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Citation

Cecchi-Pestellini, C., and A. Dalgarno. 2000. H3+ in Diffuse Interstellar Gas. Monthly Notices of the Royal Astronomical Society 313, no. 1 (March 21): L6–L8.

Published Version

doi:10.1046/j.1365-8711.2000.03320.x

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H_3^+ in diffuse interstellar gas

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Accepted 1999 December 14. Received 1999 December 10; in original form 1999 October 22

ABSTRACT

A model is constructed of the material in front of the star Cygnus OB2 no. 12 in which dense cores are embedded in diffuse clumps of gas. The model reproduces the measured abundances of H_3^+ , C_2 and CO, and predicts a column density of 9×10^{10} cm⁻² for HCO⁺.

Key words: molecular processes - ISM: clouds - ISM: molecules.

1 INTRODUCTION

The successful detection of the molecular ion H_3^+ in the interstellar medium (Geballe & Oka 1996; McCall et al. 1998) confirms the importance of cosmic-ray induced ion–molecule chemistry in the determination of the molecular composition in interstellar clouds. The abundance of H_3^+ observed along the line of sight to the star Cygnus OB2 no. 12 is 3.8×10^{14} cm⁻² (Geballe et al. 1999).

This value, comparable to that measured in dense clouds (Geballe & Oka 1996), is unexpectedly high, because the absence of the 3.0- and 4.27- μ m features of H₂O and CO₂ ices and the presence of the 3.4- μ m hydrocarbon feature (Whittet et al. 1997) strongly suggest that the intervening medium is a low-density diffuse gas (McCall et al. 1998).

An initial interpretation of the data by McCall et al. (1998), made by adopting a model of a gas of uniform density, used a total hydrogen number density of 10 cm^{-3} and a column path length between 400 and 1200 pc. As McCall et al. (1998) pointed out, the suggested path length is apparently inconsistent with observations of CH, C₂ and CO. Further, at a density of 10 cm^{-3} , photodissociation will limit the abundance of molecular hydrogen that is needed to form H₃⁺.

We propose an alternative model of the gas in which clumps of matter exist with a mean visual extinction of 1.6 mag embedded in a tenuous interclump medium. The mean clump hydrogen density is 100 cm^{-3} . The clumps contain dense cores with densities ranging from 10^3 to 10^6 cm^{-3} . The model is consistent with the presence of the 3.4- μ m feature (Whittet et al. 1997) and the absence of ices (Whittet 1992).

2 THE MODEL FOR H_3^+

We adopt a chemical network constructed from 36 species consisting of the elements H, He, C and O. We select from the UMIST data file (Millar et al. 1997) all the reactions that couple the species. We terminate the hydrocarbon chemistry at $C_2H_2^+$. We modified the UMIST data file by incorporating the branching ratios for dissociative recombination of Andersen et al. (1996), Vejby-Christensen et al. (1997), Larson et al. (1998) and Derkatch et al. (1999). We describe the depth-dependent H₂ and CO photodissociation rates by self-shielding functions (van Dishoeck & Black 1988; Sternberg & Dalgarno 1995). From a consideration of the thermal balance we obtained a mean temperature of 35 K.

The chemical structure and ionization balance depend on the element depletion. A gas phase abundance for carbon atoms to hydrogen of $1.4(\pm0.2) \times 10^{-4}$ has been derived by Cardelli et al. (1996) for five lines of sight, a ratio that agrees with the value of 1.3×10^{-4} found for ζ Ophiuchi (Snow & Witt 1996). For oxygen we adopt 3.3×10^{-4} (Snow & Witt 1996).

The H₃⁺ ions are produced by the reaction of H₂ with the H₂⁺ ions resulting from the cosmic-ray ionization of H₂. In diffuse gas with a visual extinction less than $A_V = 2$ mag, the fractional ionization $x = n_e/n_H$ is nearly constant and H₃⁺ is removed largely by dissociative recombination with electrons at a rate αn_e , where $\alpha = 1.2 \times 10^{-7} \sqrt{300/T}$ cm³ s⁻¹ (Sundström et al. 1998). Hence if ζ s⁻¹ is the cosmic-ray ionization rate, the steady state abundance of H₃⁺ is approximately

$$n({\rm H}_3^+) = \frac{\zeta n({\rm H}_2)}{\alpha \, x n_{\rm H}} \approx 4\zeta \frac{n({\rm H}_2)}{n_{\rm H}} \times 10^{10} \,{\rm cm}^{-3}.$$
 (1)

The abundance of H_3^+ follows the increase in the fraction of hydrogen that is converted to molecular form with increasing depth into the individual clumps and tends to a constant value independent of density. At larger visual extinction, atomic ions are converted to molecular ions and the fractional ionization decreases. Removal of H_3^+ then occurs preferentially by proton transfer in reactions with neutral species, and the density of H_3^+ is constant at about $2 \times 10^{12} (\zeta/\delta) \, \mathrm{cm}^{-3}$, where δ is the depletion factor.

Fig. 1 shows the calculated densities of H, H₂ and H₃⁺ for an isolated clump of visual extinction $A_V = 1.6$ mag and a density of 100 cm^{-3} as a function of distance from the centre of the clump outwards to radius r_c . The abundance of H₃⁺ follows the decrease

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Figure 1. Volume density of H, H₂ and H₃⁺ as a function of clump radius. The density of the clump is taken as 100 cm^{-3} and the ionization rate is $4 \times 10^{-17} \text{ s}^{-1}$.



Figure 2. Same as Fig. 1 for a clump density of 10 cm^{-3} .

in the H_2 molecular fraction. Fig. 2 is similar to Fig. 1 but for a density of 10 cm^{-3} . There is little conversion of H into H_2 and the density of H_3^+ is very small.

The integrated column densities of H_3^+ for clumps with A_V between 0.6 and 2 mag expressed as fractions of the total H column densities are shown in Fig. 3 as functions of the cloud density for an ionizing frequency of $4 \times 10^{-17} \text{ s}^{-1}$. Significant amounts of H_3^+ are produced for volume densities exceeding about 25 cm^{-3} . The volume density of H_3^+ tends to a constant value for clump densities larger than about 100 cm^{-3} . As a consequence, the integrated column densities of H_3^+ decrease with increasing clump density.

Low densities are not conducive to the formation of H_3^+ , and they require anomalously large values for the clump mass and dimension if the correct visual magnitude is to be obtained. We show in Fig. 4 the dependence of fractional abundances on clump mass for $A_V = 1.6$ mag.

We solved the H_3^+ radiative transfer problem with 9 spherical clumps along the line of sight with a mean chord length of 6.7 pc, equal to two-thirds of the diameter, and a hydrogen density of 100 cm^{-3} . We assume that the background gas has a small density such that it does not contribute to the extinction. The total visual extinction is 10.2 mag. If we choose $\zeta = 6 \times 10^{-17} \text{ s}^{-1}$, we predict a column density of H_3^+ of $3.8 \times 10^{14} \text{ cm}^{-2}$, in agreement with the value observed by Geballe et al. (1999).



Figure 3. Fractional column densities of H_3^+ as functions of the clump density for clumps of total visual extinction $A_V = 2$, 1.4, 1 and 0.6 mag (top to bottom).



Figure 4. Fractional abundance of H_3^+ as a function of the clump mass.

Other than H_2 , H_2^+ and OH, molecular species are nearly absent from the clump gas. To explain the measured abundances of C₂ (Gredel & Münch 1994) and CO (McCall et al. 1998), we postulate a nesting structure (Houlahan & Scalo 1992) in which the clumps of density 10^2 cm^{-3} contain cloudlets at a density of about 10^{4} cm⁻³, embedded in which are high-density cores with a density of 10^5 cm^{-3} or greater. The aggregate contribution of the cloudlets to the visual extinction is 0.9 mag, and that of the highdensity cores 0.1 mag. The major source of C₂ is the dissociative recombination of $C_2H_2^+$, the formation of which requires the presence of atomic carbon. It is produced in the cloudlets but not in the dense cores, where the carbon is largely taken up as CO. With a cosmic ray ionization rate of $6 \times 10^{-17} \text{ s}^{-1}$, we can accurately reproduce the measured abundance of 2×10^{14} cm⁻² (Gredel and Münch 1994) for C2 with a density in the cloudlet of 7×10^3 cm⁻³, and we can reproduce the measured abundance of $2.6 \times 10^{16} \text{ cm}^{-2}$ (McCall et al 1998) for CO with a density of 10^5 cm⁻³ or greater in the core. The core contains a column density of no more than 10^{11} cm⁻² of H₃⁺ and the cloudlet no more than $10^{12} \,\mathrm{cm}^{-2}$.

We predict a column density for OH of $6 \times 10^{13} \text{ cm}^{-2}$ produced mostly in the clump gas, a column density for C₂H of $2 \times 10^{13} \text{ cm}^{-2}$ produced mostly in the cloudlet, and a column density for HCO⁺ of $9 \times 10^{10} \text{ cm}^{-2}$ produced mostly in the high-density core. The core has a density greater than the critical density for the 1-0 rotational transition of HCO⁺, so that HCO⁺ may be detectable in emission at the 1-0 frequency.

ACKNOWLEDGMENTS

This research has been supported by the Division of Astronomy of the US National Science Foundation. We are grateful to T. Oka, B. J. McCall and D. A. Williams for their comments on an earlier version of this manuscript.

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