A complete 3mm line survey of the B1-b and TMC-1 cores

New discoveries with the IRAM 30m and Yebes 40m telescopes

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Abstract. We present the 3mm spectral line survey performed at the IRAM 30m telescope towards the dense cores B1-b and TMC-1. Within the 46 GHz observed, we have identified more than 500 lines arising from more than 60 molecules. We have also detected tens of unidentified lines, allowing the discovery of new molecular species in space. In this contribution we discuss two examples: the case of H_2NC and CH_3CO^+. In the latter, the 30m data was used in combination with the 7mm survey data from the Yebes 40m telescope, which provides lower energy transitions. Our deep 3mm and 7mm spectral surveys reveal a forest of lines at 50-100 mK, showing that dark clouds cannot be considered poor line sources anymore.

1 Introduction

Cold (T_{kin} ∼10 K) and dense (n ∼10^{4-5} cm^{-3}) cores are the sites where low-mass protostars and planetary systems like ours will eventually form. These regions are relatively simple since they lack of the physical complexity and energetic events associated with the star formation process. They also present a rather simple chemical scheme, dominated by gas-phase chemical reactions, mainly exothermic ion-molecule and neutral-neutral reactions, due to their low temperatures. Nevertheless, these quiet and cold regions are chemically rich and complex. Spectral line surveys are the best tool to obtain the complete view of the molecular inventory of dense cores. They require sensitive and large bandwidth receivers, but also high spectral resolution is needed in order to resolve the narrow lines arising from these cold sources. In 2011 a major upgrade at the IRAM 30m telescope was completed, with the installation of the EMIR receivers and FFTS spectrometers with a narrow spectral mode, allowing simultaneous observations of 7.2 GHz per frequency setup at high resolution. The extension of the 3mm band limits down to 72 GHz, performed in 2018, also improved the performance of the 30m, by accessing to the fundamental transitions of several deuterated species. With these improvements, the IRAM 30m telescope has become a powerful instrument to perform systematic spectral line surveys.

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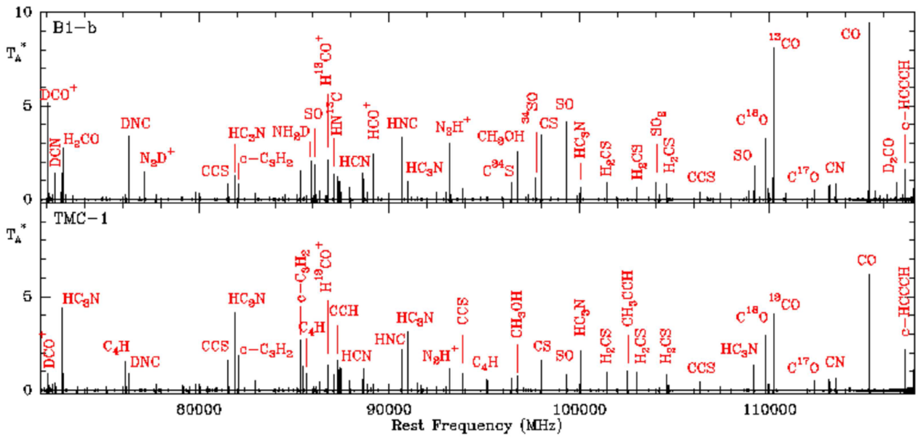

Figure 1. Complete 3mm spectral line survey observed towards B1-b and TMC-1.

2 The 3mm line survey

Figure 1 shows the full 3mm band observed towards B1-b and TMC-1, with labels indicating the strongest identified lines. In total we have covered 46 GHz, between 71.6 and 117.6 GHz. The final rms obtained in our data ranges between 3-5 mK below 110 GHz, increasing to more than 10 mK at the highest frequencies. Thanks to the high sensitivity reached in our spectra, we are able to confidently detect weak lines of ~20-30 mK (see Fig. 2). Table 1 shows the list of identified molecules in both sources. Different colours indicate those species detected only in B1-b (red) or TMC-1 (blue), and recent new detections are also highlighted. Except for H_2NC, all the new species were detected in combination with data from the 7mm spectral survey performed at the Yebes 40m telescope. In total, we have identified 579 lines in B1-b arising from 62 molecular species (127 if we include isotopic substitutions), and 512 lines from 66 molecules (125 including isotopologues) towards TMC-1. As seen in Fig. 1 and Table 1, deuterated substitutions and oxygen-bearing species, including complex molecules typical of hot cores and hot corinos, are mainly detected towards B1-b. On the other hand, TMC-1 is more prolific in carbon chains. These differences could be related to their different physical properties and evolution. While TMC-1 is a starless core, B1-b contains two very young protostars, one of them showing strong emission from COMs as seen by ALMA ([12]). Nevertheless, these objects are not resolved by the 30m beam, and we are essentially observing the cold protostellar envelope. It is also worth noting that although CH_3OCOH and CH_3OCH_3 are not detected in our 3mm line survey towards TMC-1, they have been observed through lower energy transitions with the Yebes 40m telescope (see [1]).

3 First detection of H_2NC

After the extension of our 3mm survey to low frequencies, we detected a series of unidentified lines around 72.2 GHz, which could not be assigned to any molecule. A similar pattern was also observed towards the envelope of the Class 0 protostar L483, which shows stronger and narrower lines than B1-b, and also a larger number of components (see Fig. 2). The observed spectra is typical of a molecule with a complex fine and hyperfine structure. The large splitting betweeen line components suggest that they correspond to a low rotational transition,

Table 1. Identified molecules within the 3mm line survey.

2 atoms	3 atoms		4 atoms		5 atoms		6 atoms	7 atoms	8 atoms
CN	C_2H	DCO^+	NH_2D	$HOCO^+$	CH_3O	C_4H	CH_3OH	CH_3CCH	**CH_2CHCCH**[j]
CO	C_2D	HNO	NHD_2	$DOCO^+$	l-C_3H_2	C_4D	CH_2DOH	CH_2DCCH	CH_3OCOH
CS	HCN	C_2O	H_2CN	H_2CS	l-C_3HD	HC_3N	CH_3OD	CH_3CCD	CH_2CCHCN
SiO	DCN	HCS	**H_2NC**[a]	HDCS	c-C_3H_2	DC_3N	CHD_2OH	CHD_2CCH	
NS	HNC	HSC	$HCNH^+$	D_2CS	c-C_3HD	HCCNC	**CH_2CCH**[g]	CH_3CHO	
NS^+	DNC	HCS^+	H_2CO	C_3N	c-C_3D_2	HNC_3	CH_3CN	CH_2CHCN	
SO	N_2H^+	C_2S	D_2CO	**C_3N^-**[b]	H_2CCN	$NCCNH^+$	CH_2DCN	HC_5N	
SO^+	N_2D^+	OCS	l-C_3H	C_3O	H_2CCO	**HC_3O^+**[e]	**CH_3CO^+**[h]		
	HCO	SO_2	c-C_3H	CNCN	HDCCO	**H_2CCS**[c]	CH_3SH		
	HCO^+		c-C_3D	**HCCS**[c]	HCOOH	**HCSCN**[f]	l-H_2C_4		
			HCCO	**$HCCS^+$**[d]			HC_3NH^+		9 atoms
			HNCO	HNCS			**$HCCNCH^+$**[i]		CH_2CHCH_3
			HCNO	HSCN			HCCCHO		CH_3OCH_3
			HOCN	C_3S			c-H_2C_3O		CH_3C_4H
			DNCO						

Notes. Species only detected in B1-b are indicated in red, while those observed only in TMC-1 are indicated in blue. Bold text highlights recent discoveries. **References.** (a): [4] (b): [6] (c): [8] (d): [5] (e): [7] (f): [9] (g): [2] (h): [10] (i): [3] (j): [11]

and our first hypothesis was to consider this as the $N = 1-0$ rotational transition of a linear or quasi-linear species. We requested IRAM 30m time to search for the two immediately higher transitions, in order to confirm this hypothesis. These new observations allowed the detection of a series of lines at the expected frequencies of the $N = 2-1$ and $N = 3-2$ transitions at 144 and 216 GHz, respectively (see [4]). With multiple transitions at hand we investigated the potential carrier, and performed high-level ab initio calculations for all possible candidates. Among them, H_2NC, a high energy isomer of H_2CN, had the closest value to the observed rotational constant. Furthermore, it is an open-shell species containing three nuclei with non-zero nuclear spin, whose predicted fine and hyperfine splitting is consistent to the observed one. Assuming H_2NC as the carrier of the observed unidentified transitions, we analysed the observed frequencies with the appropriate Hamiltonian in order to obtain the complete set of spectroscopic parameters. The results show an excellent agreement between the theoretical and astronomical values (see [4]).

The observed abundance ratio H_2NC/H_2CN is 1.0±0.3 and 1.25±0.30 for B1-b and L483, respectively ([4]). These two isomers have also been observed in the z=0.89 galaxy in front of the quasar PKS 1830-211, where the derived H_2NC/H_2CN ratio is 0.27±0.08. Since the chemical composition of this lensing galaxy is characteristic of diffuse or translucent clouds ([14]), this situation reminds that of the HNC/HCN abundance ratio, which is ∼1 in cold dense clouds and <1 in diffuse clouds. Our observations in B1-b and L483 show that the strongest hyperfine component of H_2NC is 3-4 times more intense than the strongest one of H_2CN. Therefore, H_2NC should be easily observable in those sources where H_2CN is detected. It is interesting to note that neither H_2NC nor H_2CN are detected towards TMC-1. Ohishi et al. ([13]) reported the discovery of H_2CN, although the lines were marginally detected and they should result in antenna temperatures above 20 mK in our 30m spectra. Therefore, the detection of H_2CN in TMC-1 by [13] is questionable.

4 Discovery of CH_3CO^+

The detection of the acetyl cation, CH_3CO^+, is one example of the fruitful combination of the IRAM 30m and Yebes 40m telescopes. Within the unidentified lines in our spectral surveys of TMC-1 at the 3mm and 7mm bands, we found two series of four lines that are harmonically related. The observed spectra (see Fig. 2) reminds that of the $K = 0$ and $K = 1$ components of the rotational transitions of a symmetric rotor. Indeed, if we assume that the carrier is the same for both series of lines and that it has a C_{3v} symmetry, all lines can be fitted with

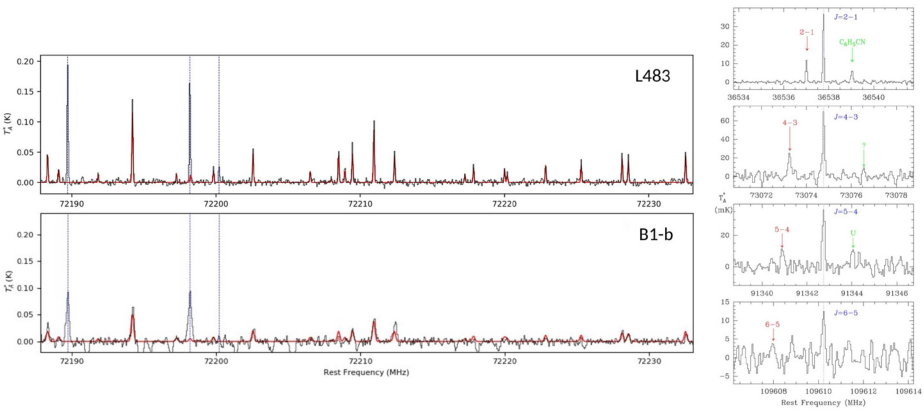

Figure 2. *(left):* Series of unidentified lines observed towards L483 (top panel) and B1-b (bottom panel), later assigned to the $1_{0,1} - 0_{0,0}$ transition of H_2NC. Lines in blue correspond to hyperfine components of the $N = 1 - 0$ transition of CCD. *(right):* Observed lines of CH_3CO^+ towards TMC-1. The blue labels correspond to the series of lines we assign to the A species of CH_3CO^+, while the red ones correspond to those of the E species.

a single rotational constant and two distortion constants. The derived rotational constant B from astronomical observations is 9134 MHz, suggesting that the molecule should contain at least three atoms betweeen C, N, and O. Several candidates were proposed based on their similar rotational constants, and we computed their spectroscopic molecular parameters using high-level ab initio calculations (see [10]). The best agreement is found for CH_3CO^+, which possible chemical precursor ketene (H_2CCO) is one of the most abundant O-bearing species in TMC-1 ([7]). In order to support this possible assignment, we performed microwave laboratory experiments to detect CH_3CO^+ ([10]). In total, 79 lines were observed in the laboratory with quantum numbers in the ranges J =10-27 and $K \leq 6$. Thus, the detection in space of the acetyl cation is secure and based on astronomical, theoretical and experimental data.

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