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THE COSMIC ABUNDANCE OF DEUTERIUM

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ABSTRACT

The cosmic abundance of deuterium may be derived from the measured ratio of the abundances of the molecules HD and H_2. The derivation is sensitive to the magnitude of the ionizing flux and to the depletion of oxygen and carbon. The abundance of OH is also sensitive to these parameters and should be useful in revealing the amount of deuterium which can exist in atomic form. Observational upper limits on the concentration of OH in regions where HD and H_2 have been observed place a lower bound on the deuterium abundance ratio [D]/[H], while the assumption that ionization of hydrogen is caused only by the observed high-energy cosmic rays provides an upper bound. Observations of the ζ Oph cloud indicate that $2 \times 10^{-6} < [D]/[H] < 2 \times 10^{-4}$.

Subject headings: abundances — interstellar matter — molecules, interstellar

I. INTRODUCTION

The presence of the molecule HD with an abundance relative to H_2 of about 10^{-6} has been established by the spectrophotometric observations of Spitzer *et al.* (1973), who point out that in order to derive the cosmic abundance [D] of deuterium from the HD/H_2 ratio it is necessary to take account of the self-shielding of the H_2 molecule and of chemical fractionation processes. The correction for self-shielding alone leads to a ratio [D]/[H] of about 5×10^{-3}. Watson (1973) has argued that the correction for chemical fractionation can reduce the derived ratio by a factor of 100. We demonstrate that the correction is sensitive to the ionizing flux and to the abundance of oxygen and that the question might be resolved by a positive measurement of the column density of the OH molecule.

We adopt as a specific example the dominant cloud component in front of ζ Oph.

II. THE ζ OPH CLOUD

The relative abundances of H_2 and H depend essentially on the ultraviolet flux that dissociates the molecular hydrogen and on the gas density in the cloud (Hollenbach, Werner, and Salpeter 1971). The populations of the high rotational levels of H_2 also depend upon the ultraviolet flux; the radiative lifetimes are much shorter than the collision times, and the populations are controlled by the efficiency of ultraviolet fluorescence through the Lyman and Werner systems followed by rotation-vibration cascading (Black and Dalgarno 1973).

We assume that hydrogen molecules are formed by recombination on grains (Hollenbach and Salpeter 1971). Then in order to reproduce the column abundances of H_2, of H and of the $J = 6$ rotational level of H_2 measured toward ζ Oph (Spitzer *et al.* 1973), we obtain at the center of the main cloud, a density, $n(H_2)$, of H_2 of 1560 cm^{-3}; a density, n(H), of H of 880 cm^{-3}; and a rate of radiative dissociation of H_2 of 2.2×10^{-14} s^{-1}, corresponding to an ultraviolet energy density of 5.6×10^{-16} ergs cm^{-3} Å^{-1} at 1000 Å. The corresponding rate of radiative dissociation of HD at the center of the cloud is 2×10^{-10} s^{-1} so that in the absence of chemical fractionation, [D]/[H] would equal 4×10^{-3}, in harmony with the estimate of Spitzer *et al.* (1973).

It has been argued (Dalgarno, Black, and Weisheit 1973; Watson 1973) that the chemical process that is largely responsible for the fractionation is

$$D^+ + H_2 \rightleftarrows H^+ + HD, \tag{1}$$

a process now known to be rapid in the forward exothermic direction with a rate coefficient of about 8×10^{-10} cm^3 s^{-1} (Fehsenfeld *et al.* 1973). D^+ ions are produced by direct ionization, but a larger source is the fast charge-transfer reaction

$$H^+ + D \rightleftarrows H + D^+, \tag{2}$$

which has a rate coefficient of 2×10^{-9} cm^3 s^{-1}. In regions of low fractional ionization, reaction (2) and

$$H^+ + O \rightarrow H + O^+ \tag{3}$$

can dominate radiative recombination

$$H^+ + e \rightarrow H + h\nu \tag{4}$$

in removing H^+. Protons are produced by direct ionization, by reaction (1) and by the reverse of reaction (2). The rate coefficients of reaction (3) and its reverse were taken from Field and Steigman (1972).

In diffuse clouds, the electrons are produced by ultraviolet photoionizations of elements such as carbon so that the proton density is directly proportional to the ionization rate ζ_0 s^{-1} per H_2 molecule. Then $n(D^+)/n(D)$ is proportional to ζ_0 and $n(D)$ to ζ_0^{-1}, $n(D^+)$ being determined in steady-state conditions by the measured ratio of $n(HD)$ to $n(H_2)$.

In the absence of H_2, reaction (3) is followed by its reverse (Field and Steigman 1972); but in the presence of H_2, the charge transfer to atomic oxygen initiates the sequence

$$O^+ + H_2 \rightarrow OH^+ + H, \tag{5}$$

$$OH^+ + H_2 \rightarrow H_2O^+ + H, \tag{6}$$

$$H_2O^+ + H_2 \rightarrow H_3O^+ + H \tag{7}$$

(cf. Herbst and Klemperer 1973). The recombinations of OH^+, H_2O^+, and H_3O^+ occur dissociatively. If hydrogen molecules are 100 times more abundant than electrons, the scheme (5), (6), and (7) proceeds rapidly toward the saturated molecular ion H_3O^+ with the eventual production of OH and H_2O.

The OH is destroyed by photodissociation and by the reactions

$$C^+ + OH \rightarrow CO + H^+, \tag{8}$$

$$O + OH \rightarrow O_2 + H. \tag{9}$$

Reaction (8) is another minor source of H^+. Details of the calculations will be presented elsewhere, but it is clear that the equilibrium abundance of OH is a measure of the density of H^+ and hence of the ionizing flux ζ_0 on which the efficiency of the deuterium fractionation (1) depends.

The chemical scheme outlined above is capable of producing OH faster at low temperatures than the endothermic process $O + H_2 \rightarrow OH + H$ suggested by Carroll and Salpeter (1966), and should generally be rather more efficient than formation on grains (Watson and Salpeter 1972*a*, *b*), by inverse predissociation (Julienne, Krauss, and Donn 1971), or by negative-ion reactions (Dalgarno and McCray 1973).

The results of detailed calculations are reproduced in table 1 for $\zeta_0 = 10^{-15}$ and 10^{-17}, for the cosmic element abundances $[H]:[O]:[C] = 1:6 \times 10^{-4}:3 \times 10^{-4}$,

TABLE 1

ζ OPH CLOUD*

PARAMETER	$\zeta_0 = 10^{-17}$			$\zeta_0 = 10^{-15}$		
	$d = 1$	$d = 3$	$d = 10$	$d = 1$	$d = 3$	$d = 10$
$T = 50°$ K:						
$n(\mathrm{OH})/n(\mathrm{H_2})$	3.6–9	1.0–8	2.3–8	3.5–7	8.9–7	1.6–6
[D]/[H]	1.5–4	5.2–5	1.8–5	1.7–6	7.9–7	5.3–7
$T = 100°$ K:						
$n(\mathrm{OH})/n(\mathrm{H_2})$	1.2–8	3.6–8	6.5–8	1.1–6	3.1–6	4.6–6
[D]/[H]	4.7–4	1.5–4	6.2–5	5.0–6	1.9–6	1.1–6

* Central densities: $n(\mathrm{H}) = 880\ \mathrm{cm}^{-3}$, $n(\mathrm{H_2}) = 1560\ \mathrm{cm}^{-3}$, $n(\mathrm{HD}) = 6.24 \times 10^{-4}\ \mathrm{cm}^{-3}$.

with [O] and [C] depleted by factors, *d*, of unity, 3, and 10, and for temperatures $T = 50°$ and 100° K. In all cases, HD is produced much more frequently by reaction (1) than by grain recombination and our conclusions are not affected by uncertainties in the relative efficiencies with which $\mathrm{H_2}$ and HD are formed in recombination.

Herbig (1968) has placed an upper limit of $8.3 \times 10^{13}\ \mathrm{cm}^{-2}$ on the column density of OH toward ζ Oph. If steady-state conditions apply, it follows that the penetrating ionizing flux in the cloud cannot exceed $5 \times 10^{-16}\ \mathrm{s}^{-1}$. Depletion of oxygen and carbon by a factor of 10 would decrease the upper limit to $9 \times 10^{-17}\ \mathrm{s}^{-1}$.

The cosmic abundance ratios [D]/[H] that we derive from the measured $n(\mathrm{HD})/n(\mathrm{H_2})$ ratio are presented in table 1. In the absence of depletion, [D]/[H] ranges from 1.7×10^{-6} to 1.5×10^{-4} as ζ_0 varies from 10^{-15} to 10^{-17} for $T = 50°$ and from 5.0×10^{-6} to 4.7×10^{-4} for $T = 100°$ K. $T = 100°$ K is probably more appropriate for the ζ Oph cloud.

The sensitivity to T is a result mainly of the temperature dependence of reaction (3). The rate coefficient of (3) is in any case uncertain, and the different limits can be regarded as a reflection of that uncertainty.

Regardless of depletion, the OH abundance limit implies the lower bound $[\mathrm{D}]/[\mathrm{H}] > 2.2 \times 10^{-6}$ for $T = 50°$ K and 2.0×10^{-5} for $T = 100°$ K. If we adopt as a minimum flux the value $\zeta_0 = 10^{-17}$ that results from high-energy cosmic rays (Spitzer 1968), we obtain the upper bounds $[\mathrm{D}]/[\mathrm{H}] < 1.5 \times 10^{-4}$ and 4.7×10^{-4}, respectively.

Depletion of carbon and oxygen below the solar abundance would decrease the derived ratio by somewhat more than the depletion factor. With the Doppler broadening parameter of $2.3\ \mathrm{km\ s}^{-1}$ obtained by Hobbs (1973) from high-resolution observations of the CH^+ line, the OAO absorption data (Morton *et al.* 1973) are consistent with a depletion factor that may be as small as 3. Thus we conclude that if steady-state conditions prevail and T is close to 100° K, $n(\mathrm{OH})/n(\mathrm{H_2}) > 3 \times 10^{-8}$ and $2 \times 10^{-5} < [\mathrm{D}]/[\mathrm{H}] < 2 \times 10^{-4}$. If the rate coefficient of reaction (3) is reduced by a factor of 10, these bounds are reduced by a factor of about 3.

The observations of Spitzer *et al.* (1973) show that $n(\mathrm{HD})/n(\mathrm{H_2})$ varies by a factor of 20 from region to region. If the deuterium abundance ratio and the penetrating ionizing flux are constant throughout the Galaxy, the observations may reflect local variations in the ultraviolet photon fluxes, in the total densities, and in the temperature. Calculations for other interstellar clouds are in progress. Measurements of the OH abundance in the clouds containing HD would be very instructive.

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