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Letter to the Editor

Molecular abundances in the Magellanic Clouds

II. Deuterated species in the LMC*

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Abstract. The first definite discoveries of extragalactic deuterium are reported. DCO^+ has been detected in three and DCN has been measured in one star-forming region of the Large Magellanic Cloud (LMC). While the HCO^+/DCO^+ abundance ratios are found to be 19 ± 3, 24 ± 4, and 67 ± 18 for N113, N44BC and N159HW, respectively, a HCN/DCN abundance ratio of 23 ± 5 is obtained for N113. These results are consistent with a gas temperature of about 20 K and a D/H ratio of about 1.5×10^{-5}, consistent with that observed in the Galaxy. If the cloud temperature is closer to 30 K, then a D/H ratio is required to be up to an order of magnitude larger. Because this ratio provides a lower limit to the primordial D/H ratio, it indicates that the baryon mass density alone is unable to close the universe.

Key words: ISM: abundances – ISM: molecules – Galaxies: abundances – Magellanic Clouds – Cosmology: observations – Radio lines: ISM

1. Introduction

The primordial ratio of the number of deuterium to hydrogen nuclei (D/H) created in big bang nucleosynthesis is the most sensitive measure of the cosmological baryon-to-photon ratio, η, and the cosmological density of baryons, Ω_b. In the interstellar medium of our Galaxy D/H = $1.6 \pm 0.3 \times 10^{-5}$ (Linsky et al. 1995), which places a strict lower limit on the primordial abundance, because stars reduce the proportion of D in the ISM. On the other hand, quasar absorption line systems should provide suitable targets to determine primordial D abundances because they can sample metal-poor gas at early epochs where the destruction of D should be negligible. Carswell et al. (1994) and Songaila et al. (1994) obtained a high D/H $\approx 2.5 \times 10^{-4}$ ratio from a possible deuterium absorption feature toward the quasar Q0014+813. More recent observations by Rugers & Hogan (1996) and Tytler et al. (1996) do not provide clear evidence in favor or against high D/H ratios at large redshifts and it is still difficult to rule out entirely the possibility that the D feature is contaminated by H having a velocity different from that of the principal hydrogen lines. Therefore, a direct measurement of atomic deuterium toward high redshift quasars is a potentially powerful, though not yet fully explored means of studying D/H.

Irrespective of the validity of a high or low cosmological D/H value, the ratio appears to be small enough to preclude any easy detection of deuterated molecular species in interstellar space. Nevertheless, the zero-point energy difference between hydrogen- and deuterium-bearing molecules means that deuterated species can become heavily fractionated in cool environments. Models of fractionation (Brown & Rice 1986; Millar et al. 1989) indicate that the underlying D/H ratio is consistent with that suggested by Linsky et al. (1995), implying that the baryon mass density is not large enough to close the universe. Hence measurements of deuterated species have become an important tool to study the physical properties and the chemical and dynamical history of Galactic molecular clouds (e. g. Wootten 1987; Millar et al. 1989). In a previous study Mauersberger et al. (1995) presented sensitive upper limits to the DCN/HCN ratio in NGC 253 and

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* Based on observations with the Swedish-ESO Submillimeter Telescope (SEST) at the European Southern Observatory (ESO), La Silla, Chile

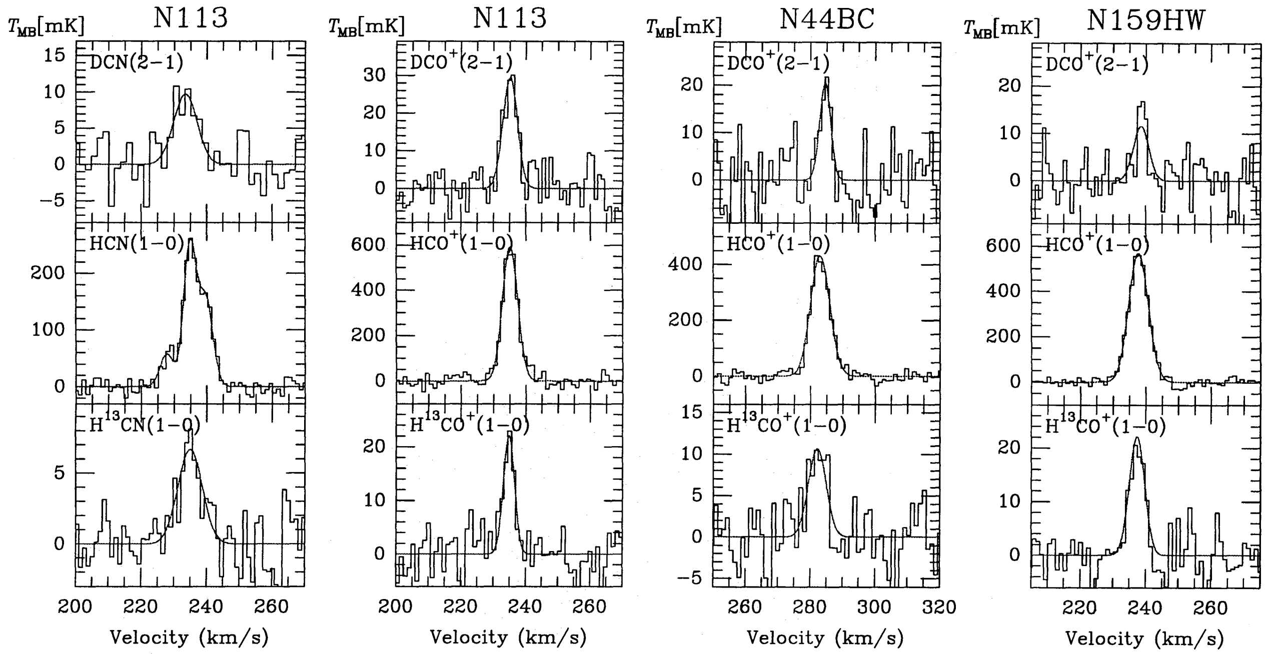

Fig. 1. The observed spectra of selected hydrogen-, deuterium-, and ^{13}C-bearing molecules toward N113 ($\alpha_{1950} = 5^h13^m38\overset{s}{.}7$, $\delta_{1950} = -69°25'57''$), N44BC ($\alpha_{1950} = 5^h22^m10\overset{s}{.}6$, $\delta_{1950} = -68°00'32''$), and N159HW ($\alpha_{1950} = 5^h40^m04\overset{s}{.}4$, $\delta_{1950} = -69°46'54''$) in the LMC

IC 342, which are consistent with the warm, metal rich environment of this starburst nucleus.

2. Observations

The data were taken in January and March 1996, using the 15-m Swedish-ESO Submillimetre Telescope (SEST) at La Silla, Chile. Two SIS receivers, one at $\lambda = 3$ and one at 2 mm, yielded overall system temperatures, including sky noise, of order $T_{sys} = 250$ K on a main beam brightness temperature (T_{MB}) scale. The backend was an acousto-optical spectrometer which was split into 2 × 1000 contiguous channels for simultaneous 3 and 2 mm observations. The channel separation of 43 kHz corresponds to 0.09 and 0.15 km s^{-1} at 145 and 88 GHz, respectively. The corresponding antenna beamwidths were 35″ and 55″ at the observed line frequencies taken from Lovas (1992).

The observations were carried out in a dual beam-switching mode (switching frequency 6 Hz) with a beam throw of 11′40″ in azimuth. The on-source integration time of each spectrum varied from 8 minutes for HCO$^+$ to 18 hours for H^{13}CN toward N113. All spectral intensities obtained were converted to a T_{MB} scale, correcting for main beam efficiencies of 0.74 at 85–100 and 0.67 at 130–150 GHz (Dr. L.B.G. Knee, priv. comm.). The pointing accuracy, obtained from measurements of the SiO maser sources R Dor and U Men, was better than 10″.

3. Results

Toward the prominent star-forming region N113 we have detected HCO$^+$, HCN, and their rare isotopic species H^{13}CO$^+$, DCO$^+$, H^{13}CN, and DCN. HCO$^+$, H^{13}CO$^+$, and DCO$^+$are also observed toward N159HW (position defined by Hunt & Whiteoak 1994) and N44BC. The spectra and line parameters obtained from Gaussian fits are displayed in Fig. 1 and Table 1.

Assuming optically thin line emission, we can derive from the line intensity ratios of the ^{13}C- and deuterium-bearing species the ratio of column densities. We find

$$\frac{N_1}{N_2} = \alpha \frac{B_2}{B_1} \frac{g_{l_1}}{g_{u_1}} \frac{g_{u_2}}{g_{l_2}} \frac{(1 - e^{-h\nu_2/kT_2})}{(1 - e^{-h\nu_1/kT_1})} \frac{(J_{\nu_2,T_2} - J_{\nu_2,2.7})}{(J_{\nu_1,T_1} - J_{\nu_1,2.7})} \frac{I_1}{I_2},$$

$$\alpha = \frac{e^{2\,hB_1/kT_1}}{3} \qquad \text{and} \qquad J_{\nu,T} = \frac{h\nu}{k}\left(e^{h\nu/kT} - 1\right)^{-1} \quad (1)$$

(N: column density; B: rotational constant; g_l and g_u: statistical weights of lower and upper states; T: excitation temperature; I: integrated line intensity; indices 1 and 2 refer to the deuterium-bearing and to the ^{13}C-bearing or main isotopic species, respectively). Both HCO$^+$ and HCN have large electric dipole moments (of order 3 Debye) and are excited well beyond 2.7 K only at high densities. At $n(H_2) = 10^5$ cm^{-3} radiative transfer calculations with a Large Velocity Gradient (LVG) model, spherical cloud geometry, and collision cross sections from Green & Thaddeus (1974) yield excitation temperatures of order 4 K for T_{kin} = 20–40 K in the optically thin limit, both for

Table 1. Parameters of the Observed Molecular Lines

Molecule & Transition			Frequency [GHz]	T_{MB} [mK]	r.m.s. [mK]	v_{LSR} [$km\,s^{-1}$]	$\Delta v_{1/2}$ [$km\,s^{-1}$]	$\int T_{MB}\,dv$ [$K\,km\,s^{-1}$]
N113								
DCN [a)]	J=2–1		144.077321	10	8	233.4	8.4	0.086 ± 0.011
		F=1–1	88.630416	153				
HCN [b)]	J=1–0	F=2–1	88.631847	247	19	234.9	4.7	2.33 ± 0.04
		F=0–1	88.633936	57				
$H^{13}CN$ [a)]	J=1–0		86.340184	6.7	3	235.0	8.8	0.065 ± 0.006
DCO^+	J=2–1		144.828000	29	10	235.1	5.3	0.166 ± 0.011
HCO^+	J=1–0		89.188518	593	39	235.1	5.5	3.56 ± 0.06
$H^{13}CO^+$	J=1–0		86.754294	22	6	234.8	4.1	0.105 ± 0.008
N44BC								
DCO^+	J=2–1		144.828000	20	12	284.5	4.0	0.084 ± 0.014
HCO^+	J=1–0		89.188518	432	25	283.0	7.0	3.16 ± 0.04
$H^{13}CO^+$	J=1–0		86.754294	11	6	282.2	6.5	0.067 ± 0.009
N159HW								
DCO^+	J=2–1		144.828000	12	8	238.5	5.6 [c)]	0.054 ± 0.010
HCO^+	J=1–0		89.188518	569	23	237.8	7.0	4.29 ± 0.04
$H^{13}CO^+$	J=1–0		86.754294	22	5	237.4	5.6	0.122 ± 0.009

a) The hyperfine components of DCN and $H^{13}CN$ line cannot be resolved.
b) The three HCN hyperfine transitions (F=1–1, F=2–1, F=0–1) have been resolved by a Gaussian fit. While T_{MB} values for each component are given, the total integrated line intensity refers to the entire line.
c) During the Gaussian fit value of $\Delta v_{1/2}$ has been fixed by using that determined from the $H^{13}CO^+$(1–0) transition.

the J=1–0 transition of $H^{13}CN$ and for the 2–1 transition of DCN. These results also hold for HCO^+. While smaller densities would lead to excitation temperatures almost undistinguishable from those of the microwave background (and thus to negligible emission), gas at even higher densities is likely not common enough to contribute significantly to the observed emission. We thus find, neglecting differences in beam sizes, for HCO^+

$$\frac{N(DCO^+)}{N(H^{13}CO^+)} \approx 1.68 \frac{I(DCO^+)}{I(H^{13}CO^+)} \qquad (2)$$

and for HCN

$$\frac{N(DCN)}{N(H^{13}CN)} \approx 1.67 \frac{I(DCN)}{I(H^{13}CN)}. \qquad (3)$$

With $^{12}C/^{13}C \approx 50$ (Johansson et al. 1994; this is consistent with the line intensity ratios dereived from Table 1) we then obtain $N(HCO^+)/N(DCO^+) \approx 19 \pm 3$ and $N(HCN)/N(DCN) \approx 23 \pm 5$ for N113, while $N(HCO^+)/N(DCO^+) \approx 24 \pm 4$ and 67 ± 18 for N44BC and N159HW, respectively.

4. Discussion

The detection of DCO^+ and DCN in the LMC is a useful tool to study D/H on a larger spatial scale and in a less 'chemically' processed environment than that provided by the Galaxy. Gensheimer et al. (1996) observed a high deuteration of water toward a number of Galactic hot cores despite a high kinetic temperature. While this can be explained in terms of a recent evaporation of grain mantles, this effect probably plays no role toward our LMC sample since we are looking on a much larger region which may much better reflect the average conditions of the interstellar gas than the highly biassed sample by Gensheimer et al. (1996). Due to the lower metallicity in the LMC, we expect grain surface reactions to be of lesser importance than for the Galactic interstellar medium. The process of chemical fractionation has, however, to be accounted for quantitatively. To this end, we have re-visited earlier models of deuterium chemistry (Millar et al. 1989; Howe & Millar 1992) with conditions appropriate for clouds in the LMC (Paper I) and with an elemental D to H ratio of 1.5×10^{-5}. We have updated the chemistry to include the fast dissociative recombination of H_3^+ (and H_2D^+) and more accurate rate coefficients for neutral-neutral reactions. Although the general trends of fractionation can be understood, especially for simple species like HCO^+ detailed models are necessary for quantitative comparison with the observations (Millar et al. 1989).

Table 2. Calculated abundance ratios

Temperature	10 K			20 K			30 K		
Time (yr)	$R(H_3^+)$	$R(HCO^+)$	$R(HCN)$	$R(H_3^+)$	$R(HCO^+)$	$R(HCN)$	$R(H_3^+)$	$R(HCO^+)$	$R(HCN)$
10^5	3.8	12.8	24.9	8.3	23.7	61.1	167	309	246
3.2×10^5	3.7	10.3	14.9	8.2	17.7	32.5	166	257	253
10^7	4.3	9.3	20.0	8.6	14.8	37.5	166	251	476

a) The ratio R(HX) is defined as the abundance ratio of HX to DX, and is tabulated for HX = H_3^+, HCO^+ and HCN

Because deuterium fractionation depends on small differences in zero-point energies, the process is sensitive to the kinetic temperature, $T_{\rm kin}$, of the molecular gas. Multi-transition studies of CO in N113 have not been made so that $T_{\rm kin}$ is unknown, but a value of around 20 K is expected since the cloud is associated with an H II region (for detailed modelling, see Lequeux et al. 1994). To cover the range of possibilities, we present the results of time-dependent chemical kinetic calculations at 10, 20 and 30 K for three model times in Table 2.

At low temperatures there are two main routes to D fractionation:

$$H_3^+ + HD \longleftrightarrow H_2D^+ + H_2 \qquad (4)$$
$$H_3^+ + D \longrightarrow H_2D^+ + H \qquad (5)$$

where we have calculated the rate coefficient, k_{-4}, for the back reaction of H_2D^+ with H_2 using the data presented by Sidhu et al. (1992). This rate coefficient is very sensitive to temperature and has values of 2.1×10^{-18}, 2.4×10^{-13} and 8.3×10^{-12} cm^{3}s^{-1} at 10, 20 and 30 K, respectively. For $T \gtrsim 25$ K, the back reaction is fast and $R(H_3^+)$ is large, ≈ 165 at 30 K. DCO^+ is formed through reactions involving $H_2D^+$and D atoms, with these species contributing 64% (36%) at 10 K, 54% (46%) at 20 K and 44% (56%) at 30 K, to the formation rate of DCO^+.

Our results show that the deuterium fractionation is larger than that observed in N113 for HCO^+ and HCN for $T \leq 20$ K and smaller for $T = 30$ K; the observed result that fractionation is larger in DCO^+ than DCN is reproduced.

Our results are consistent with $T \sim 20$ K for a D/H ratio of 1.5×10^{-5}. However, the temperatures of the LMC clouds are not, as yet, well constrained. The observed abundance ratios could be reproduced in warmer clouds if the D/H ratio is larger than our adopted value. At a cloud temperature of 30 K, one would need a D/H ratio about 10 times larger, i. e. on the order of 1.5×10^{-4}. If there temperature is 20–30 K as suggested by Lequeux et al. (1994) for the cloud cores (for HCN, see also Chin et al. 1996), then it appears that the D/H ratio in the LMC is similar to or larger than that in our Galaxy. This would be consistent with the LMC gas being less processed through stars than that in our Galaxy. Thus, the evidence from the LMC is consistent with an open universe as long as the cosmological constant is small.

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