source. The data used here correspond to the 86–94 GHz band, which have an angular and spectral resolution of 29' and 0.6 km s^{−1} respectively, and typical 1 σ rms values of about 0.03 K.

The sources, classified as IRDCs, HMPOs, HMCs and UCHII, are presented in Table 2, where the coordinates and distances are included. The classification is based on the guidelines introduced by Beuther et al. (2007) and Zinnecker & Yorke (2007) according to the physical conditions of the evolutionary sequence in the formation of high-mass stars. IRDCs are sources that consist of cold and dense gas and dust that emit mainly at (sub)millimeter wavelengths. According to Gerner et al. (2014), the IRDCs of this sample consist of starless IRDCs as well as IRDCs already starting to harbor point sources at m-wavelengths.

HMPOs are sources hosting an actively accreting massive protostar(s), which shows an internal emission source at mid-infrared. HMCs are much warmer than HMPOs and can be distinguished from a chemical point of view. At this stage, the central source(s) heats the surroundings evaporating molecular-rich ices. Finally, the UV radiation from the embedded massive protostar(s) ionizes the surrounding gas and gives rise to an UCHII region. Even though there might be overlaps among HMPO, HMC and even the UCHII stage, such classification was followed by Gerner et al. (2014) based on physical quantities, especially the temperature, which rises from IRDCs to HMPOs to UCHII regions, and based on the chemistry that can differentiate HMPOs (chemically poorer sources) from HMCs (molecularly richer sources). The sample includes 19 IRDCs, 20 HMPOs, 7 HMCs and 9 UCHII regions. In addition to the possible overlaps among the types of sources, it is possible that within the beam of the observational data lies more than one type of source. This is the case for HMC034.26, a region hosting several H II regions and a hot core. Thus, it is necessary to be careful with any analysis in relation to the evolutionary stages.

The quality of these IRAM data and the variety of sources in the sample included in such a catalog allow us to perform a new analysis of several molecular species in order to probe the molecular gas conditions and the chemistry related to IRDCs, HMPOs, HMCs and UCHII regions with the aim of probing chemical tools.

Additionally, we used infrared (IR) data to complement the information obtained from the molecular lines with the aim of probing, in these wavelengths, the activity of the star-forming regions. Data at the Ks band extracted from the UKIRT Infrared Deep Sky Survey (UKIDSS) (Lawrence et al. 2007) and IRAC-Spitzer 4.5 μ m data obtained from the Galactic Legacy Infrared Midplane Survey Extraordinaire (GLIMPSE) survey (Churchwell et al. 2009) were used.

3.1. Infrared and Submillimeter Continuum Emission

Given that jets and outflows affect the star-forming regions' chemistry, we looked for evidence of such processes by using IR data to have additional information on

each source, besides its classification, to interpret and complement the molecular analysis. Data at the Ks band extracted from the UKIDSS were used to search for signs of jets (e.g., Paron et al. 2022) mainly in HMPOs, and also in HMCs and UCHII regions. IRAC-Spitzer 4.5 μ m data, obtained from the GLIMPSE survey, were employed to analyze whether the sources present extended 4.5 μ m emission, likely indicating outflow activity (e.g., Davis et al. 2007). Additionally, each source was checked to see if it is cataloged as an “EGO–likely MYSO outflow candidate” according to the catalog of Cyganowski et al. (2008).

In Table 2 (Cols. 6 and 7), we indicate the kind of emission at the Ks and 4.5 μ m bands observed within the beam size of the IRAM data centered at the position of each source. If one or several point sources appear within the IRAM beam, we indicate this as “points.” Extended emission, suggesting the presence of jets and outflows, is signified as “ext.,” and if this extended emission presents a jet-like morphology, it is stated as “jets.” Diffuse emission without any clear morphology is indicated as “diff.” While “no” means that there is no emission, an “x” indicates there are no data at the corresponding wavelength. In the case of the 4.5 μ m emission, if the source is cataloged as an “EGO–likely MYSO outflow candidate,” this is indicated with “EGO” in Col. 7.

As an example, Figure 1 [Figure 1: see original paper] displays two sources in the Ks band: on the left HMPO20126 shows a jet-like feature and some extended emission at the 4.5 μ m band, while on the right HMC45.47 appears with extended emission at both bands, and it is cataloged as an EGO.

Additionally, in Table 2 (Col. 8), we include the peak flux of the submillimeter emission obtained from the APEX Telescope Large Area Survey of the Galaxy (ATLASGAL) compact source catalog (Contreras et al. 2013; Urquhart et al. 2014) for sources whose coordinates indicated in Cols. 2 and 3 lie within the IRAM beam centered at the source position.

3.2. HCN/HNC Ratio and TK

Following the same procedure as done by Hacar et al. (2020) when they tested the HCN/HNC kinetic temperature in a large sample of dense molecular clumps extracted from the MALT90 survey (see their Section 4.4), we derived the TK for each source of the sample presented here. The correlation to derive TK proposed by the authors is as follows: if the integrated intensity ratio of the isomers HCN and HNC (hereafter $I(\text{HCN})/I(\text{HNC})$) is ≤ 4 , TK is estimated as $\text{TK} = 10 \times I(\text{HCN})/I(\text{HNC})$; and if $I(\text{HCN})/I(\text{HNC}) > 4$, $\text{TK} = 3 \times (I(\text{HCN})/I(\text{HNC}) - 4) + 40$ is used. As done by Hacar et al. (2020), we integrated the HCN ($J = 1-0$), including all hyperfine components and HNC ($J = 1-0$) over a given velocity interval (in Appendix we include some spectra indicating the integrated area in both isomers). The obtained integrated emission values, and the respective ratios, are presented in Table 3 (Cols. 2, 3 and 4, respectively), and the obtained kinetic temperatures following the mentioned relations are presented in Table 4. Typical errors in $I(\text{HCN})$ and $I(\text{HNC})$ are about 0.2 and 0.1 K km s $^{-1}$,

respectively, which yield errors between 1 and 5%, and in some cases at most 10%, in the TK.

From now on, the obtained errors in the measured and derived parameters appear as bars in the figures, and for a better display, we do not include them in the tables.

In the further analysis and comparisons, following Hacar et al. (2020), we do not consider values of kinetic temperatures obtained from the HCN/HNC ratio (hereafter TK(HCN/HNC)) lower than 15 K. These values are due to I(HCN)/I(HNC) ratios close to unity, which according to the authors, the uncertainties in the method grow for such cases, likely due to the combination of excitation and opacity effects. In Section 4.1.1, based on the inspection of the HCN and HNC spectra of sources for which $\text{TK}(\text{HCN}/\text{HNC}) < 15$ K, we discuss this issue.

In order to compare the TK(HCN/HNC), we sought the dust temperature of each source. Dust temperature (T_{dust}) values were obtained from the maps¹ generated by the point process mapping (PPMAP) algorithm (Marsh et al. 2015) applied to the Herschel infrared Galactic Plane Survey (Hi-GAL) maps in the wavelength range 70–500 μm (Marsh et al. 2017). T_{dust} values are included in Table 4, and they represent average values on the dust temperature map over the IRAM beam size centered at the source position. Additionally, we also compared with the ammonia kinetic temperature (TK(NH₃)) derived by Urquhart et al. (2011) in several sources of the sample analyzed here that are contained in the Red MSX Source survey (Hoare et al. 2005; Mottram et al. 2006; Urquhart et al. 2008).

Figure 2 [Figure 2: see original paper] exhibits the comparisons between TK(NH₃) and T_{dust} (upper panel), T_{dust} and TK(HCN/HNC) (middle panel), and TK(NH₃) and TK(HCN/HNC) (bottom panel). Table 5 presents the average temperature values with their errors. As mentioned above, sources with values $\text{TK}(\text{HCN}/\text{HNC}) < 15$ K were not considered, either in the figures or in the calculated average.

3.3. Molecules as “Chemical Clocks” ?

Following Yu & Wang (2015), we performed a similar analysis using the HNC, C₂H, HC₃N, H₁₃CO⁺ and N₂H⁺ emissions measured toward the sources presented in Table 2.

This is: (1) we compared the molecular emissions with the flux at the submillimeter continuum, (2) we analyzed the line widths of the C₂H, HC₃N, H₁₃CO⁺ and N₂H⁺, and (3) we analyzed the column densities (extracted from Gerner et al. 2014) of C₂H and N₂H⁺ by comparing with that of the H₁₃CO⁺.

Figure 3 [Figure 3: see original paper] displays the integrated intensities of

¹<http://www.astro.cardiff.ac.uk/research/ViaLactea/>

HNC, C₂H, HC₃N and N₂H⁺ (presented in Table 3) versus the 870 m peak flux obtained from the ATLASGAL compact source catalog (presented in Col. 8 in Table 2).

We fitted the line emission of C₂H, N₂H⁺, H₁₃CO⁺ and HC₃N with Gaussian functions to obtain the full width at half maximum (FWHM) line widths (Δv) in each source (in Appendix we include some spectra showing the Gaussian fittings). In the case of the C₂H and N₂H⁺, which have hyperfine components, the fitting was done with multiple Gaussian functions, and the Δv values used in this analysis correspond to the main components. These values are presented in Table 6. The absence of values in some sources is due to a lack of emission or the hyperfine components being completely blended with the main component. Table 7 expresses the average line widths for each kind of source, and with the aim of analyzing their behavior, following the analysis reported in Yu & Wang (2015), we present plots that display relations among the measured Δv in Figure 4 [Figure 4: see original paper].

From Gerner et al. (2014) we obtained the column densities of C₂H, N₂H⁺ and H₁₃CO⁺ for each source. We used the column densities obtained as “iteration 1” according to the model used by the authors, which are the values derived with the mean temperatures from the best-fit models of “iteration 0.” Values indicated as upper limits are not included in our analysis. Figure 5 [Figure 5: see original paper] displays the column densities of C₂H and N₂H⁺ versus the H₁₃CO⁺ column density. Error bars are not included, given that the authors did not inform them in their work. Finally, Figure 6 [Figure 6: see original paper] depicts the relative abundance of [C₂H]/[H₁₃CO⁺] versus [N₂H⁺]/[H₁₃CO⁺].

4. Discussion

Unlike low-mass stars, the formation of high-mass stars is not yet fully understood, and different scenarios have been proposed (see e.g., Tan et al. 2014; Motte et al. 2018). Probing the chemical conditions of high-mass star-forming regions at different evolutionary stages is an important issue to advance knowledge on the formation of this kind of star, and to explore such chemical conditions, it is necessary to use efficient tools.

In this context, we decided to test the HCN/HNC ratio as a thermometer of the gas, as well as the use of the emission of H₁₃CO⁺, HC₃N, N₂H⁺ and C₂H as “chemical clocks.” The obtained results from each study are discussed in what follows.

4.1. Testing the use of HCN/HNC Ratio as a Thermometer

Employing simple molecules, ubiquitous in star-forming regions, to derive their physical parameters is a helpful strategy for methodically analyzing many regions and avoiding complex calculations. In this context, we use the HCN/HNC intensity ratio formulation proposed recently by Hacar et al. (2020) to estimate the kinetic temperature (TK(HCN/HNC)).

As done by the authors, we probed them through comparisons with dust temperature (T_{dust}) and TK obtained from the ammonia emission ($\text{TK}(\text{NH}_3)$), when those parameters were available toward the sources of the analyzed sample. It is worth noting that the useful kinetic temperature range derived from the ammonia is between 15 and 40 K (Ho & Townes 1983; Urquhart et al. 2011), in coincidence with the valid range indicated for $\text{TK}(\text{HCN}/\text{HNC})$.

Despite the limited amount of sources satisfying that the obtained TK from the HCN/HNC ratio is >15 K with measured values of T_{dust} and $\text{TK}(\text{NH}_3)$ (see Table 4), some conclusions can be extracted. Also, from the sources with $\text{TK}(\text{HCN}/\text{HNC}) < 15$ K or lower than expected, we can obtain important conclusions about this tool.

The comparison between T_{dust} and $\text{TK}(\text{NH}_3)$ (see upper panel of Figure 2) indicates that, within a range of 0-5 K of difference between both temperatures, the molecular gas and the dust could be considered to be thermally coupled, allowing us to suggest that in general this property could be extrapolated to the whole sample. This supports that comparison between $\text{TK}(\text{HCN}/\text{HNC})$, which is obtained from the gas emission, and the T_{dust} can be made.

Valid kinetic temperature values obtained following the HCN/HNC ratio (i.e., >15 K) seem to be more accurate for IRDCs and HMPOs than for HMCs and UCHII regions. By analyzing the average values (see Table 5), TK obtained from the dust and ammonia emissions increases from IRDCs to UCHII regions as expected, but $\text{TK}(\text{HCN}/\text{HNC})$ increases only from IRDCs to HMPOs, and then it decreases in HMCs and UCHII regions. This suggests that in such sources, using the HCN-HNC tool to derive TK may not be appropriate, and it may underestimate the actual temperature value.

Hacar et al. (2020) calculated the $\text{TK}(\text{HCN}/\text{HNC})$ toward a large sample of dense clumps extracted from the MALT90 survey (Foster et al. 2011; Jackson et al. 2013), and compared them with the T_{dust} measurements derived by Guzmán et al. (2015). At this point, they stated that the comparison between TK and T_{dust} should be done with caution given the fact that the beam resolution of the MALT90 targets and the measurement sensitivity within this beam do not allow resolving the temperature of individual clumps. However, they pointed out that a correspondence between both temperatures prevails despite the mentioned observational caveats.

Nevertheless, they do not discuss the optical depth issue in the MALT90 sample as they did for their Orion results. This is an important matter to be considered, mainly when we work with a sample of different kinds of sources. As Hacar et al. (2020) mention, the increase of the HCN $J = 1-0$ line opacity, while the HNC $J = 1-0$ line likely remains optically thin, would reduce the HCN/HNC ratio, decreasing the values of $\text{TK}(\text{HCN}/\text{HNC})$. This phenomenon is observed in sources with $\text{TK}(\text{HCN}/\text{HNC}) < 15$ K (see Section 4.1.1) and in some other sources that, although the TK obtained from the HCN-HNC tool is greater than 15 K, their values are well below the temperatures obtained from the dust

and/or ammonia (about 10 K of difference). This is the case of HMCs and UCHII regions in our sample, in which, in general, it is observed that the HCN hyperfine line $F = 1-1$ appears absorbed, indicating high optical depths (for an example, see Figure A5).

4.1.1. Sources with $TK(\text{HCN}/\text{HNC}) < 15 \text{ K}$ In our sample, there are several sources such that the HCN/HNC ratio yields kinetic temperatures lower than 15 K, which were neither included in the analysis nor the comparisons with T_{dust} and $TK(\text{NH}_3)$ performed above. These sources have $I(\text{HCN})/I(\text{HNC})$ ratios close to unity or even lower than one, which according to Hacar et al. (2020), in those cases, the uncertainties seem to increase, likely due to the combination of excitation and opacity effects. The percentages of sources with this issue are: 58%, 30%, 28% and 11% for IRDCs, HMPOs, HMCs and UCHII regions, respectively, suggesting that this may be a condition that is more pronounced at earlier stages.

Taking into consideration the HCN hyperfine line anomalies (Walmsley et al. 1982; Loughnane et al. 2012), which prevent obtaining reliable values of HCN opacities, we carefully analyzed each HCN and HNC spectrum to look for signatures of high optical depths. We found that the HCN spectra of sources with $TK(\text{HCN}/\text{HNC}) < 15 \text{ K}$ have pronounced saturation and/or self-absorption features in some cases at both the main component and hyperfine lines (see Figure 7 [Figure 7: see original paper] for an example), and in other cases in the hyperfine line $F = 1-1$. In the case of the HNC, we did not find such spectral features.

We point out that the use of the HCN/HNC ratio as a universal thermometer in the ISM should be taken with care. We suggest that such a thermometer could be used only in some IRDCs and HMPOs (when the derived kinetic temperature is not lower than 15 K; see Section 4.1.1) and in more evolved regions, for instance, HMCs and UCHII regions, this tool underestimates the temperature. Thus, we conclude that the HCN-HNC tool as a kinetic temperature estimator should be used only after a careful analysis of the HCN spectrum, checking that no line, either the main or the hyperfine ones, presents absorption features; otherwise, it is not a useful tool for calculating kinetic temperatures.

4.2. An Exploration of Molecules as “Chemical Clocks”

Molecular species such as HNC, HCN, H^{13}CO^+ , C_2H and HC_3N are relatively easy to observe and they give us a significant amount of scope to search for differences in the chemistry as a function of the evolutionary stage in massive star-forming regions (Sanhueza et al. 2012; Yu & Wang 2015; Urquhart et al. 2019). After performing a similar analysis as presented by Yu & Wang (2015) on our sample of massive star-forming regions, we discuss our results below.

First, from the comparison between the molecular integrated intensities and the 870 μm peak flux (see Figure 3 [Figure 3: see original paper]), we found that,

in general, the integrated intensities of N₂H⁺, C₂H, HNC and HC₃N increase with the submillimeter peak flux. In the case of IRDCs, HMPOs and HMCs, this increment correlates with the evolutionary stage of the sources, i.e., the position of each kind of source in the plots seems to be sectorized. UCHII regions show the same trend, but their points are overlapped with those of the other sources in all cases except for the N₂H⁺ case. Yu & Wang (2015) found that the N₂H⁺ integrated intensities of H II regions tend to be lower than those for MYSOs. This behavior seems to occur with the UCHII regions of our sample in comparison with the other sources, suggesting that the destruction path due to electronic recombination, where N₂H⁺ is destroyed by free electrons from the surroundings (Vigren et al. 2012), could be ongoing in the UCHII regions.

This result complements what was presented by Yu & Wang (2015) with sources at earlier stages, and suggests that the relation between the molecular integrated intensities and the 870 μm peak flux could be useful to distinguish regions among IRDCs, HMPOs and HMCs.

The comparisons between the column densities obtained from Gerner et al. (2014) also show an interesting trend regarding the evolutionary stage of the sources. Yu & Wang (2015) stated, based on astrochemical models (e.g., Bergin et al. 1997; Nomura & Millar 2004), that the H₁₃CO⁺ column density reflects the amount of H₂ density in a clump because its abundance seems to not vary much with time. In line with their work, we compared N(C₂H) and N(N₂H⁺) with N(H₁₃CO⁺) (see Figure 5 [Figure 5: see original paper]). The N(H₁₃CO⁺) values of our sample range in a wider interval of values (from some 10¹² cm⁻² for IRDCs to values close to 10¹⁴ cm⁻² for HMCs) than the N(H₁₃CO⁺) presented by Yu & Wang (2015). An increase in the N(C₂H) and N(N₂H⁺) with the N(H₁₃CO⁺) is observed. In the case of N(C₂H) versus N(H₁₃CO⁺) relation, such an increment also presents a conspicuous correlation with the evolutionary stage from IRDCs to HMCs in which the positions of each kind of source are sectorized in the plot. In the UCHII regions, both column densities have similar values compared with those of HMCs and the largest ones of HMPOs. A similar behavior, with larger dispersion, is observed in the comparison between N(N₂H⁺) versus N(H₁₃CO⁺). The N₂H⁺ and H₁₃CO⁺ column density increment from IRDCs to HMCs could be explained by their progressive formation through the H₃⁺ + 13CO → H₁₃CO⁺ + H₂, and H₃⁺ + N₂ → N₂H⁺ + H₂ mechanisms (Jørgensen et al. 2004). Then, the break on the constant increment in the column density values in the UCHII regions compared with the previous sources can be due to the beginning of the destruction of such molecules by electronic recombination (Yu & Xu 2016).

It is worth noting that the discussed behavior in the column densities (which have molecular excitation assumptions) regarding the correlation with the evolutionary stage from IRDCs to HMCs is quite similar to the comparison between the integrated intensities and the peak submillimeter flux (which are direct measurements). Thus, in the line of a chemical clock analysis, even though more statistics are necessary, we propose that these relations, mainly the N(N₂H⁺)

versus $N(\text{H13CO}^+)$ and the $I(\text{C2H})$ versus $F870 \text{ m}$, in which the different kinds of sources (IRDCs, HMPOs and HMCs) are clearly separated, could be used to differentiate them, which can be useful in works handling a large amount of sources of unknown, or not completely known, nature.

The comparison between the relative abundance ratios $[\text{C2H}]/[\text{H13CO}^+]$ versus $[\text{N2H}^+]/[\text{H13CO}^+]$ (Figure 6 [Figure 6: see original paper]) presents a high dispersion, mainly along the y-axis, i.e., in the $N(\text{C2H})/N(\text{H13CO}^+)$ ratio, and does not show a remarkable difference as it was found between MYSOs and H II regions by Yu & Wang (2015). However, along the x-axis, i.e., in the $N(\text{N2H}^+)/N(\text{H13CO}^+)$ ratio, some trend can be appreciated, mainly such a ratio seems to be larger in IRDCs in comparison with the other kind of sources. In the line of a chemical clock analysis, we suggest that this abundance ratio can be used to differentiate the earliest stage of the star-forming regions.

The molecular line widths (FWHM) are usually associated with the kinematics of the molecular gas and can be affected by multiple events, such as shocks, outflows, rotation of the clump, line widths and turbulence. In this work, we assume that they originate mainly from the increasing turbulence that arises as a consequence of evolving star formation stages (Sanhueza et al. 2012; Yu & Wang 2015). With this in mind, by analyzing the average line width of N2H^+ , HC3N , H13CO^+ and C2H (see Table 7), it can be appreciated that in the four species, the line width rises until reaching the HMC stage. Such an increase could be a consequence of the gas dynamics related to the star-forming processes that take place in the molecular clumps (Fontani et al. 2002; Pirogov et al. 2003). Particularly, our $\Delta v(\text{N2H}^+)$ average values are in quite good agreement with those presented by Sanhueza et al. (2012): the average value that we obtained for IRDCs is similar to that obtained by the authors in their so-called “quiescent” and “intermediate” clumps, while the value that we obtained for HMPOs is in agreement with the values of their “active” clumps. Finally, our $\Delta v(\text{N2H}^+)$ average values obtained for HMCs and UCHII regions are slightly larger than the value obtained for their “red” clumps. Following Sanhueza et al. (2012), we can confirm that the line widths of N2H^+ slightly increase with the evolution of the clumps.

As found by Sanhueza et al. (2012) in their sample of clumps embedded in IRDCs, we observed that in our sources, the H13CO^+ and HC3N have slightly narrower line widths than N2H^+ (see panels d and f in Figure 4 [Figure 4: see original paper]). This hints that they trace similar optically thin gas emanating from the internal layers of the regions, and according to our findings, it seems to be independent of the kind of source. Yu & Wang (2015) found that the best Δv correlation is between C2H and N2H^+ for their sample of EGOs. In our case, we did not find such a good correlation between these molecular species (see panel e in Figure 4). The C2H line widths are slightly narrower than those of the N2H^+ . Sanhueza et al. (2012) also remarked that the C2H appears to present the best correlation with N2H^+ among all the studied Δv relations. However, by inspecting their $\Delta v(\text{C2H})$ versus $\Delta v(\text{N2H}^+)$ plot, we observe a

similar behavior as our plot, where most of the points tend to be below the unity line.

In the spectra of these four molecular species toward the whole sample, we did not find line wings that may probe outflows, except the HC3N spectra of HMPO18247, HMC029.96 (see Figure A6) and UCH10.30, and in the H13CO+ spectrum of HMC34.26, in which small spectral wings appear. UCH10.30 is an EGO; the other sources present 4.5 m extended emission and diffuse emission at the Ks band.

Besides these sources, it can be noticed that the near-infrared (near-IR) evidence of jets or/and outflows does not have any direct correlation with spectral features in the emission of N2H+, HC3N, H13CO+ or C2H.

5. Summary and Concluding Remarks

We presented a spectroscopic molecular line analysis of 55 high-mass star-forming regions with the aim of probing some chemical tools that were recently proposed to characterize such regions. The analyzed sources are classified as IRDCs, HMPOs, HMCs and UCHII regions, according to an evolutionary progression in high-mass star formation. The main results can be summarized as follows:

1. The emissions of the HCN and HNC isomers were used to estimate the kinetic temperature through a new “thermometer” whose formulation was proposed by Hacar et al. (2020), and we investigated its use in the presented sample of sources. By comparing the TK derived from the HCN/HNC ratio with temperatures obtained from the dust and ammonia emission, we found that the use of such a ratio as a universal thermometer in the ISM should be taken with care. The HCN optical depth is a big issue to be taken into account. Line saturation may explain the derived temperature values below 15 K, which must be discarded, and mainly correspond to IRDCs and HMPOs. In addition, we found that, although the TK obtained from the HCN-HNC tool is greater than 15 K, its value could be far from the temperatures obtained from the dust or ammonia, yielding lower temperatures. This is the case of HMCs and UCHII regions of our sample, in which, in general, it is observed that the HCN hyperfine line F = 1-1 appears absorbed. In conclusion, we point out that the HCN-HNC tool as a kinetic temperature estimator should be used only after a careful analysis of the HCN spectrum, checking that no line, either the main or the hyperfine ones, presents absorption features.
2. Additionally, we analyzed the molecular species N2H+, HC3N, H13CO+ and C2H in the sample of sources focusing on their use as “chemical clocks.” The comparison of the molecular integrated intensities of HC3N, N2H+, C2H and also of HNC with the 870 m peak flux, as well as the relations of the column densities of C2H and N2H+ with that of the H13CO+, can be useful to distinguish regions among IRDCs, HMPOs and HMCs, which

complement the Yu & Wang (2015) results. On the other hand, from the $[\text{C2H}]/[\text{H13CO}^+]$ versus $[\text{N2H}^+]/[\text{H13CO}^+]$ relation, we can point out that even though the $[\text{C2H}]/[\text{H13CO}^+]$ ratio shows a large dispersion along the analyzed sources, the $[\text{N2H}^+]/[\text{H13CO}^+]$ ratio seems to be larger in IRDCs in comparison with the other kind of sources analyzed in this work. Finally, regarding the molecular line widths, we found that the Δv rises from the IRDC to the HMC stage, which could be due to the increasing turbulence as a consequence of the evolution of the star-forming processes.

In conclusion, this work explores chemical tools, some of them based on direct measurements, to be applied in different ISM environments. In that sense, we probed such tools in a new sample of sources with respect to previous works, and these results not only contribute to more statistics in the literature but also complement such works with other types of sources. Using direct tools, like, for instance, the ratios of different molecular parameters that can be directly measured from the observations, can be very useful mainly when a large sample of sources is handled. If it is proven that such tools are reliable, they can be used to obtain important statistical information in a simple way. Our work points to this and encourages performing similar works in larger samples of sources of different types.

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Appendix: Example Spectra

In this appendix we include some spectra of the analyzed molecular lines as an example of each kind of source, showing the integrated area in the case of the HCN and HNC emissions and the Gaussian fittings for H13CO^+ , C2H , HC3N and N2H^+ . Spectra of IRDC18151 are shown in Figures A1 and A2, of HMPO20126 in Figures A3 and A4, of HMC029.96 in Figures A5 and A6, and of UCHII 45.45 in Figures A7 and A8.

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