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Laboratory and astrophysical detection of the hyperfine structure of the $J = 1$–0 rotational transition of $HC^{17}O^+$

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Abstract. The three hyperfine components of the $J = 1 \leftarrow 0$ rotational transition of $HC^{17}O^+$ have been resolved in laboratory leading to a value of the quadrupole coupling constant eQq of 4.595 MHz, which is far below the previous estimate of an upper limit of 12 MHz by Guélin et al. (1982a). The $HC^{17}O^+$ (1–0) spectrum has been observed toward the "molecular peak" of L1544 and analyzed on the basis of the laboratory hyperfine frequencies.

Key words. molecular data – methods: laboratory – ISM: individual(L1544), molecules – radio lines: ISM

1. Introduction

HCO^+ is one of the most abundant ions in molecular clouds, its chemistry is straightforward and well understood (e.g. Watson 1977; Wootten et al. 1979), and it is easily observable with current antennas. Formyl ion isotopes have been used to study physical and chemical properties of star forming regions (e.g. Butner et al. 1995; Hogerheijde et al. 1997; Gregersen et al. 1997), shocks produced by protostellar jets (e.g. Girart et al. 1998) and by supernovae (e.g. Koo & Moon 1997), disks around T-Tauri stars (e.g. Duvert et al. 2000), translucent molecular clouds (Turner 1995), diffuse clouds (Lucas & Liszt 1996), chemistry in comets (e.g. Lovell et al. 1997; Womack et al. 1997).

The main destruction route for HCO^+ is dissociative recombination, so its abundance is closely related to the electron density of the studied region. In dense clouds, the $[DCO^+]/[HCO^+]$ abundance ratio has been frequently used to estimate the ionization degree (e.g. Guélin et al. 1982b; Dalgarno & Lepp 1984; Wootten et al. 1982; Caselli et al. 1998; Williams et al. 1998), which is thought to be the fundamental parameter regulating the rate of star formation through the process of ambipolar diffusion (e.g. Shu et al. 1987). It is thus important to accurately determine column densities of these species to better understand physical and chemical properties of molecular clouds.

However, in dense regions, low J transitions of the most abundant isotopomers (HCO^+ and $H^{13}CO^+$) may be optically thick and affected by foreground absorption due to the presence of cold and low density core envelopes (e.g. Tafalla et al. 1998; Caselli et al. 1999). In these cases it is necessary to detect thinner lines such as those of the rarer $HC^{18}O^+$ and $HC^{17}O^+$. Because of the presence of hyperfine structure (caused by the electric quadrupole and the magnetic dipole interactions of the ^{17}O nucleus which has a spin of 5/2), observations of $HC^{17}O^+$ lines will furnish a direct measure of the optical depth, once the hyperfine structure is known from laboratory measurements.

So far, the $J = 1 \rightarrow 0$ rotational transition of $HC^{17}O^+$ has been observed in Sagittarius B2 by Guélin et al. (1982a). The coarse spectral resolution did not allow these authors to resolve the three hyperfine components and at that time there were no laboratory work on this molecular ion. Plummer et al. (1983) measured the $J = 2 \rightarrow 3$ transition of $HC^{17}O^+$, but this higher J transition did not show any evidence of hyperfine structure.

In this paper we report laboratory measurements and astronomical detection toward a dense cloud core of the $HC^{17}O^+$ (1–0) hyperfine structure.

2. Laboratory measurements

The laboratory spectrum was observed with a frequency-modulated millimeter-wave spectrometer (Cazzoli & Dore 1990) equipped with a double-pass negative glow discharge cell (Dore et al. 1999). The radiation source was a Gunn oscillator working in the region 78–116 GHz (J. E. Carlstrom Co) and the signal, detected by a liquid-helium-cooled InSb hot electron bolometer (QMC Instr. Ltd. type QFI/2), was demodulated at 2-f by a lock-in amplifier.

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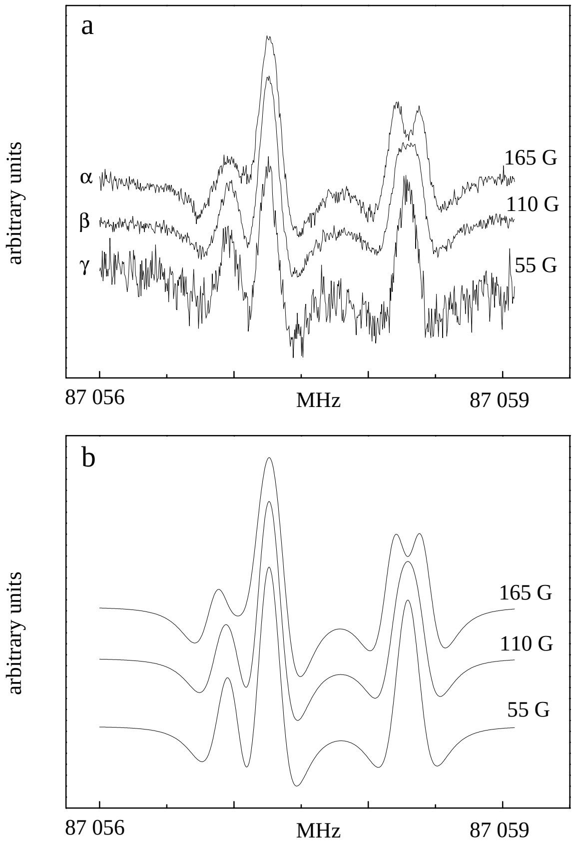

Fig. 1. a) Hyperfine structure of the $J = 0 \rightarrow 1$ transition of $HC^{17}O^+$. Trace α: time constant 30 msec, averaging time 370 s, axial magnetic field 165 Gauss; trace β: 30 msec, 925 s, 110 G; trace γ: 30 msec, 740 s, 55 G. **b)** Simulation spectra at the different values of the axial magnetic field. They were computed by summing a modulated Voigt profile for each Zeeman component, weighted by the relative intensity of the component. To compute the frequencies of the Zeeman components of each hyperfine transition, the treatment of Gordy & Cook (1984a) was followed using the value of the molecular rotational g factor of $C^{17}O$ ($g_J = -0.2623$), and the value of the nuclear g factor ($g_I = -0.7575$) derived from the nuclear magnetic moment of ^{17}O

$HC^{17}O^+$ was produced by discharging a 1:2 mixture of CH_4 and O_2 (sample with 76% of ^{17}O) in Ar buffer gas with a total pressure of about 6 mTorr. The discharge current was a few mA, the cell was cooled at 77 K by liquid nitrogen circulation, and an axial magnetic field up to 165 G was applied throughout the length of the discharge. This longitudinal magnetic field, which allows observation of the ion by drastically improving its production, is responsible of the splitting and enlargement of the hyperfine components of the $J = 0 \rightarrow 1$ rotational transition. This effect, shown in Fig. 1, arises because of the Zeeman interaction between the magnetic field and the magnetic dipole moment of the ^{17}O nucleus, which is coupled to the molecular axis by nuclear quadrupole interaction (Gordy & Cook 1984a); the Zeeman observable $\Delta M_F = \pm 1$ components (the axial field is perpendicular to the electric vector of the microwave radiation) are symmetrically distributed around the unperturbed hyperfine line, whose frequency is the center of the blended multiplet. A quantitative description of this finer splitting is provided in Fig. 1, where simulation spectra based on Eq. (11.34) of Gordy & Cook (1984a) are displayed.

The measured hyperfine frequencies are listed in Table 1 along with the frequency of the $J = 2 \rightarrow 3$ transition observed by Plummer et al. (1983). They were analyzed by using Pickett's SPFIT fitting program (Pickett 1991), which is equivalent to use standard forms of the quadrupole and spin-rotation energies (Gordy & Cook 1984b) and, in addition, accounts for the shift of the apparent line center of the $J = 2 \rightarrow 3$ transition from the unperturbed frequency. The determined spectroscopic constants are reported in Table 2 along with the hyperfine constants of $C^{17}O$ for comparison purposes. The values of eQq for the two isoelectronic species are similar, and a reconsideration of the previous estimate of Guélin et al. (1982a) (i.e., 12 MHz) indicates that their scaling of the eQq constant of $HC^{14}N$ was badly affected by an inaccurate value of the ratio $Q(^{17}O)/Q(^{14}N)$ of the ^{17}O and ^{14}N electric quadrupole moments: an updated value of the ratio is -1.27 (Lide 1998), instead of -2.6, leading to an estimated value of 6 MHz. Measurements of additional rotational transitions to refine these constants are in progress.

Table 1. Transition frequencies of $HC^{17}O^+$

$J'' \rightarrow J'$	$F'' \rightarrow F'$	Frequency (MHz)
$0 \rightarrow 1$	$5/2 \rightarrow 3/2$	87 056.966(20)
	$5/2 \rightarrow 7/2$	87 057.258(20)
	$5/2 \rightarrow 5/2$	87 058.294(20)
$2 \rightarrow 3$		261 164.92(10)[a]

[a] Plummer et al. (1983).

Table 2. Ground state spectroscopic constants of $HC^{17}O^+$ and hyperfine constants of $C^{17}O$

Constant (MHz)		$HC^{17}O^+$	$C^{17}O^a$
B	rotational	43 528.928	···
D_J	centrifugal distortion	0.079	···
eQq	quadrupole coupling	4.595	4.337
C_I	spin–rotation	−0.020	−0.0304

[a] Frerking & Langer (1981).

3. Detection toward L1544

Observations of $HC^{17}O^+$ (1–0) toward the starless core L1544, in the Taurus Molecular Cloud, were carried out during November 1998, using the IRAM 30–m telescope. The $HC^{17}O^+$ (1–0) line was observed together with the $J = 2$–1 and 3–2 lines of DCO^+ as part of a project aimed to study physical and chemical characteristics of L1544

(Caselli et al., in prep.). At the frequency of the J = 1–0 line of $HC^{17}O^+$, the angular resolution (the half power beam width, HPBW) was 28 arcsec, or ~0.02 pc at the distance of Taurus (140 pc), and the spectral resolution was 0.034 $\mathrm{km\,s^{-1}}$. The data were acquired in frequency switching mode with a frequency throw of 1.0 MHz at 3 mm. The pointing was checked at 1–2 hours intervals and found good to ~4 arcsec. We looked for $HC^{17}O^+$ (1–0) toward the L1544 "molecular peak" (with coordinates: RA(1950) = $5^{\mathrm{h}}1^{\mathrm{m}}12\overset{\mathrm{s}}{.}5$, Dec(1950) = $25°6'40''$), i.e. the position where the integrated intensity of the mapped molecular species (such as NH_3, DCO^+, N_2H^+, and N_2D^+; Caselli et al., in prep.) reaches its maximum value.

The observed $HC^{17}O^+$(1–0) spectrum, smoothed at a spectral resolution of 20 kHz, is shown in Fig. 2. Albeit the moderate signal to noise (S/N) ratio of the hyperfines, the line is clearly detected. In fact, the intensity integrated over the three hyperfines (hf) is $I \pm \sigma_I = 0.040 \pm 0.004$ K $\mathrm{km\,s^{-1}}$ ([1]).

Figure 2 also shows the fit to the three $HC^{17}O^+$ (1–0) hyperfines, obtained with the "hfs" fitting program in CLASS (Forveille et al. 1989). This program computes lines with hyperfine structure with the assumption of Gaussian velocity distribution and equal excitation temperatures. Variables are excitation temperature, LSR velocity, line width, and total optical depth (i.e. the sum of the peak optical depths of the hf components), whereas the frequencies of the hyperfines are kept fixed at the laboratory values, neglecting the corresponding uncertainties. Because of the poor sensitivity of the $HC^{17}O^+$(1–0) spectrum, the determination of the optical depth from the hfs fit is affected by large errors. However, the line is likely to be thin (as the intensity ratio between the hf components suggests) and optically thin conditions have been assumed to determine the other parameters.

The fit to the $HC^{17}O^+$ spectrum in Fig. 2 takes into account the presence of two velocity components along the line of sight toward L1544, which have been observed in other molecular tracers (e.g. $HC^{18}O^+$, see Caselli et al. 1999). Fit results are listed in Table 3: the main beam brightness temperature (T_{mb}) of the J = 1–0 line (i.e. T_{mb} of the main hf component divided by its statistical weight), the LSR velocity (V_{LSR}) and the intrinsic line width (Δv) of the two velocity components. As already stated, the error associated with the measured radial velocity does not include the uncertainty on the measured frequencies (20 kHz, or ~0.07 km $\mathrm{s^{-1}}$, see Table 1), which should be added in quadrature to obtain the correct value. Inside the errors, V_{LSR} and Δv values of the two velocity components coincide with those relative to the $HC^{18}O^+$(1–0) line observed in the same direction (Caselli et al., in prep.), indicating the good agreement between laboratory and astrophysical measurements.

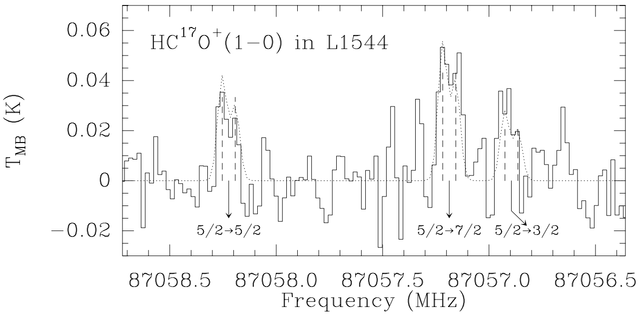

Fig. 2. $HC^{17}O^+$ (1–0) spectrum toward the "molecular peak" of L1544, observed at the IRAM 30–m antenna. The spectrum is in units of main beam brightness temperature. The dotted spectrum represents the hfs fit (see text) to the three hyperfine components of the J = 1–0 line using the parameters measured in the laboratory. Dashed lines indicate the splitting of the three hyperfines due to the presence of two velocity components along the line of sight. The relative intensities of the three groups of lines reflect their statistical weight, suggesting that the observed emission is optically thin

In the L1544 study (Caselli et al., in prep.), the detection of $HC^{17}O^+$ allowed us to estimate the optical depth of the $HC^{18}O^+$ (1–0) line, more accurately determine the $HC^{18}O^+$ (and thus HCO^+) column density, and better constrain electron fraction. In general, $HC^{17}O^+$ observations are advised when accurate estimates of HCO^+ column density are needed, and doubts on the thickness of $HC^{18}O^+$ lines are present (e.g. in cases of asymmetric or double peaked profiles, as found in L1544).

Table 3. Results of the hfs fit to the $HC^{17}O^+$ (1–0) line

Component	T_{mb} (K)	V_{LSR} ($\mathrm{km\,s^{-1}}$)	Δv ($\mathrm{km\,s^{-1}}$)
1	0.13 ± 0.02	7.14 ± 0.02	0.17 ± 0.04
2	0.09 ± 0.02	7.35 ± 0.03	0.17 ± 0.06

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[1] $\sigma_{\mathrm{I}} = \mathrm{rms} \times \sqrt{N_{\mathrm{ch}}} \times \Delta v_{\mathrm{res}}$, where rms is the 1σ level of the noise in the off–line channels (0.011 K), N_{ch} is the number of channels in the integrated intensity (31), and Δv_{res} is the velocity resolution of the spectrum (smoothed at 0.067 $\mathrm{km\,s^{-1}}$).

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