Revealing the Molecular Universe: One Antenna Is Never Enough
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D. C. Backer and J. L. Turner and J. M. Moran

The Distribution of Deuterium in the ISM: One Nucleon is Never Enough

T. G. Phillips and D. C. Lis

Downs Laboratory of Physics, California Institutue of Technology, Pasadena, CA

Abstract. The tendency for deuterium to be concentrated into the cold dense regions of the galaxy is due to the lower ground state energy of the heavier molecules. Such chemical fractionation leads to [D/H] values as high as 1! In turn this allows the detection of species such as ND_3, H_2D^+ and D_2H^+. The fraction of the interstellar medium (ISM) with such large deuteration is hard to estimate, but may be sufficient to cause both spatially variable and generally low [D/H] values in the diffuse ISM.

1. Introduction

The fractional abundance of deuterium is a parameter in theories of the evolution of the Universe, and is therefore of fundamental interest. The Galactic [D/H] value is usually measured by optical or UV spectroscopy in diffuse regions of the interstellar medium (ISM) near the Sun (generally within 1 or 2 kpc). However, spectroscopic observations of the ground-state of deuterium have shown that the distribution of this molecule in the dense ISM is quite inhomogeneous. In part, this may be due to varying astration rates on a galactic scale (10 kpc). However, observations also show an amazingly large variation on the scale of the size of molecular clouds (10 to 100 pc). In the cores of dark molecular clouds, where densities are large and temperatures low, the [D/H] ratio in the gas phase can reach unity! This implies that the [D/H] value may be low in the outer, diffuse parts of the clouds. We will describe some of the observations leading to this possible conclusion.

Simple molecules containing H or D are light and therefore rotate rapidly, with fundamental frequencies approaching the THz range. Figure 1 shows a cartoon spectrum, in the millimeter/submillimeter band, of a molecular cloud at 30 K (Phillips & Keene 1992). The "line forest" due to the rotation spectra of heavy molecules is replaced at shorter wavelengths by the fast rotating hydrides (and deuterides).

In order to observe the interstellar medium spectra at submillimeter wavelengths the effects of the Earth's atmosphere, which are mainly absorption by H_2O and O_2 lines, must be avoided. The atmospheric transmission from Mauna Kea and also from airplane altitude is shown in Figure 2. From Mauna Kea, in very good weather, zenith transmission in the atmospheric submillimeter "windows" can be ∼50%.

Telescopes for submillimeter wavelength spectroscopy have been sited on the volcanic mountain of the Big Island of Hawaii, Mauna Kea; e.g., the Caltech Sub-

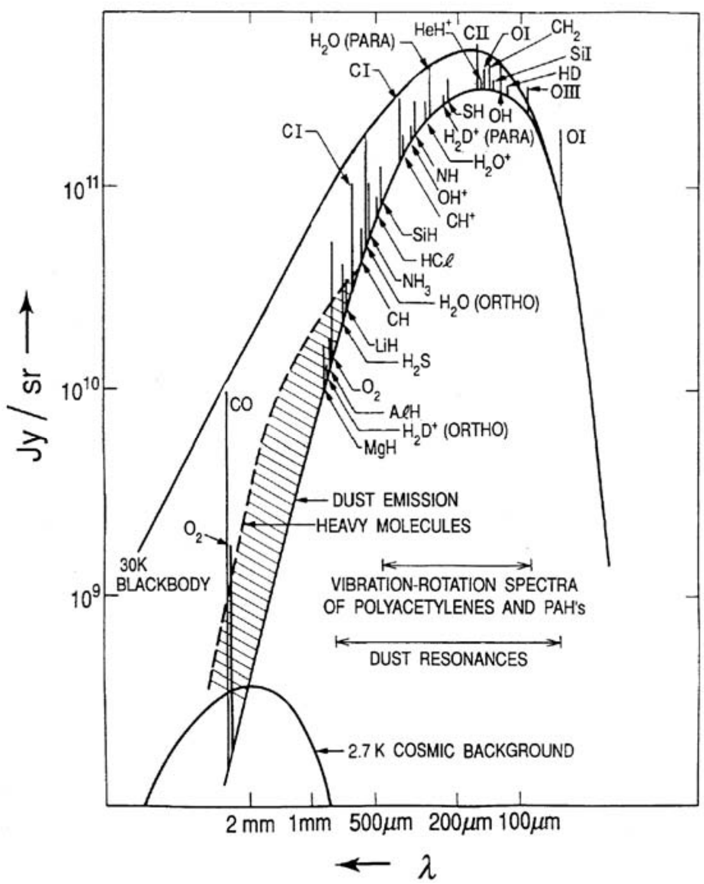

Figure 1. A cartoon view of the emission spectrum of a 30K ISM cloud, as it would appear if broadband high-resolution spectroscopy were possible throughout the submillimeter wavelength region (from Phillips & Keene 1992).

millimeter Observatory (CSO), the James Clerk Maxwell Telescope (JCMT) and the Smithsonian Submillimeter Array (SMA). The transmission from SOFIA, NASA's converted 747SP, is shown also in Figure 2. It is a lot better than from Mauna Kea, but the clearest view will be from space, employing the ESA/NASA satellite, Herschel. Figure 3 shows pictures of the CSO, SOFIA and Herschel. Together with the new European telescope APEX on the Atacama/Chajnantor plateau, they will provide a powerful capability in submillimeter spectroscopy, but at the moment only the CSO and JCMT are fully operational. In due course, the most powerful instrument will be the giant interferometer ALMA on the Atacama/Chajnantor plateau in Chile.

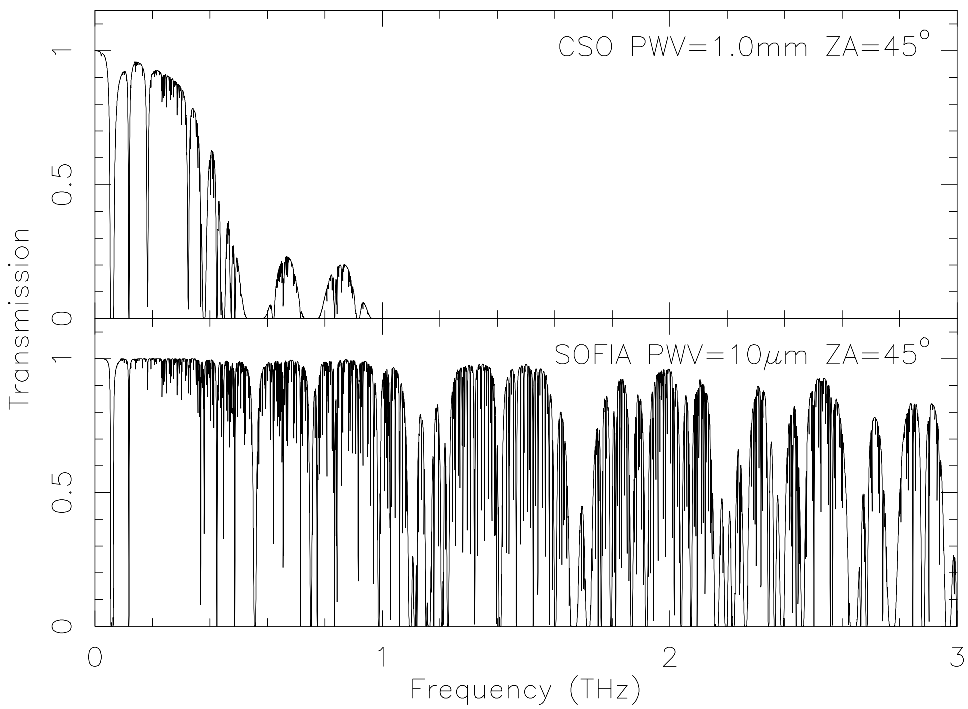

Figure 2. Atmospheric transmission throughout the submillimeter band from Mauna Kea and a high-altitude airplane, with partial pressures of water vapor of (top) λ 1mm and (bottom) λ 10μm, respectively.

2. Deuterium in Molecules

Since the original detection of the rotation transitions of HCN and DCN (Jefferts, Penzias & Wilson 1973) in the dense interstellar medium, it has become clear that the [D/H] value is considerably increased compared to the consensus value of 1.5×10^{-5} (Linsky 1998) for the dense ISM. By now nearly 30 deuterated species have been detected in the dense ISM, as shown in Table 1. The reason for the increase in [D/H] is known to be the tendency for the molecular system to minimize its free energy, so that in the cold dense regions reactions leading to the substitution of H by D in molecules are preferred compared to the reverse (Solomon & Woolf 1973). The basic chemical reaction scheme is as follows:

$$\mathrm{H^+ + D \Longleftrightarrow H + D^+},$$

$$\mathrm{D^+ + H_2 \Longleftrightarrow HD + H^+ + \Delta E_1},$$

$$\mathrm{D^+ + HD \Longleftrightarrow D_2 + H^+ + \Delta E_2}.$$

An H_2 molecule is very light and vibrates rapidly. The ground state is considerably higher in energy than that of the HD (Fig. 4), so the second reaction above will proceed to the right. Thus, initially, most of the D will be in the

Figure 3. From the bottom, clockwise: Caltech Submillimeter Observatory (CSO), Herschel Space Observatory (HSO), and Stratospheric Observatory for Infrared Astronomy (SOFIA).

form of HD, in the cold, dense regions. In the ion-molecule reaction scheme, the abundant ion is H_3^+ and the reaction

$$H_3^+ + HD \Longleftrightarrow H_2D^+ + H_2 + \Delta E_a$$

proceeds again to the right.

Table 1. Deuterated molecules detected in the ISM.

HD	DCN	CH_3OD	CH_2DCCH
H_2D^+	DNC	CH_2DOH	CH_3CCD
D_2H^+	C_2D	CHD_2OH	HDCS
NH_2D	DCO^+	CD_3OH	D2CS
ND_2H	N_2D^+	HDS	C_4D
HDO	HDCO	D_2S	DC_3N
ND_3	D_2CO	CH_2DCN	DC_5N

However, in most of the ISM the H_3^+ abundance is limited by reaction with other molecules, such as CO, which are abundant, e.g.,

$$H_3^+ + CO \Longleftrightarrow HCO^+ + H_2 \quad \text{and}$$

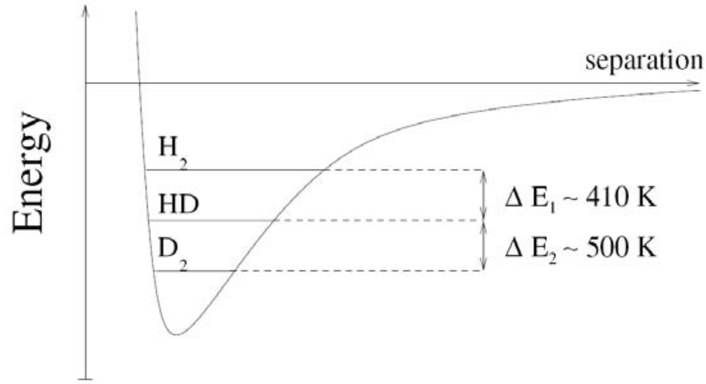

Figure 4. H_2, HD, and D_2 potential energy diagram (from Phillips & Vastel 2003).

$$H_2D^+ + CO \Longleftrightarrow DCO^+ + H_2.$$

Thus, the deuteration moves into heavy molecules and the H_2D^+ abundance is limited. The role of dust grains must also be considered since it is known that many molecules will condense out on the grains and will be depleted in the cold dense regions. The most abundant trace molecule, CO, is shown to be depleted in such extreme regions by factors of 10 or more (Bacmann et al. 2002). Phillips & Vastel (2003) noted that in regions with depleted CO, HD becomes the most abundant trace molecule, and the H_3^+ reaction chain should include D_2H^+ and D_3^+:

$$H_3^+ + HD \Longleftrightarrow H_2D^+ + H_2 + \Delta E_a,$$

$$D_2H^+ + HD \Longleftrightarrow D_2H^+ + H_2 + \Delta E_b,$$

$$H_2D^+ + HD \Longleftrightarrow D_3^+ + H_2 + \Delta E_c.$$

Roberts, Herst & Millar (2003) included those higher deuteration species in their calculations and found that the gas phase of the cold regions becomes even more deuterium rich, with [D/H] in the gas phase approaching unity.

3. Multiply Deuterated Molecules

As seen in Table 1, cases of double deuteration (ND_2H, D_2CO, CHD_2OH, D_2S) exist, but it was the triply deuterated case of ND_3 (also CD_3OH) that brought home the extraordinary situation of the presence of molecules of normally 10^{-15} abundance relative to their hydrogenated parent. Figure 5 shows the first detection of ND_3 in Barnard 1, including the nitrogen hyperfine structure (Lis et al. 2002).

The natural extension of the basic chemistry to the abundant deuterium case leads to the presence of D_2, D_2H^+ and D_3^+. As for H_2 and H_3^+, the species

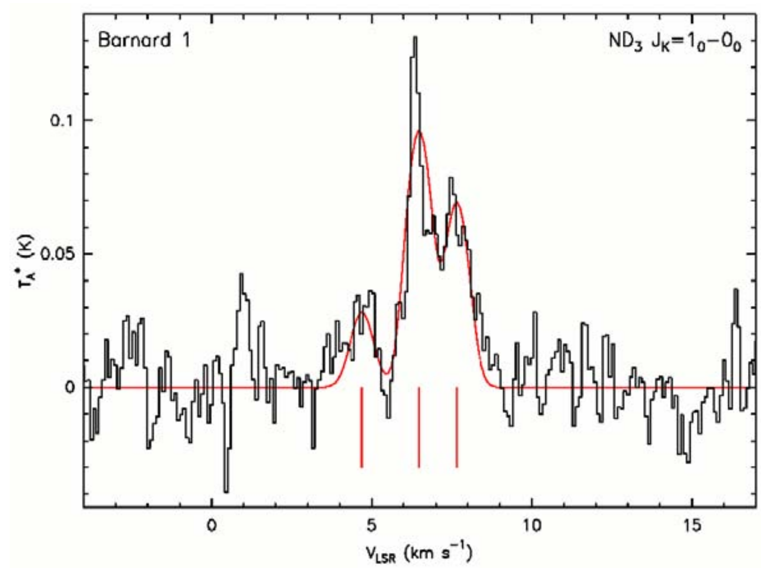

Figure 5. Detection of ND_3 in the Barnard 1 cloud (from Lis et al. 2002).

D_2 and D_3^+ cannot be observed in pure rotational spectroscopy because they are symmetric and have no dipole moment. However, D_2H^+, like H_2D^+, has allowed transitions in the submillimeter band. Therefore the detection of $H_2D_3^+$ was a test of the Roberts et al. model. The potential energy level diagram for H_3^+ isotopic variants is shown in Figure 6. The ground state ortho transition of H_2D^+ is now routinely observed at 372 GHz. The equivalent transition of D_2H^+ is the 692-GHz, ground state para line. However, the precise frequency was not known. This was quickly remedied by Hirao & Amano (2003) who provided the relevent frequency from their lab spectroscopy system. A detection of the 692 GHz line in the cold dense ISM followed immediately (Vastel, Phillips & Yoshida 2004). Spectra of H_2D^+ and D_2H^+ in Lynds 1689N are shown in Figure 7.

4. Consequences of Inhomogeneous Deuterium Distribution

The accepted values of [D/H] are obtained primarily from UV absorption spectroscopy of foreground diffuse gas in the Milky Way, using satellites (IUE, EUVE, HST, FUSE, and Copernicus), giving values of $\sim 1.5\times10^{-5}$ (Linsky 1998; Moos et al. 2002). However, considerable dispersion exists in such measurements (Steigman 2003), with published values varying from 5×10^{-6} to 4×10^{-5}. Most measurements are for sources at distances extending from 100 pc to 500 pc from the Sun, but a recent FUSE case includes one at ∼2 kpc (Hoopes et al. 2003). [D/H] ratios measured in high-redshift systems also show large dispersion (e.g., Tytler et al. 1999). It is accepted that deuterium is produced during the Big Bang, and it is generally believed that, since the Big Bang, deuterium has been destroyed, but not created, in the nuclear reactions occurring in stars. There are calculations of the effect of nuclear burning on [D/H] values, but it is argued

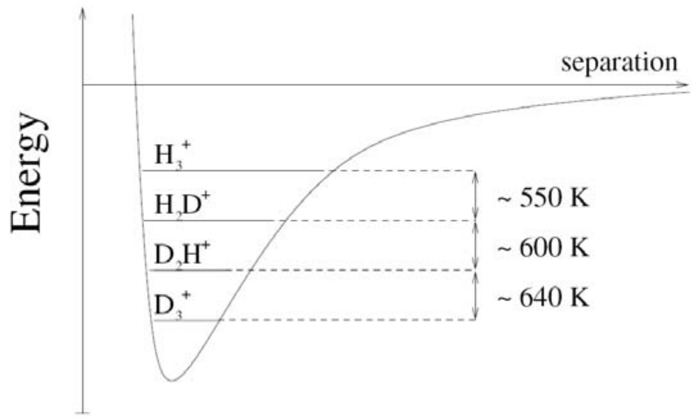

Figure 6. Potential energy diagram for H_3^+ isotopologues (from Phillips & Vastel 2003).

that this does not explain the measured dispersion (Vidal-Madjar 2000; Fields et al. 2001).

The unexpected variation between lines of sight could be due to the proximity to cold, dense regions. Also, if it turns out that the effect is significant, increasing the cosmic value of [D/H] would decrease the baryon density (Fig. 8).

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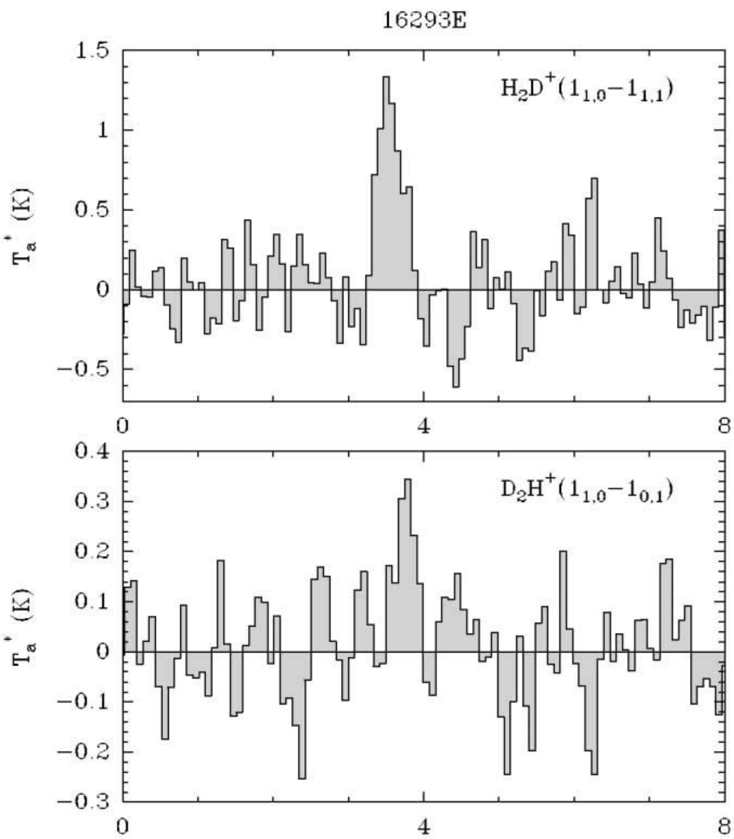

Figure 7. H_2D^+ and D_2H^+ spectra in Lynds 1689N (from Phillips & Vastel 2003).

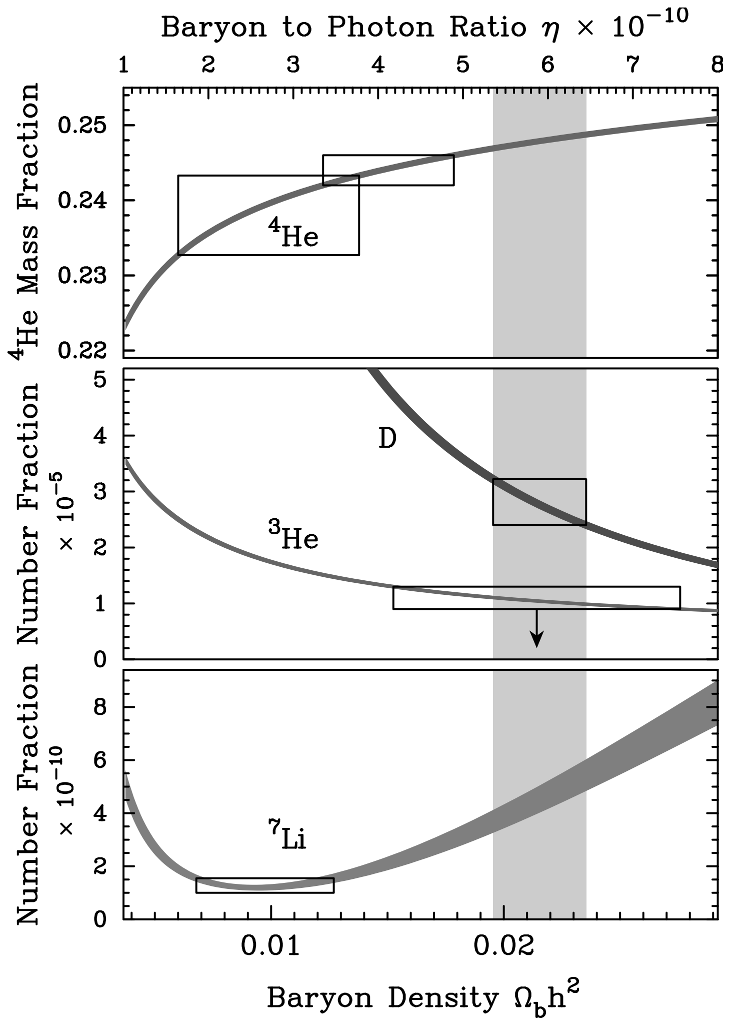

Figure 8. Predicted and measured abundances of the light nuclei as a function of baryon density (from Kirkman et al. 2003). Boxes mark measurements and uncertainties, while the gray strip mark the predicted value based primarily on the deuterium abundance.