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, $\eta$, and the cosmological density of baryons, $\Omega_b$. In the interstellar medium of our Galaxy D/H = 1.6 ± 0.3 × 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 ≈ 2.5 × 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...
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 $T_{\text{sys}} = 250$ K on a main beam brightness temperature ($T_{\text{MB}}$) scale. The backend was an acousto-optical spectrometer which was split into $2 \times 1000$ 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 $T_{\text{MB}}$ 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$^+$ and H$^{13}$CO$^+$ 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

$$N_1 = \frac{\alpha B_2 g_1 g_{u_2} (1 - e^{-h\nu_2/kT_2}) (J_{\nu_2, T_2} - J_{\nu_2, 2.7}) I_1}{B_1 g_1 g_{u_2} (1 - e^{-h\nu_1/kT_1}) (J_{\nu_1, T_1} - J_{\nu_1, 2.7}) I_2},$$

$$\alpha = \frac{e^2 h B_1/kT_1}{3}$$

and

$$J_{\nu, T} = \frac{h\nu}{k} \left( e^{h\nu/kT_1} - 1 \right)^{-1}$$

$N$: column density; $B$: rotational constant; $g_1$ and $g_{u_2}$: 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 $T_{\text{kin}} = 20–40$ K in the optically thin limit, both for
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$^+$

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

(2)

and for HCN

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

(3)

With $^{12}\text{C}/^{13}\text{C} \approx 50$ (Johansson et al. 1994; this is consistent with the line intensity ratios derived from Table6) we then obtain $N(\text{HCO}^+)/N(\text{DCO}^+) \approx 19 \pm 3$ and $N(\text{HCN})/N(\text{DCN}) \approx 23 \pm 5$ for N113, while $N(\text{HCO}^+)/N(\text{DCO}^+) \approx 24 \pm 4$ and $67 \pm 18$ 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 biased 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 $1.5 \times 10^{-5}$. We have updated the chemistry to include the fast dissociative recombination of H$_3^+$ (and H$_2$D$^+$) 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).

| 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 $^a$ $^b$ $^c$)  | $J=2-1$        | 144.077321    | 10          | 8                   | 233.4                | 8.4                  | 0.086 ± 0.011        |
|                      | $F=1-1$        | 88.630416     | 153         |                     |                      |                      |                      |
|                      | $F=2-1$        | 88.631847     | 247         | 19                  | 234.9                | 4.7                  | 2.33 ± 0.04          |
|                      | $F=0-1$        | 88.633936     | 57          |                     |                      |                      |                      |
| H$^{13}$CN $^a$ $^b$ | $J=1-0$        | 86.340184     | 6.7         | 3                   | 235.0                | 8.8                  | 0.065 ± 0.006        |
| DCO$^+$ $^b$ $^c$    | $J=2-1$        | 144.828000    | 29          | 10                  | 235.1                | 5.3                  | 0.166 ± 0.011        |
| HCN $^b$ $^c$        | $J=1-0$        | 89.185185     | 593         | 39                  | 235.1                | 5.5                  | 3.56 ± 0.06          |
| H$^{13}$CO$^+$ $^b$  | $J=1-0$        | 86.754294     | 22          | 6                   | 234.8                | 4.1                  | 0.105 ± 0.008        |
| **N44BC**            |                |               |             |                     |                      |                      |                      |
| DCO$^+$ $^b$ $^c$    | $J=2-1$        | 144.828000    | 20          | 12                  | 284.5                | 4.0                  | 0.084 ± 0.014        |
| HCO$^+$ $^c$         | $J=1-0$        | 89.185185     | 432         | 25                  | 283.0                | 7.0                  | 3.16 ± 0.04          |
| H$^{13}$CO$^+$ $^c$  | $J=1-0$        | 86.754294     | 11          | 6                   | 282.2                | 6.5                  | 0.067 ± 0.009        |
| **N159HW**           |                |               |             |                     |                      |                      |                      |
| DCO$^+$ $^c$         | $J=2-1$        | 144.828000    | 12          | 8                   | 238.5                | 5.6 $^c$            | 0.054 ± 0.010        |
| HCO$^+$ $^c$         | $J=1-0$        | 89.185185     | 569         | 23                  | 237.8                | 7.0                  | 4.29 ± 0.04          |
| H$^{13}$CO$^+$ $^c$  | $J=1-0$        | 86.754294     | 22          | 5                   | 237.4                | 5.6                  | 0.122 ± 0.009        |

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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.
Because deuterium fractionation depends on small differences in zero-point energies, the process is sensitive to the kinetic temperature, $T_{\text{kin}}$, of the molecular gas. Multi-transition studies of CO in N113 have not been made so that $T_{\text{kin}}$ 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:

\[ \text{H}_2^+ + \text{HD} \leftrightarrow \text{H}_2 \text{D}^+ + \text{H}_2 \] \hspace{1cm} (4)

\[ \text{H}_2^+ + \text{D} \rightarrow \text{H}_2 \text{D}^+ + \text{H} \] \hspace{1cm} (5)

where we have calculated the rate coefficient, $k_{-4}$, for the back reaction of H$_2$D$^+$ with H$_2$ using the data presented by Sidhu et al. (1992). This rate coefficient is very sensitive to temperature and has values of $2.1 \times 10^{-18}$, $2.4 \times 10^{-13}$ and $8.3 \times 10^{-12}$ cm$^3$s$^{-1}$ at 10, 20 and 30 K, respectively. For $T \gtrsim 25$ K, the back reaction is fast and $R(\text{H}_2^+)$ is large, $\approx 165$ at 30 K. DCO$^+$ is formed through reactions involving H$_2$D$^+$ 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 $T \lesssim 20$ 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 $1.5 \times 10^{-5}$. 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 $1.5 \times 10^{-4}$. 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.

**Acknowledgements.** We like to thank Drs. J.L. Linsky and T.L. Wilson for useful comments. TJM is supported by a grant from PPARC. RM was supported by a Heisenberg fellowship of Deutsche Forschungsgemeinschaft.

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