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Detection of the HC_3NH^+ and HCNH^+ ions in the L1544 pre-stellar core

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ABSTRACT

The L1544 pre-stellar core was observed as part of the ASA (Astrochemical Surveys At IRAM) Large Program. We report the first detection in a pre-stellar core of the HCNH^+ and HC_3NH^+ ions. The high spectral resolution of the observations allows us to resolve the hyperfine structure of HCNH^+ . Local thermodynamic equilibrium (LTE) analysis leads to derive a column density equal to $(2.0 \pm 0.2) \times 10^{13} \text{ cm}^{-2}$ for HCNH^+ and $(1.5 \pm 0.5) \times 10^{11} \text{ cm}^{-2}$ for HC_3NH^+ . We also present non-LTE analysis of five transitions of HC_3N , three transitions of H^{13}CN and one transition of HN^{13}C , all of them linked to the chemistry of HCNH^+ and HC_3NH^+ . We computed for HC_3N , HCN and HNC a column density of $(2.0 \pm 0.4) \times 10^{13} \text{ cm}^{-2}$, $(3.6 \pm 0.9) \times 10^{14} \text{ cm}^{-2}$ and $(3.0 \pm 1.0) \times 10^{14} \text{ cm}^{-2}$, respectively. We used the gas-grain chemical code NAUTILUS to predict the abundances of all these species across the pre-stellar core. Comparison of the observations with the model predictions suggests that the emission from HCNH^+ and HC_3NH^+ originates in the external layer where non-thermal desorption of other species was previously observed. The observed abundance of both ionic species ($[\text{HCNH}^+] \approx 3 \times 10^{-10}$ and $[\text{HC}_3\text{NH}^+] \approx [1.5 - 3.0] \times 10^{-12}$, with respect to H_2) cannot be reproduced at the same time by the chemical modelling within the error bars of the observations only. We discuss the possible reasons for the discrepancy and suggest that the current chemical models are not fully accurate or complete. However, the modelled abundances are within a factor of 3, consistent with the observations, considering a late stage of the evolution of the pre-stellar core, compatible with previous observations.

Key words: astrochemistry – line: identification – molecular data – radiative transfer.

1 INTRODUCTION

Protonated hydrogen cyanide, HCNH^+ , was first discovered in the interstellar medium towards Sgr B2 by Ziurys & Turner (1986) using the $J = 1-0$, $2-1$ and $3-2$ pure rotational transitions at 74, 148 and 222 GHz, respectively. They derived a fractional abundance of 3×10^{-10} . Since the initial detection, HCNH^+ has also been observed in the TMC-1 dark cloud (Schilke et al. 1991; Ziurys, Apponi & Yoder 1992) as well as the DR 21(OH) compact H II region (Schilke et al. 1991; Hezareh et al. 2008) with abundances of 1.9×10^{-9} and $\sim 10^{-10}$, respectively. This ion appears to be one of the key species in the ion-molecule network of interstellar chemistry. It was also thought to be the main precursor to both HCN and HNC , both formed through rapid dissociative recombination of HCNH^+ (Herbst 1978).

Protonated Cyanoacetylene (HC_3NH^+) has been searched towards a sample of dark cloud, evolved star, high-mass star-forming region by Turner, Amano & Feldman (1990) with no conclusive detection due to the high rms of their observations. Also, Amano et al. (1990) performed a deep search of the 5–4 transition at 43.3 GHz towards TMC-1 resulting in an upper limit only. HC_3NH^+ was later detected in the same cloud by Kawaguchi et al. (1994) through the 5–4 (43.3 GHz) and 4–3 (34.6 GHz) transitions consistent with an abundance of 1×10^{-10} . It is the largest ion detected so far in space. It is thought to play a role in the production of the cyanopolyyynes (HC_{2n+1}N , where n is an integer; Turner et al. 1990) that are ubiquitous in cold dark clouds.

L1544 is a prototypical pre-stellar core in the Taurus molecular cloud complex ($d \sim 140$ pc) and is on the verge of gravitational collapse (Caselli et al. 2002a, 2012, and references within). It is characterized by a high central density (larger than a few 10^6 cm^{-3}), a low temperature (~ 7 K), a high CO depletion and a large degree of molecular deuteration (Caselli et al. 2003; Crapsi et al. 2005;

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Vastel et al. 2006). Its physical and dynamical structure has been reconstructed by Caselli et al. (2012) and Keto, Rawlings & Caselli (2014) taking into account the numerous observations that have been made towards L1544 as well as the first detection of water in a pre-stellar core. The observed water line shows an inverse P-Cygni profile (Caselli et al. 2012; Quénard et al. 2016), characteristic of gravitational contraction, confirming that L1544 is on the verge of collapse. Keto & Caselli (2010) and Keto et al. (2014) have shown that L1544 is in slow contraction from unstable quasi-static hydrodynamic equilibrium (an unstable Bonnor–Ebert sphere).

As part of the IRAM-30-m Large Program ASAI¹ (Lefloch et al. in preparation), a highly sensitive, unbiased spectral survey of the molecular emission of the L1544 pre-stellar core has been performed with a high spectral resolution. From this survey, Vastel et al. (2014) reported the detection of many oxygen-bearing complex organic molecules (COMs) and suggested that they were produced through the release, in the gas phase, of methanol and ethene through non-thermal desorption processes. The sensitivity of these IRAM observations also led to the detection of the hyperfine structure of CH_2CN (Vastel et al. 2015a) as well as HOCO^+ (Vastel et al. 2016) that were likely emitted in the external layer through the same non-thermal desorption processes as for the COMs. In this study we report on the detection of the HCNH^+ and HC_3NH^+ ions for the first time in a pre-stellar core. These ions are involved in the chemistry of HCN and HNC, both important species in the formation of larger and more complex nitrogen-bearing molecules.

2 OBSERVATIONS

We used the observations published by Vastel et al. (2014) combined with more recent observations. The latest were performed in 2015 December at the IRAM-30-m towards L1544 ($\alpha_{2000} = 05^{\text{h}}04^{\text{m}}17\overset{\text{s}}{.}21$, $\delta_{2000} = 25^\circ10'42\overset{\text{s}}{.}8$). We used the broad-band receiver EMIR at 3 mm, connected to an FTS spectrometer in its 50 kHz resolution mode. The beam of the observations is 33 arcsec, 28 arcsec and 26 arcsec at 75, 87 and 95 GHz, respectively. Weather conditions were very good with 2 to 3 mm of precipitable water vapour. System temperatures were between 80 and 110 K, resulting in an average rms of ~ 4 mK in a 50 kHz frequency bin. In order to obtain a flat baseline, observations were carried out using a nutating secondary mirror, with a throw of 3 arcmin. No contamination from the reference position was observed. Pointing was checked every 1.5 h on the nearby continuum sources 0439+360 and 0528+134. Pointing errors were always within 3 arcsec. We adopted the telescope and receiver parameters (main-beam efficiency, half power beam width, forward efficiency) from the values monitored at IRAM-30-m (<http://www.iram.fr>). Line intensities are expressed in units of main-beam brightness temperature.

HCNH^+ contains a nitrogen atom and exhibits electric quadrupole hyperfine structure, resolved in our observations, whose frequencies and other spectroscopic parameters have been retrieved from the CDMS data base² (Cologne Database for Molecular Spectroscopy, Müller et al. 2001) based on astronomical observations of Ziurys et al. (1992). They have detected the electric quadrupole structure in this ion, through the observation of the $J=1-0$ transition towards the cold dark cloud TMC-1, enabling the determination of the quadrupole coupling constant. The HCNH^+ rest frequencies from the CDMS data base are the following: $F = 0-1: 74\ 111.5427$,

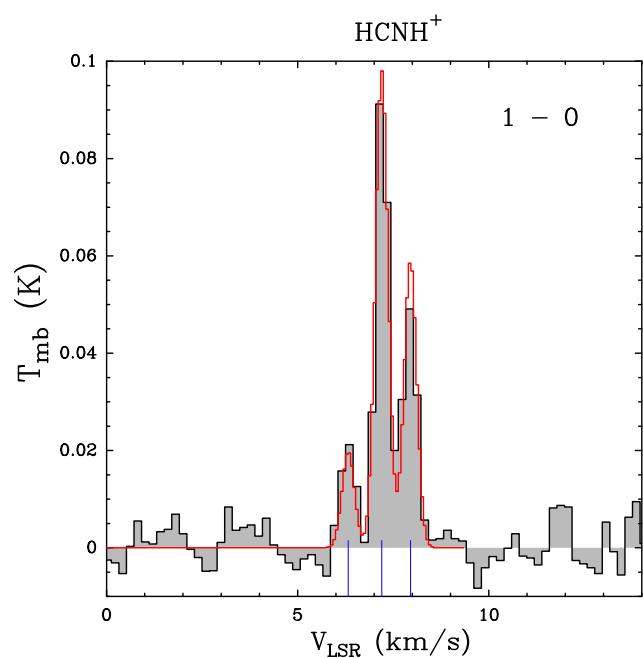


Figure 1. Observed spectra of the HCNH^+ 1–0 HFS transitions at 74.1 GHz. Temperatures are in main beam. The red line shows the LTE fit at 10 K using the following frequencies: $F = 0-1$ at 74 111.54 MHz, $F = 2-1$ at 74 111.33 MHz, $F = 1-1$ at 74 111.14 MHz. Intensities are given in units of main-beam temperature in K.

$F = 2-1: 74\ 111.3258$ and $F = 1-1: 74\ 111.1812$ MHz. The V_{LSR} in L1544 is not constant due to gas motion and it could modify the frequency at which a given line is detected. We measured the V_{LSR} (7.2 ± 0.1 km s⁻¹) for the strongest hyperfine structure (hereafter HFS) transition ($F = 2-1$) of HCNH^+ . The best fit for the $F = 0-1$ transition is consistent with the CDMS frequency at 74 111.54 MHz. The best fit for the $F = 1-1$ transition ($74\ 111.14 \pm 0.01$ MHz) is offset by ~ 0.04 MHz compared to the CDMS data base (74 111.1812 MHz), within the uncertainty of 75 kHz quoted from Ziurys et al. (1992).

In addition, we report observations of related species: HNC, HCN, HN^{13}C , H^{13}CN and HC_3N . These species are important to understand the chemical origin of HCNH^+ and HC_3NH^+ and better constrain the chemical models, as discussed in the following sections. The spectroscopic parameters for these species, as well as for HC_3NH^+ , were also taken from the CDMS data base. Unfortunately, HCN^+ and HNC^+ are not available in the data bases but we are using HC_3N , HCN and HNC to study the trends of the related species HCNH^+ and HC_3NH^+ .

Table 1 reports the spectroscopic parameters as well as the properties of the detected lines, obtained by Gaussian fitting, using the Levenberg–Marquardt algorithm. For the line identification, we used the CASSIS³ software developed at IRAP (Vastel et al. 2015b). The detected spectra are shown in Figs 1–4.

3 RESULTS

We performed an LTE analysis of the observed line intensities for HCNH^+ , HC_3NH^+ and HC_3N using CASSIS, assuming no beam dilution. Note that it is consistent with the chemical modelling

¹ Astrochemical Surveys At IRAM: <http://www.oan.es/asai/>

² <http://www.astro.uni-koeln.de/>

³ <http://cassis.irap.omp.eu>

Table 1. Properties of the observed HC_3NH^+ , HCNH^+ , HCN, HNC, H^{13}CN , HN^{13}C and HC_3N lines ($E_{\text{up}} \leq 35$ K, $A_{\text{ul}} \geq 10^{-7} \text{ s}^{-1}$). Uncertainties are given at the 1 sigma level and only include statistical fluctuations of the Gaussian fits of the lines. The rms has been computed over 20 km s $^{-1}$. The dash symbol means that the line shows self-absorption, so no fit has been performed.

Transitions (J'F'-J,F)	Frequency (MHz)	E_{up} (K)	A_{ul} (s $^{-1}$)	$S\mu^2$	V_{peak} (km s $^{-1}$)	FWHM (km s $^{-1}$)	$\int T_{\text{mb}} dV$ (mK km s $^{-1}$)	rms mK
HCNH^+								
1,0–0,1	74 111.54	3.56	1.33×10^{-7}	0.028				11 ± 3
1,2–0,1	74 111.33	3.56	1.33×10^{-7}	0.14	7.20 ± 0.10	0.39 ± 0.11	42 ± 8	4.3
1,1–0,1	74 111.14	3.56	1.33×10^{-7}	0.084				27 ± 3
HC_3NH^+								
9,8–8,7	77 920.63	18.70	6.67×10^{-6}	20.5873	7.22 ± 0.05	0.37 ± 0.07	6.4 ± 2.1	3.7
9,9–8,8	77 920.63	18.70	6.68×10^{-6}	23.0409				
9,10–8,9	77 920.63	18.70	6.76×10^{-6}	25.7870				
10,9–9,8	86 578.14	22.85	9.22×10^{-6}	23.1953	7.20 ± 0.05	0.41 ± 0.07	5.1 ± 1.6	3.6
10,10–9,9	86 578.14	22.85	9.23×10^{-6}	25.6626				
10,11–9,10	86 578.14	22.85	9.23×10^{-6}	28.3923				
11,10–10,9	95 235.53	27.42	1.24×10^{-5}	25.7988	7.26 ± 0.05	0.63 ± 0.05	12.0 ± 2.3	3.8
11,11–10,10	95 235.53	27.42	1.24×10^{-5}	28.2748				
11,12–10,11	95 235.53	27.42	1.25×10^{-5}	30.9885				
HC_3N								
8–7	72 783.82	15.72	2.94×10^{-5}	111.429	7.23 ± 0.01	0.51 ± 0.01	2013 ± 5	5.1
9–8	81 881.47	19.65	4.21×10^{-5}	125.314	7.23 ± 0.01	0.54 ± 0.01	1610 ± 3	3.7
10–9	90 979.02	24.02	5.81×10^{-5}	139.252	7.33 ± 0.05	0.50 ± 0.03	1367 ± 2	1.7
11–10	10 0076.39	28.82	7.77×10^{-5}	153.179	7.24 ± 0.02	0.49 ± 0.03	939 ± 2	3.9
12–11	10 9173.63	34.06	1.04×10^{-4}	167.109	7.23 ± 0.01	0.46 ± 0.03	617 ± 2	3.2
HCN								
1,1–0,1	88 630.42	4.25	2.41×10^{-5}	8.922	–	–	698 ± 5	5.1
1,2–0,1	88 631.85	4.25	2.41×10^{-5}	14.869	–	–	1083 ± 5	5.1
1,0–0,1	88 633.94	4.25	2.41×10^{-5}	2.974	–	–	802 ± 5	5.1
H^{13}CN								
1,1–0,1	86 338.73	4.14	2.22×10^{-5}	8.890	7.14 ± 0.01	0.52 ± 0.02	209 ± 2	4.0
1,2–0,1	86 340.16	4.14	2.22×10^{-5}	14.883	7.12 ± 0.01	0.56 ± 0.02	303 ± 2	4.0
1,1–0,1	86 342.25	4.14	2.23×10^{-5}	2.976	7.17 ± 0.01	0.51 ± 0.01	112 ± 2	4.0
HNC								
1–0	90 663.57	4.35	2.69×10^{-5}	9.302	–	–	2384 ± 5	4.3
HN^{13}C								
1–0	87 090.83	4.18	2.38×10^{-5}	9.302	7.16 ± 0.03	0.82 ± 0.05	1212 ± 5	4.1

performed in Section 4. Considering the low temperatures in the L1544 pre-stellar core, we used a 10 K excitation temperature for the detected transition of HCNH^+ in order to determine its column density: $N(\text{HCNH}^+) = (2.0 \pm 0.2) \times 10^{13} \text{ cm}^{-2}$. From the HC_3NH^+ (9–8), (10–9) and (11–10) transitions, the excitation temperature must be in the [10–15 K] range with a column density $N(\text{HC}_3\text{NH}^+) = [1–2] \times 10^{11} \text{ cm}^{-2}$ to reproduce the observations. We checked that a change in the excitation temperature in the range [5–15 K] does not change the resulting column densities of HCNH^+ and HC_3NH^+ by more than a factor of ~ 1.4 . Fig. 1 shows the LTE model with an excitation temperature of 10 K for the HCNH^+ transition over-plotted with the observations. All lines are optically thin.

For HC_3N , we carried out a non-LTE analysis using the LVG code by Ceccarelli et al. (2003). For that, we used the collision coefficients with H_2 (Faure, Lique & Wiesenfeld 2016) and derived a kinetic temperature of 12 ± 2 K and a density of $(5 \pm 3) \times 10^4 \text{ cm}^{-3}$ with a column density $N(\text{HC}_3\text{N}) = [1.6–2.4] \times 10^{13} \text{ cm}^{-2}$. We also performed an LTE analysis to compare with the non-LTE result. In order to fit simultaneously all five HC_3N transitions, the

excitation temperature must be $T_{\text{ex}} = 8.5 \pm 0.5$ K with $N(\text{HC}_3\text{N}) = (1.9 \pm 0.2) \times 10^{13} \text{ cm}^{-2}$. Therefore, the LTE and non-LTE results give similar column densities.

We present in Fig. 4 the HCN, H^{13}CN , HNC and HN^{13}C (1–0) transitions obtained with our ASAI observations. The HCN and HNC line profiles show self-absorption and the so-called hyperfine anomalies (Guilloteau & Baudry 1981; Gonzalez-Alfonso & Cernicharo 1993), indicating opacity effect. Therefore, to determine the HCN and HNC column densities, we used their respective isotopologues. For HCN we used the collision rates from Green & Thaddeus (1974) with Helium, scaled by a factor of 1.363 to reproduce the collisions by H_2 . The resulting HCN column density is $[2.7–4.4] \times 10^{14} \text{ cm}^{-2}$ using a $^{12}\text{C}/^{13}\text{C} = 68$ for a kinetic temperature between 8 and 10 K and a density between 5×10^4 and 10^5 cm^{-3} . The H^{13}CN line is optically thick and the column density is therefore uncertain. For HN^{13}C we used the collision rates from Dumouchel, Klos & Lique (2011). The resulting HNC column density is $[2–4] \times 10^{14} \text{ cm}^{-2}$ using a $^{12}\text{C}/^{13}\text{C} = 68$ for a kinetic temperature between 8 and 10 K and a density between 5×10^4 and 10^5 cm^{-3} . The HN^{13}C is moderately optically thick with a low value

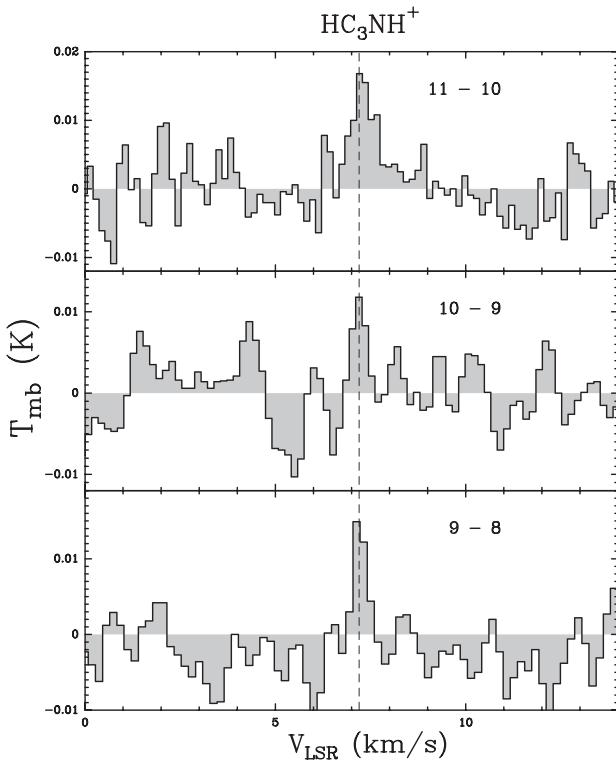


Figure 2. Observed spectra of the HC_3NH^+ 9–8 (bottom), 10–9 (middle) and 11–10 (up) transitions at 77.9 GHz, 86.8 GHz and 95.2 GHz, respectively. The dashed line shows a V_{LSR} of 7.2 km s^{-1} . Intensities are given in units of main-beam temperature in K.

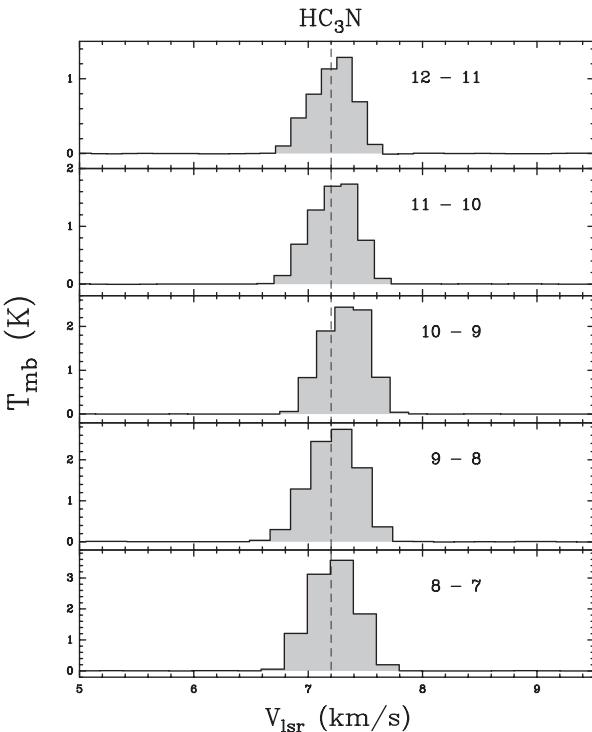


Figure 3. Observed spectra of the HC_3N transitions at 72.8 GHz (8–7), 81.9 GHz (9–8), 91 GHz (10–9), 100.1 GHz (11–10) and 109.2 GHz (12–11). The dashed line shows a V_{LSR} of 7.2 km s^{-1} . Intensities are given in units of main-beam temperature in K.

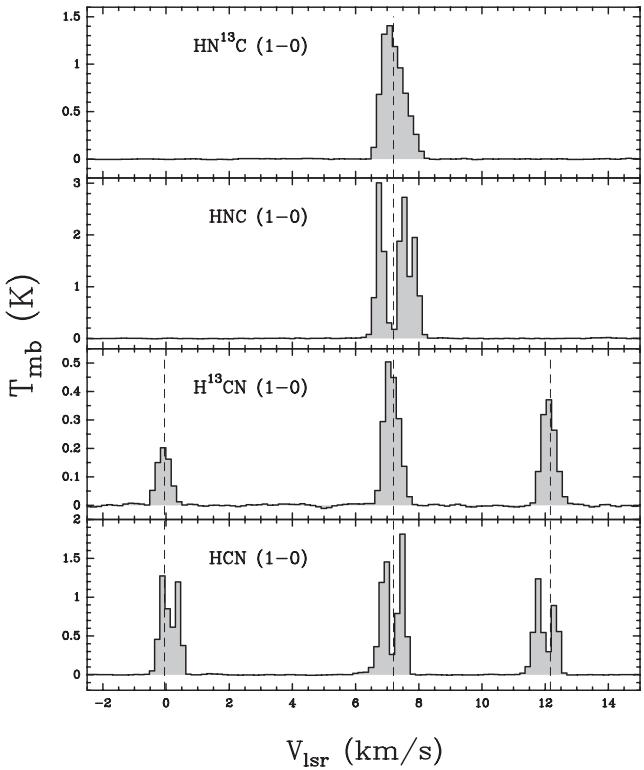


Figure 4. Observed spectra of the HCN, H^{13}CN , HNC and HN^{13}C 1–0 transition at 88.6, 86.3, 90.7 and 87.1 GHz respectively. Intensities are given in units of main-beam temperature in K. The dashed line shows a V_{LSR} of 7.2 km s^{-1} for both HNC and HN^{13}C and indicates the same velocity for the hyperfine structure of the HCN and H^{13}CN 1–0 transition.

for the excitation temperature at 4 K. Such low excitation temperatures were also reported by Padovani et al. (2011). Both HCN and HNC have previously been observed by Hily-Blant et al. (2010) using the IRAM-30-m telescope with a spectral resolution of 20 kHz of the $J=1-0$ HN^{13}C and H^{13}CN species. Assuming $T_{\text{ex}} = 8 \text{ K}$ and a $^{12}\text{C}/^{13}\text{C} = 68$, they derived $N(\text{HCN}) = [1.9–2.9] \times 10^{13} \text{ cm}^{-2}$ and $N(\text{HNC}) = [3.8–5.8] \times 10^{13} \text{ cm}^{-2}$ leading to a HNC/HCN ratio of ~ 2.0 . The resulting excitation temperature from our analysis is much lower than the 8 K value assumed by Hily-Blant et al. (2010). We note that lowering their excitation temperature to 3.5–4 K (instead of their assumed value of 8 K) would increase their HCN column density by a factor of 5. We use the results from our observations and analysis in this work.

We also present the observed column densities for HCO^+ , N_2H^+ (two other relevant ions in this pre-stellar core) and CO. These three species will allow us to test the completeness and robustness of the chemical study. To perform the comparison with the modellings, we have taken the observations derived by Caselli et al. (2002a,b). In their study, the authors obtained $N(\text{HCO}^+) = [0.3–1.0] \times 10^{14} \text{ cm}^{-2}$ ($T_{\text{ex}} \sim 8 \text{ K}$), $N(\text{N}_2\text{H}^+) = [0.3–2.0] \times 10^{13} \text{ cm}^{-2}$ ($T_{\text{ex}} = 5 \text{ K}$) and $N(\text{CO}) = [0.6–1.7] \times 10^{18} \text{ cm}^{-2}$ ($T_{\text{ex}} = 10 \text{ K}$).

4 CHEMICAL MODELLING

4.1 Description of the modelling

In this section, we aim at deriving the spatial variation of the abundance of HCN^+ and HC_3NH^+ for several chemical ages of the pre-stellar core. We do not pretend here to describe the situation

Table 2. Initial gas phase elemental abundances assumed relative to the total nuclear hydrogen density n_{H} .

Species	EA1	EA2
He	1.40×10^{-1}	9.00×10^{-2}
N	2.14×10^{-5}	7.60×10^{-5}
O	1.76×10^{-4}	2.56×10^{-4}
C ⁺	7.30×10^{-5}	1.20×10^{-4}
S ⁺	8.00×10^{-8}	1.50×10^{-5}
Si ⁺	8.00×10^{-9}	1.70×10^{-6}
Fe ⁺	3.00×10^{-9}	2.00×10^{-7}
Na ⁺	2.00×10^{-9}	2.00×10^{-7}
Mg ⁺	7.00×10^{-9}	2.40×10^{-6}
Cl ⁺	1.00×10^{-9}	1.80×10^{-7}
P ⁺	2.00×10^{-10}	1.17×10^{-7}
F ⁺	6.68×10^{-9}	1.80×10^{-8}

with a self-consistent model, but just to shed light on the formation pathways of both ionic species HC_3NH^+ and HCNH^+ . We will confront the predicted column densities with the observed values.

To do so, we have used the gas-grain chemical code NAUTILUS (Hersant et al. 2009; Ruaud, Wakelam & Hersant 2016) to predict the abundances of both species in the cold core. NAUTILUS allows us to compute the evolution of the chemical composition of the gas and the icy mantle of the grains. Details of the processes included in the model can be found in Ruaud et al. (2016). Note that we have used NAUTILUS in its two-phase model, meaning that there is no distinction between the surface and the bulk of the mantle of the grains. Briefly, gas species can stick on the grain mantles where they can diffuse (depending on the species), be photo-dissociated and undergo chemical reactions. In addition, frozen species are injected into the gas phase by thermal and non-thermal processes. For the latter, we considered: (i) photo-desorption by direct and cosmic-ray-induced UV photons, with a fixed yield equal to 10^{-4} ; (ii) direct cosmic ray desorption, following the formalism by Hasegawa & Herbst (1993); (iii) chemical desorption, following the formalism by Garrod, Wakelam & Herbst (2007), in which a fixed 1 per cent of the species formed on the grain surfaces are injected into the gas-phase, regardless of the species. The gas phase reactions are based on the kida.uva.2014 network⁴ (see Wakelam et al. 2015) while the surface network is based on Garrod & Herbst (2006). The full network contains 736 species (488 in the gas phase and 248 at the surface of the grains) and 10 466 reactions (7552 pure gas phase reactions and 2914 reactions of interactions with grains and reactions at the surface of the grains).

The chemical model is divided into two phases. The first phase corresponds to the evolution of the chemistry in a diffuse or molecular cloud (hereafter ambient cloud), depending on the initial H density assumed (see below). We let the chemical composition evolve until 1×10^6 years. The abundances from this first step are then used as initial abundances for the second step where we consider the physical structure of the L1544 pre-stellar core, as determined by Keto et al. (2014).

Ambient cloud phase: the first phase takes into account photo-processes, for both the gas and the grain surface chemistry. We adopted two different sets of initial atomic abundances (with respect to the total proton density n_{H}) given in Table 2 (Wakelam & Herbst 2008).

Table 3. Chemical modelling parameters shown in this study.

Model number	Density ^a (cm^{-3})	Elemental abundances model
1	1×10^{2b}	EA1
2	3×10^{3c}	EA1
3	2×10^{4d}	EA1
4	1×10^2	EA2
5	3×10^3	EA2
6	2×10^4	EA2

^aInitial H densities used in the ambient cloud phase.

^bValue used in Vasyunin & Herbst (2013) and Jiménez-Serra et al. (2016).

^cValue used in Quénard et al. (2016).

^dValue used in Vastel et al. (2014) and Vastel et al. (2016).

(i) In model EA1, which is consistent with recent studies performed towards this core (Vasyunin & Herbst 2013; Jiménez-Serra et al. 2016), initial abundances are called low-metal abundances because they are lower by a factor of ~ 100 for heavy elements in comparison with solar elemental abundances in order to take into account elemental depletion on grains in cold interstellar cores. The carbon and oxygen abundances are respectively 7.30×10^{-5} and 1.76×10^{-4} leading to a C/O ratio of ~ 0.4 .

(ii) The model EA2, based on the high-metal abundances observed in the ζ Oph diffuse cloud, but modified based on recent observations. The carbon and oxygen abundances are respectively 1.20×10^{-4} and 2.56×10^{-4} leading to a C/O ratio of ~ 0.5 .

For both sets, the C/O ratio (~ 0.4 and ~ 0.5 for models EA1 and EA2, respectively) is consistent with recent results towards L1544 (Vastel et al. 2014). Nonetheless, by varying the initial oxygen abundance shown in Table 2, we have varied the C/O ratio to be 0.4, 0.5, 0.6, 0.9 and 1.2, but it does not change the result significantly. Therefore, in the following, we use the initial gas phase elemental abundance shown in Table 2 for a given model. The gas and grain temperatures are fixed to 20 and 10 K, respectively. The cosmic ray ionization rate is set to the standard value of $1.3 \times 10^{-17} \text{ s}^{-1}$. These values are consistent with recent studies of this core (e.g. Jiménez-Serra et al. 2016; Vastel et al. 2016). We have verified that a variation of 10 K, either for the gas or grain temperature, will not change the result significantly. In the literature, various initial H densities have been used to describe this ambient cloud phase, ranging from $n_{\text{H}} = 10^2$ to a few 10^4 cm^{-3} (Jiménez-Serra et al. 2016; Quénard et al. 2016; Vastel et al. 2016, in order of increasing initial H densities assumed in their studies). One must also note that different chemical codes have been used in these different studies. For the sake of our study, we have tested different initial H densities in the range defined above (see Table 3). The assumed size of the ambient cloud is $\sim 6 \times 10^4 \text{ au}$ or 0.3 pc (Quénard et al. 2016). This leads to A_V up to ~ 10 mag depending on the initial H density taken.

Pre-stellar phase: for the second phase, the final abundances of the first phase are used as initial abundances. The physical structure adopted in this phase (density, gas and grain temperature) is the one derived from the recent study of Keto et al. (2014) (see Fig. 5). This physical model has been widely used in recent studies to describe the structure of L1544 (e.g. Jiménez-Serra et al. 2016; Quénard et al. 2016; Vastel et al. 2016). The cosmic ray ionization rate is kept the same during this step. In this second phase, the chemistry is followed for 3 million years. At the end, the radial abundance profiles of the species for several ages of the pre-stellar core are

⁴ <http://kida.obs.u-bordeaux1.fr/networks.html>

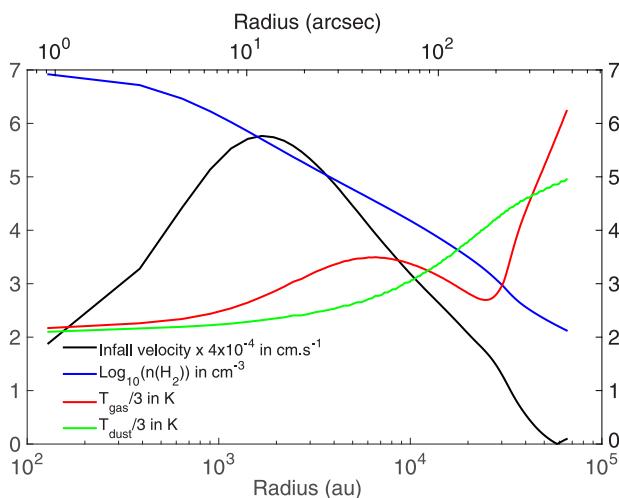


Figure 5. Gas and dust temperature, density and velocity profiles of L1544 used in this study from Keto et al. (2014).

obtained. At the end of phase 2, carbon is largely depleted into the grain mantles in the innermost part of the condensation: at 5×10^3 au, where the density is about $\sim 7 \times 10^4 \text{ cm}^{-3}$, only 0.1 per cent of carbon is in the gas phase (mainly in the form of CO), the rest is almost equally distributed into iced CO, H₂CO and CH₃OH. At about 10^4 au the gas phase carbon amounts to about 1 per cent, while in the very external regions, where UV photons penetrate, gaseous carbon varies from 10 to 90 per cent for the density varying from 2×10^4 to $1 \times 10^2 \text{ cm}^{-3}$. Similar values are also found for gaseous oxygen and nitrogen. At about 10^4 au, the most abundant gaseous O-bearing species are CO and atomic O and the N-bearing species are N₂ and atomic N, whereas the most abundant iced species are H₂O and NH₃, respectively.

4.2 Results and comparison with observations

We have considered six different chemical models using the three different initial gas densities of the ambient cloud phase presented previously and the two different sets (EA1 and EA2) of initial atomic abundances (see models shown in Table 3). To easily compare the modelled abundance with the observations, we calculated the column density along the radius of the core. We used the method described in Jiménez-Serra et al. (2016) to convert the abundance [X] (with respect to H) of a species X into column densities N(X):

$$N(X) = 2 \times \sum_{i=2}^n \left(\frac{n(\text{H})_i[X]_i + n(\text{H})_{i-1}[X]_{i-1}}{2} \right) \times (R_{i-1} - R_i), \quad (1)$$

with R the radius from the centre and i the position in the grid along the line of sight ($i = 1$ being the outermost position) composed of n shells ($n = 129$). $n(\text{H})_i$ is the gas density at radial point i and $[X]_i$ the abundance of the species. Different column densities are derived depending on the observed position towards the core. The different column densities obtained using equation (1) are then convolved with the beam size of the IRAM-30-m telescope at the frequency of the observations (~ 30 arcsec) to take this effect into account. The H₂ column density has also been calculated following the same method and we derive $N(\text{H}_2) = 6.7 \times 10^{22} \text{ cm}^{-2}$. Thus, the observed abundances (with respect to H₂) are $[\text{HCN}^+] \simeq 3 \times 10^{-10}$ and $[\text{HC}_3\text{NH}^+] \simeq [1.5 - 3.0] \times 10^{-12}$.

Fig. 6 presents the different column densities (HCN⁺, HC₃NH⁺, HCN, HNC, HC₃N, HCO⁺, N₂H⁺ and CO) for models reported in Table 3. Based on the observed HCN⁺, we have defined three vertical grey areas corresponding to three possible solutions for the age of phase 2 (solutions 1 and 2 for models 1, 2 and 3 and solution 3 for model 4, 5 and 6). No perfect agreement between the models and the observations is found to reproduce simultaneously both HCN⁺ and HC₃NH⁺ for the different ages and different initial H densities. Nonetheless, above an age of 1×10^5 yr, both HCN⁺ and HC₃NH⁺ column density predictions cross the observed column density, unfortunately not at the same age. Either HCN⁺ is underestimated or HC₃NH⁺ is overestimated by a factor of $\sim 3-15$, depending on the initial H density.

The middle panels of Fig. 6 present the column densities of HCN, HNC and HC₃N. The observed column density of HC₃N (green area) is reproduced by all three different initial densities of models 1, 2 and 3 within the same time-scale of solution 1 (shown in grey area). It is also reproduced with model 6 for solution 3. No models can reproduce HC₃N for solution 2. The observed HNC column density (red area) is reproduced with models 1 and 2 and within a factor of ~ 3 for model 3. Solution 2 reproduces the observed HNC within a factor of ~ 3 . For solution 3, model 6 is the only one reproducing the observed HNC column density below a factor of ~ 3 . For HCN (in blue), we manage to reproduce the observed column density with solution 1 (models 1 and 2) and within a factor of ~ 3 for model 3. For solutions 2 and 3 we obtain a modelling-to-observed ratio $\lesssim 5$ and $\lesssim 10$, respectively, for this species. Around 3×10^5 yr, for all models of solution 1, HC₃N, HCN and HNC are well reproduced. At the same age, for any of these models, HCN⁺ and HC₃NH⁺ tend to be under-estimated and over-estimated, respectively. Since these ionic and neutral species are closely related (see Section 5), this could possibly mean reactions linking these two sets of molecules are badly constrained. This could also indicate that other destruction routes for HCN and HNC are needed to explain the observed column densities.

The bottom panels of Fig. 6 present the column densities of HCO⁺, N₂H⁺ and CO. The observed column densities of HCO⁺ (blue area) and N₂H⁺ (red area) are well fitted with model EA1 (both solutions 1 and 2) for all three different initial densities (models 1, 2 and 3). N₂H⁺ is also reproduced with model 4, 5 and 6 (using model EA2) but HCO⁺ is under-predicted by a factor of ~ 10 for model 6 and $\lesssim 3$ for model 4 and 5. The CO column density is under-estimated for both model EA1 and EA2, by a factor of <6 and <3 , respectively. Note that the observed CO column density shown in this figure is derived from the C¹⁷O observations of L1544 derived by Caselli et al. (2002a).

Table 4 presents a summary of the modelled and observed column density agreement for all models and all molecules, confronted to the three solutions. For each molecule and each model, all predicted column densities that fall within a factor of 3 in the observed error bars are marked with a cross. From this table, we can conclude that models 1 and 2 associated with solution 1 are the best models to reproduce the observed column densities. These models correspond to ambient cloud densities of $1 \times 10^2 \text{ cm}^{-3}$ and $3 \times 10^3 \text{ cm}^{-3}$, and to abundances from model EA1. One must also note that model 6 associated with solution 3 might also be a good solution, except for HCN which is over-estimated by a factor of ~ 30 for this model.

Fig. 7 presents the column density ratios of HNC/HCN, HCN^{+/HC₃NH⁺, HC₃NH^{+/HC₃N, HCN^{+/HC₃N, HCN^{+/HCN and HCN/HC₃N as a function of time. The observed HNC/HCN ratio is 0.97 ± 0.52 , close to the modelled ratio of}}}}

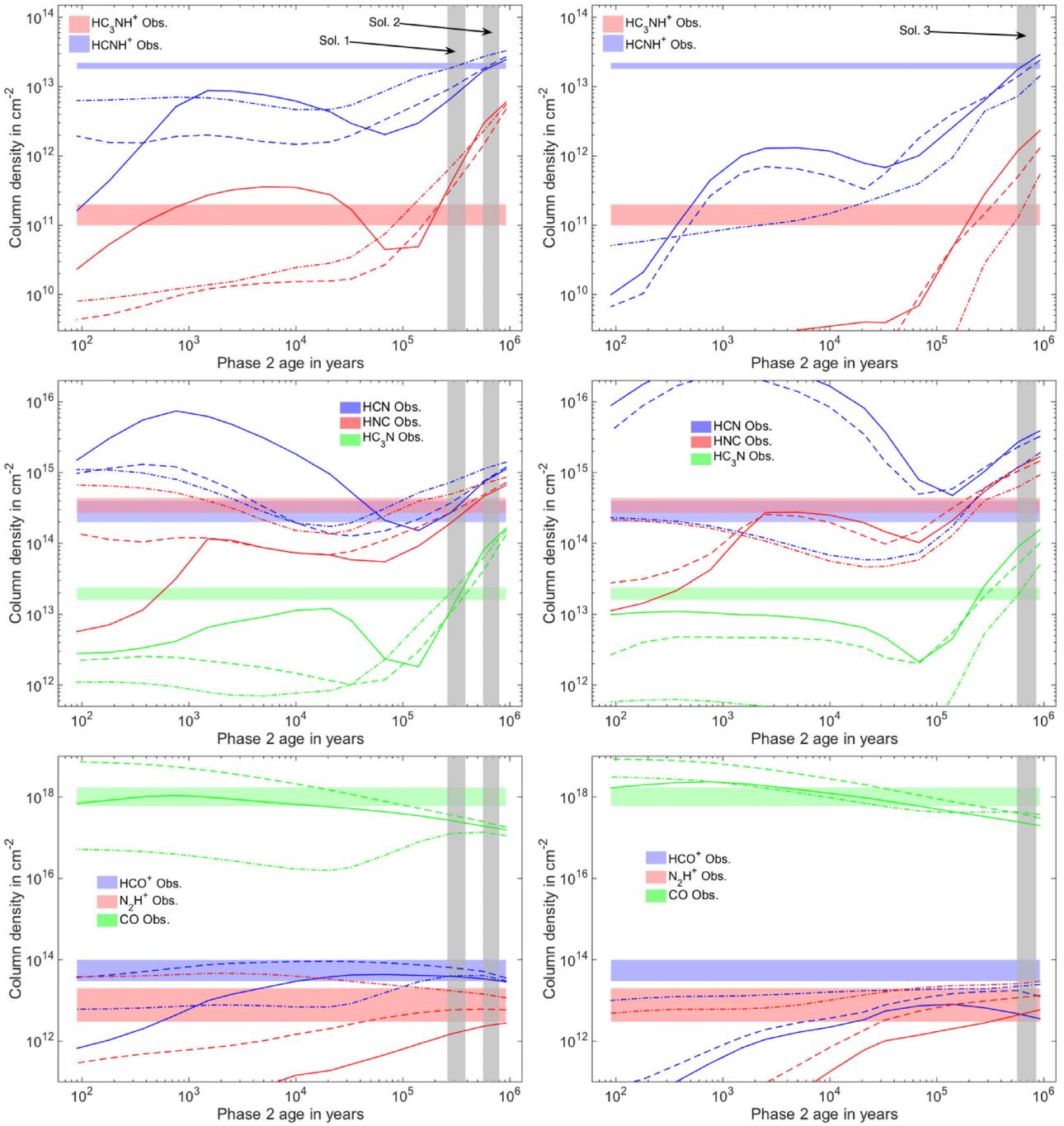


Figure 6. Column densities for HCNH^+ , HC_3NH^+ (top panels), HCN , HNC , HC_3N (middle panels), HCO^+ , N_2H^+ and CO (bottom panels) as a function of the age of phase 2 for different initial gas densities of the ambient cloud phase: $1 \times 10^2 \text{ cm}^{-3}$ (full line), $3 \times 10^3 \text{ cm}^{-3}$ (dashed line) and $2 \times 10^4 \text{ cm}^{-3}$ (dash-dotted line). The area of confidence of the observed column densities for these species is also shown. Grey areas show the time span area of confidence of each model based on the observed HCNH^+ . These areas are labelled solutions 1, 2 and 3. Left-hand panels: Model EA1 of initial atomic abundances. Right-hand panels: Model EA2 of initial atomic abundances.

$\lesssim 1$ for both EA1 and EA2 models. From our study, we also derived the observed $\text{HCNH}^+/\text{HC}_3\text{N}=1.1 \pm 0.3$, $\text{HCNH}^+/\text{HC}_3\text{NH}^+=155 \pm 65$ and $\text{HC}_3\text{NH}^+/\text{HC}_3\text{N}=(8.4 \pm 4.2) \times 10^{-3}$. The predicted ratios with model EA2 give a good agreement compared to the observed ratios, for an age $> 10^5$ yr. Model EA1 is worse than model EA2, especially for $\text{HCNH}^+/\text{HC}_3\text{NH}^+$ and $\text{HC}_3\text{NH}^+/\text{HC}_3\text{N}$. Nonetheless, the $\text{HCNH}^+/\text{HC}_3\text{N}$ is in good agreement with the observations

for both models. This might show that HC_3NH^+ is slightly better reproduced by model EA2 rather than model EA1.

4.3 Discussion

To reproduce the observed column densities, several improvements in the chemical network are required as follows.

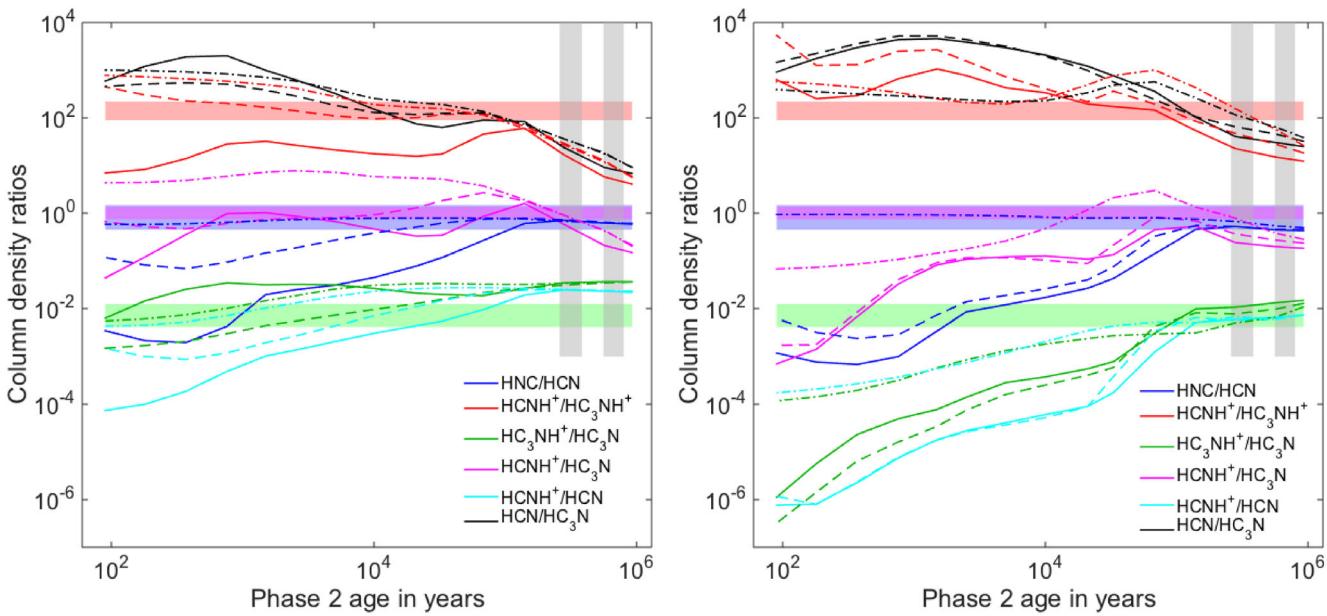


Figure 7. Evolution of the column density ratios of HNC/HCN, $\text{HCN}\text{H}^+/\text{HC}_3\text{NH}^+$, $\text{HC}_3\text{NH}^+/\text{HC}_3\text{N}$, $\text{HCN}\text{H}^+/\text{HC}_3\text{N}$, $\text{HCN}\text{H}^+/\text{HCN}$ and $\text{HCN}/\text{HC}_3\text{N}$ as a function of the age of phase 2 for different initial gas densities of the ambient cloud phase: $1 \times 10^2 \text{ cm}^{-3}$ (full line), $3 \times 10^3 \text{ cm}^{-3}$ (dashed line) and $2 \times 10^4 \text{ cm}^{-3}$ (dash-dotted line). The area corresponds to the observed ratio coming from this study and Hily-Blant et al. (2010) (cf. text). Grey areas show the time span area of confidence of each model based on the observed HCNH^+ . Left-hand panels: Model EA1 of initial atomic abundances. Right-hand panels: Model EA2 of initial atomic abundances.

Table 4. Summary of the modelled and observed column densities agreement for all models and all molecules, confronted to the three possible solutions for the age of phase 2: solutions 1 and 2 for models 1, 2 and 3 and solution 3 for models 4, 5 and 6 (see text and Table 3). A cross indicates that the modelled column density reproduces the observed value within a factor of 3.

Molecule	Model number											
	1			2			3			4		
	Solution 1			Solution 2			Solution 3					
HCNH^+	X	X	X	X	X	X	X	X	X	X	X	X
HC_3NH^+	X	X								X	X	
HCN	X	X	X	X	X							
HNC	X	X	X	X	X	X						X
HC_3N	X	X	X			X				X	X	
HCO^+	X	X	X	X	X	X				X	X	
N_2H^+	X	X	X	X	X	X	X	X	X	X	X	
CO	X	X				X		X	X	X	X	
Total	8	8	6	5	7	4	3	6	7			

(i) A better description of the physical conditions of the source may change the results, by taking into account the collapse of the core between phase 1 and phase 2, although it may imply other sources of error in the modelling.

(ii) Formation (or destruction) routes for HCNH^+ and HC_3NH^+ must be added to the chemical network. Agúndez et al. (2015) also came to this conclusion in their study of the ion NCCNH^+ in the cold dark clouds TMC-1 and L483. In their work, using a comparable chemical network (UMIST RATE12; McElroy et al. 2013), the authors well reproduced the abundance of several ions (e.g. NCCNH^+ , HCO^+ , NH_4^+) but they did not reproduce the observed HCNH^+ and HC_3NH^+ abundances by a factor of ~ 10 , which is similar to the value we find in our study.

(iii) A better estimate of reaction rates, e.g. the rate of the dissociative recombination of HC_3NH^+ with electrons (J.-C. Loison, private communication) and HCNH^+ (Loison, Wakelam & Hickson 2014) where recent rates are not available yet in the KIDA network.

These points will be developed in a forthcoming study, focused on the complex chemistry of the species involved in this study.

Fig. 8 shows the evolution of the abundance of HCNH^+ and HC_3NH^+ as a function of the radius. The area represents the abundance of both species for models with an age $\gtrsim 10^5$ yr. This figure suggests that the emission of these ions is mainly coming from the external part of the core, in a region close to $\sim 10^4$ au, in an external layer where non-thermal desorption of other species has been previously observed (Vastel et al. 2014, 2016; Jiménez-Serra et al. 2016). We have also plotted in Appendix A several figures (see Fig. A1) showing the variation of the abundance, for all models and all eight molecules, as a function of the radius for an age of phase 2 corresponding to solution 1 (3×10^5 yr).

To summarize, we can conclude that for an initial H density of 1×10^2 and $3 \times 10^3 \text{ cm}^{-3}$, coupled with the model EA1 for elemental abundances, a good agreement can be found for HCNH^+ and HC_3NH^+ (and other relevant species) for a phase 2 age larger than 10^5 yr. This is consistent with the fact that L1544 must be in an advanced pre-stellar stage since it has already begun to collapse (Caselli et al. 2012; Keto et al. 2014).

5 CHEMISTRY OF HCNH^+ AND HC_3NH^+

The formation of HCNH^+ in dense and cold regions such as L1544 is thought to be dominated by both HCN and HNC (Schilke et al. 1991; Hezareh et al. 2008; Loison et al. 2014) following:



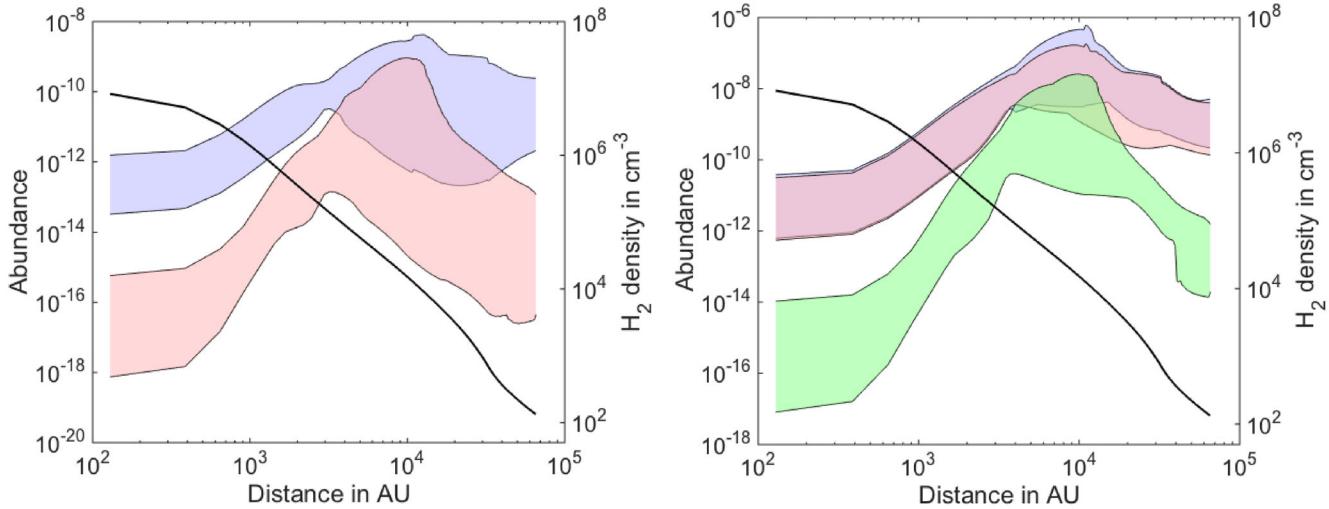
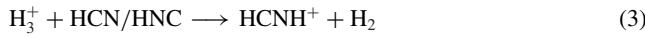


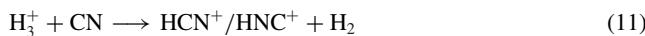
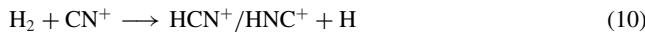
Figure 8. Evolution of the abundance as a function of the radius. Left: HCNH^+ (blue) and HC_3NH^+ (red). Right: HCN (blue), HNC (red) and HC_3N (green). The boundaries have been obtained combining the different abundance profiles for ages $\gtrsim 10^5$ yr, for both EA1 and EA2 sets. The H_2 density profile of L1544 is also shown (black line).



Its destruction is dominated by dissociative recombination (e.g. Hezareh et al. 2008; Loison et al. 2014) following:



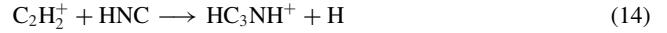
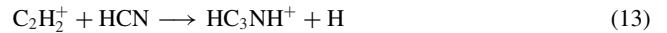
The two reactions in (2), involving HCN^+ and HNC^+ , are thought to be the main formation route of HCNH^+ in these regions (Loison et al. 2014). HCN^+ and HNC^+ are formed by:



Reactions in (9) and (10) are the main formation routes of HCN^+ and HNC^+ and they are mostly entirely destroyed by reactions (2).

The chemistry of HC_3NH^+ is poorly known compared to HCNH^+ . Several routes to form this species have been pro-

posed (Knight, Freeman & McEwan 1986; Kawaguchi et al. 1994; Osamura et al. 1999; Takagi et al. 1999):



The branching ratio of reactions (17) and (18) is ~ 70 and ~ 30 per cent, respectively, hence reaction (17) is the main outcome of $\text{HC}_3\text{N}^+ + \text{H}_2$. Once HC_3NH^+ is formed, dissociative recombination will lead to the formation of species HC_3N , HNC_3 and HCCNC (HCNCC could also be formed using this route but it is the least stable isomer; Osamura et al. 1999):



The following reaction might also be involved in the formation of HC_3NH^+ (Federer et al. 1986; Scott et al. 1999):



This reaction might be important for the formation of HC_3NH^+ (thus HC_3N), but we decided not to include it in the network because

it is still subject to discussions and its reaction rate is unknown. A forthcoming paper will study in deeper details the chemistry of both HCNH^+ and HC_3NH^+ , including the impact of the latter reaction.

Although the HCN/HNC ratio is predicted to be one via the photodissociation of HCNH^+ , observations show variations by factors up to 3, below or above unity, for the HNC/HCN ratio in dark clouds, and even larger variations in warmer sources (Hirota et al. 1998). However, the derivation of the HCN and HNC column densities based on observations of their ^{13}C isotopologues have been questioned recently by Roueff, Loison & Hickson (2015). It then appears that the deviations of the HNC/HCN ratio from unity may be an observational problem rather than an astrochemical one. The study of the spatial variations of the HCNH^+ ion is therefore of utmost importance to elucidate the origin of these variations.

From the NAUTILUS results, we derived the following reactions as the main production and destruction processes of both species. For HCNH^+ , as expected from the discussions above, the two main production reactions are reactions (2) with both HCN and HNC. In our model, the reaction with HCN and HNC is responsible for ~ 60 per cent and ~ 30 per cent of the production of HCNH^+ , respectively. The destruction follows the reactions (6), (7) and (8) by a factor of 33 per cent each, as expected by Semaniak et al. (2001) (see also W. D. Geppert's notes in KIDA website⁵). For HC_3NH^+ , it seems to be only produced from reaction (17) (by a factor close to 100 per cent) and destroyed following reactions (19) and (20) mainly. The respective factors of these reactions is ~ 56 per cent and ~ 32 per cent. The remaining ~ 12 per cent are divided into the production of different isomers such as HCCNC and HCNC.

Although dissociative recombination with electron rate constants are well known from experiments (Semaniak et al. 2001; Geppert et al. 2004; Agúndez & Wakelam 2013), formation reaction rates are poorly constrained – especially for HC_3NH^+ . The reaction rate of (2) and (17), in the KIDA network, comes from estimations. Since these reactions appear to be the main formation pathways of their respective ions, accurate laboratory measurements of these reactions could determine the precise value of their respective reaction rate, changing the estimated abundance. Moreover, reaction (17) has a branching ratio with reaction (18). A higher ratio for the latter reaction would result in a lower abundance of HC_3NH^+ . Finally, as concluded in the previous section, formation or destruction routes could also be added to this network in order to reproduce the observed column densities. A lack of laboratory experiments and observational data does not allow, to date, to disentangle which reactions dominate the formation of both HCNH^+ and HC_3NH^+ . Reaction rates are not well constrained and it may lead to numerous errors in the abundance determination.

6 CONCLUSIONS

In this paper, we presented the detection of one HFS transition of HCNH^+ and three HFS transition of HC_3NH^+ in the pre-stellar core L1544. An LTE analysis has been performed and we derive $\text{N}(\text{HCN}\text{H}^+) = (2.0 \pm 0.2) \times 10^{13} \text{ cm}^{-2}$ and $\text{N}(\text{HC}_3\text{NH}^+) = (1.5 \pm 0.5) \times 10^{11} \text{ cm}^{-2}$. We also report the detection of five transitions of HC_3N , three transitions of H^{13}CN and one transition of HN^{13}C . A non-LTE analysis gives a column density $\text{N}(\text{HC}_3\text{N}) = (2.0 \pm 0.4) \times 10^{13} \text{ cm}^{-2}$, $\text{N}(\text{HCN}) = (3.6 \pm 0.9) \times 10^{14} \text{ cm}^{-2}$ and $\text{N}(\text{HNC}) = (3.0 \pm 1.0) \times 10^{14} \text{ cm}^{-2}$ with a kinetic temperature of $11 \pm 3 \text{ K}$ and

a density of $(6 \pm 4) \times 10^4 \text{ cm}^{-3}$. Using a gas–grain chemical code, we calculated the predicted abundance in the pre-stellar core using a two-step model by varying the initial gas densities of the initial phase (within the range found in previously published works). The resulting abundances have been compared to the observed column densities and models with an age $> 10^5 \text{ yr}$, giving us a satisfactory agreement with the observations, in agreement with recent studies of this source. We have also discussed the possible predominant chemical reactions leading to the formation and destruction of both ionic species. Further investigation of the chemistry of nitrogen species (with laboratory experiments) is required to better reproduce the observations, especially for HC_3NH^+ .

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⁵ http://kida.obs.u-bordeaux1.fr/datasheet/datasheet_2815_HCNH+e+-V1.pdf

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APPENDIX A: ABUNDANCE PROFILES

We present in this appendix the abundance profiles for all six models as a function of the radius for an age of phase 2 of 3×10^5 yr, for all eight molecules. This age corresponds to solution 1, the best solution as determined by Table 4. For all eight molecules, models 1 and 2 reproduce the observed column densities within a factor of 3.

One can note that the modelled peak abundance for HCN, HNC and HC₃N is located at a radial distance of $\sim [4\text{--}5] \times 10^3$ au. At this distance, from Fig. 5, the kinetic temperature is 10 K with a H₂ density of $\sim 1 \times 10^5$ cm⁻³. Both values are consistent with the non-LTE modelling performed in Section 3 for these species.

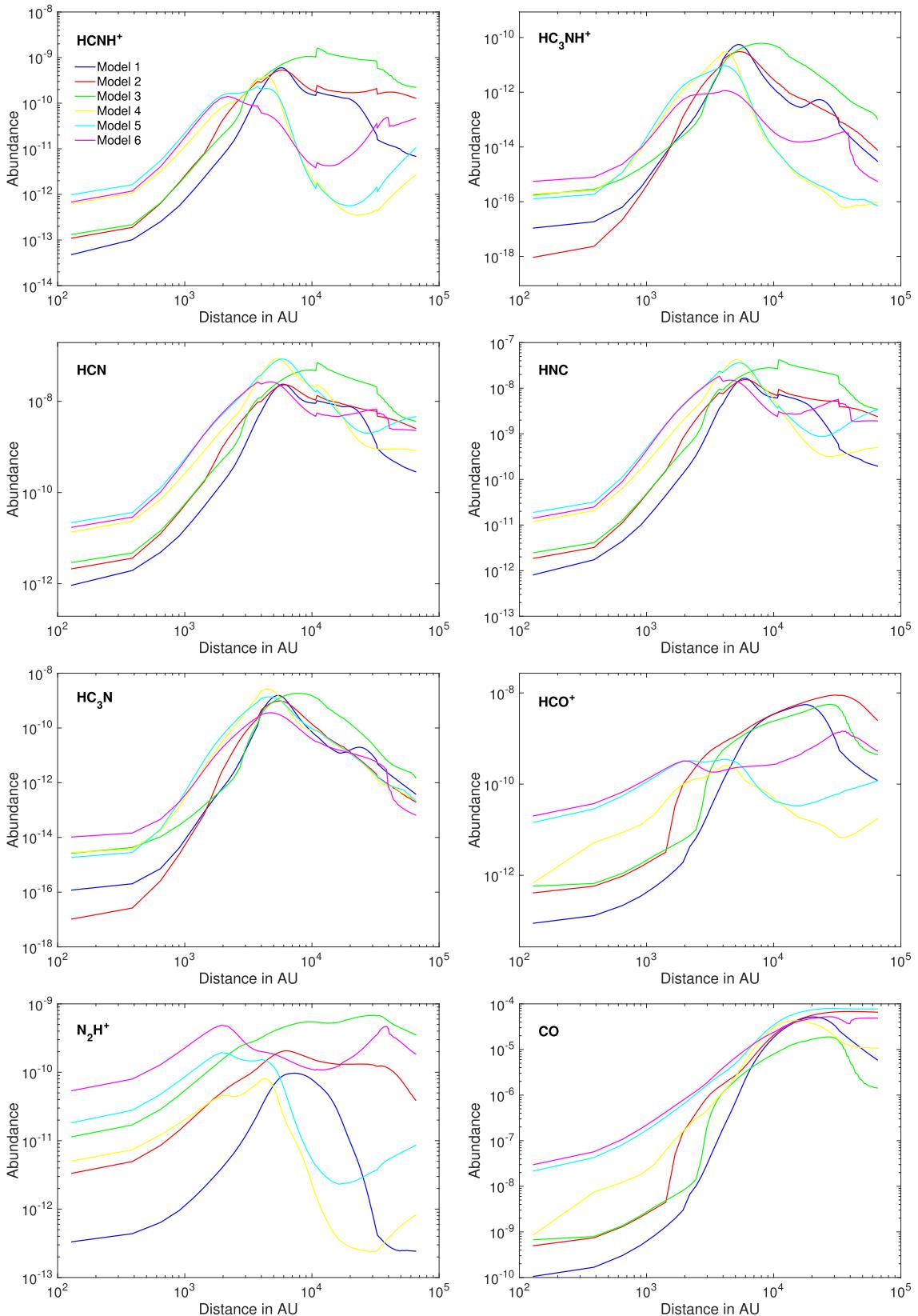


Figure A1. Abundance profiles as a function of the radius given for all models for an age of phase 2 of 3×10^5 yr.

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