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Measuring interstellar gas-phase D/H ratios in the presence of H_2 *(Research Note)*

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ABSTRACT

Aims. To clarify the circumstances under which it is acceptable to approximate the interstellar gas-phase D/H ratio by D I/H I.
Methods. Observed column densities of H I, D I, H_2 and HD are compared for six lines of sight having appreciable fractions of H_2.
Results. The overall fraction of deuterium in HD varies by a factor 3−4 but is found to be much smaller than the fraction of H in H_2 in all cases, implying that deuterium appears as D I and N(D I)/N(H I) exceeds the gas-phase D/H ratio in H_2-bearing gas.
Conclusions. Deuterium in H_2-bearing gas contributes to the observed D I absorption and the D/H ratio should be inferred from N(D)/N(H) where $N(\mathrm{D}) = (N(\mathrm{D\ I}) + N(\mathrm{HD}))$, $N(\mathrm{H}) = N(\mathrm{H\ I}) + 2N(\mathrm{H_2})$: failure to do so biases the resulting D/H ratio upward, typically by 5%−15% in present data. Along sightlines with multiple kinematic components having different molecular fractions, fractionation can cause velocity differences between D I and H I profiles. Shifts between H_2 and HD velocity centroids may arise when the molecule-bearing gas has kinematic substructure reflecting regions of different ionization balance and HD/H_2 ratios.

Key words. ISM: abundances – ISM: atoms – ISM: molecules

1. Introduction

Measurements of the primordial D/H ratio provide important constraints on Big-Bang nucleosynthesis, and measurements of the local interstellar gas phase D/H ratio $(\mathrm{D/H})_g$ provide useful information on galactic structure and chemical evolution. It is now found that $(\mathrm{D/H})_g = 1.5\times10^{-5}$ in the Local Bubble of hot gas surrounding the Sun, about half the primordial D/H value (Moos et al. 2002; Linsky 1998), but still somewhat larger than $(\mathrm{D/H})_g$ measured over longer lines of sight extending several hundred pc from the Sun. A summary of extant $(\mathrm{D/H})_g$ measurements illustrating this effect has recently been given by Wood et al. (2004) and a further example is given by Hébrard et al. (2005). The H I column density-weighted mean D I/H I ratio seen over lines of sight longer than 300 pc is 0.86×10^{-5} in the compilation of Wood et al. (2004).

As longer lines of sight are employed to reach more distant gas in studies of the D/H ratio (Hoopes et al. 2003; Wood et al. 2004; Hébrard et al. 2005; Williger et al. 2005) it is inevitable that the hydrogen column density N(H) will grow and the fraction of H-nuclei in molecular form will be larger. With the notable exception of the work of Williger et al. (2005) it is the practice at present to assert that $(\mathrm{D/H})_g = N(\mathrm{D\ I})/N(\mathrm{H\ I})$, ignoring both the deuterium and the hydrogen in the "molecular" gas. However this should not be the case. Observationally it can be shown that a much smaller overall fraction of gas-phase deuterium is incorporated in HD than hydrogen in H_2, implying that gas-phase deuterium remains mostly in the form of D I (i.e., not HD) in the diffuse ISM no matter the local fraction of H_2 (for a theoretical treatment, see Le Petit et al. 2002). In this case, D I in the H_2-bearing regions contributes a fraction of the total observed D I absorption column which is approximately equal to the overall fraction of H-nuclei in H_2, $F_{H_2} = 2N(\mathrm{H_2})/N(\mathrm{H}) = 2N(\mathrm{H_2})/(N(\mathrm{H\ I}) + 2N(\mathrm{H_2}))$, while H I in the H_2-bearing gas contributes a fraction $F_{H_2} \times (1 - F_{H_2})$ of the absorbing H I. Therefore one should take $(\mathrm{D/H})_g = N(\mathrm{D})/N(\mathrm{H})$, where $N(\mathrm{D}) = N(\mathrm{D\ I}) + N(\mathrm{HD})$, representing all of the hydrogen and deuterium (see Williger et al. 2005) although even the *ansatz* $(\mathrm{D/H})_g = N(\mathrm{D\ I})/N(\mathrm{H})$ is an improvement.

Within H_2-bearing gas it is the case that $N(\mathrm{D\ I})/N(\mathrm{H\ I}) \approx (\mathrm{D/H})_g/(1 - f_{H_2})$ (f_{H_2} is the local H_2-fraction $2n(\mathrm{H_2})/n(\mathrm{H})$) which is an arithmetic restatement of the claim that the fraction of D in HD is so much smaller than that of H in H_2. This fractionation of the atomic component of the H_2-bearing gas can induce shifts between the H I and D I gas velocity centroids along lines of sight with multiple kinematic components having different f_{H_2}. If the contribution of the H_2-bearing gas were to be isolated, the fractionation could give the misleading impression of a too-large D/H ratio if it were to be asserted that $(\mathrm{D/H})_g = N(\mathrm{D\ I})/N(\mathrm{H\ I})$.

In Sect. 2 we review extant observations of H_2, HD, D I and H I in order to define the circumstances under which the contribution of H_2-bearing gas to measured $N(\mathrm{D\ I})/N(\mathrm{H\ I})$ ratios may safely be neglected. In fact, this is permissible only when $N(\mathrm{H_2}) \ll N(\mathrm{H\ I})$, which is true only for smaller values of the hydrogen column density $N(\mathrm{H\ I}) < 1.4 \times 10^{20}\ \mathrm{cm^{-2}}$. Otherwise, there will be a perceptible effect on the measured $(\mathrm{D/H})_g$ ratios, which are biased *upward* when the contribution of the H_2-bearing gas is *neglected*: Sect. 2 assesses the magnitude of the bias along the lines of sight recently discussed by Hoopes et al. (2003), Wood et al. (2004), Hébrard et al. (2005) and Williger et al. (2005). Section 3 is a brief summary, but the result of our discussion is simple: to obtain accurate values for $(\mathrm{D/H})_g$, either avoid observing H_2-bearing gas or measure and fully include its contribution.

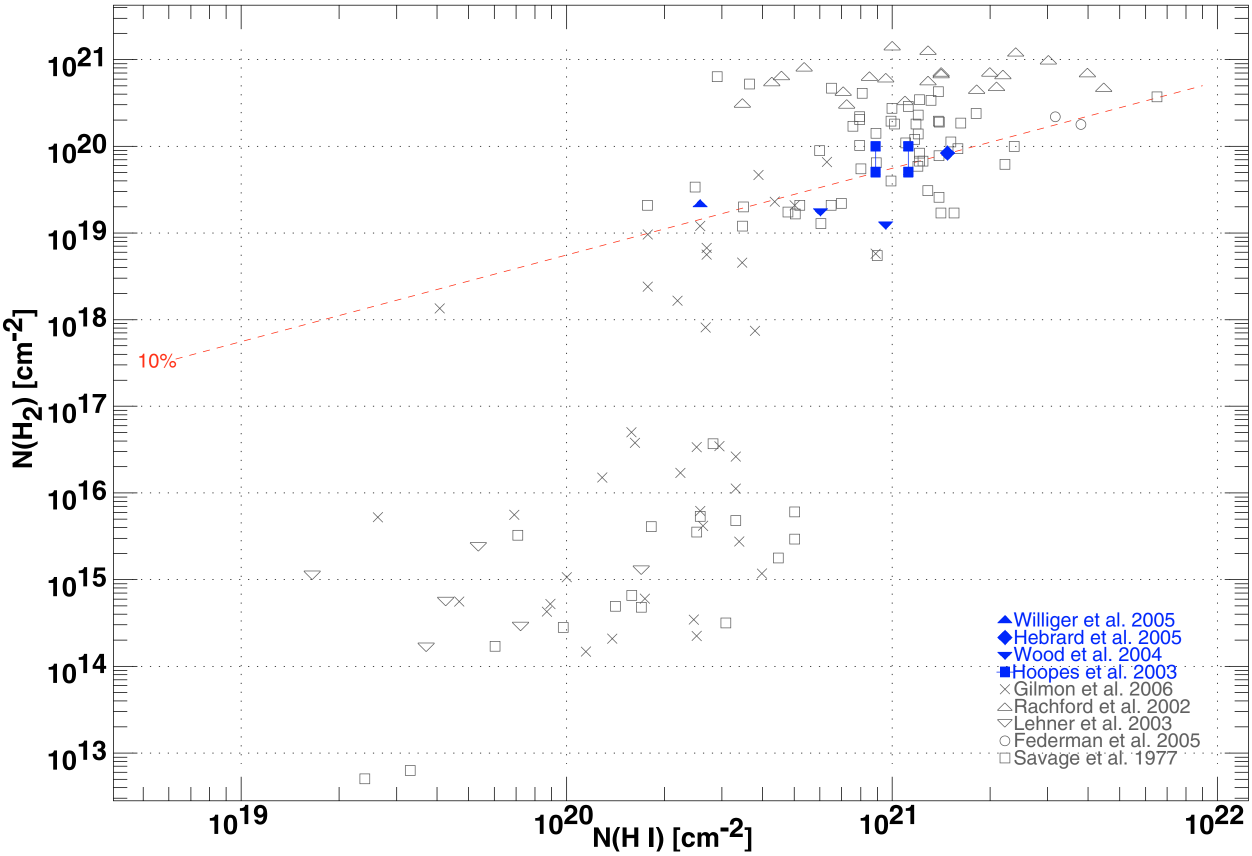

Fig. 1. Column densities of interstellar atomic and molecular hydrogen from various references as noted. Lines of sight with appreciable $N(H_2)$ and used for D/H measurements are shown as solid symbols: Hoopes et al. (2003) provided only a range of $N(H_2) = 0.5{-}1.0 \times 10^{20}$ cm^{-2} along two lines of sight. A dashed (red) line indicates where $N(H_2) = 0.1\ N(\text{H I})$.

2. Does H_2-bearing gas matter to measurements of D I/H I?

We first ask under what conditions it is unassailably correct to equate $(\text{D/H})_g = N(\text{D I})/N(\text{H I})$ in neutral gas, neglecting the possible contribution of regions having a substantial fraction of H-nuclei in molecular form. The most obvious of these would be for sightlines with negligible amounts of H_2-bearing gas. Until recently this was the case as may be seen by comparing the lines of sight tabulated by Wood et al. (2004) against the references to measurements of $N(H_2)$ cited in Fig. 1. This figure shows the run of $N(H_2)$ with $N(\text{H I})$ along most of the lines of sight where both of these have been measured. Lines of sight studied independent of considerations of the D/H ratio are shown as grayed open symbols and crosses (Savage et al. 1977; Rachford et al. 2002; Lehner et al. 2003; Federman et al. 2005; Gillmon et al. 2006).

The molecular fraction is low near the Sun, or in general when $N(\text{H}) \approx N(\text{H I}) < 1.4 \times 10^{20}$ cm^{-2}. The regime $N(\text{H I}) = 2{-}4 \times 10^{20}$ cm^{-2} is a transition region with both low and high $N(H_2)$. For $N(\text{H I}) > 4 \times 10^{20}$ cm^{-2} it is relatively rare to encounter lines of sight having $F_{H_2} < 5{-}10\%$ and measurements of $(\text{D/H})_g$ at such $N(\text{H I})$ must consider whether the deuterium in H_2-bearing gas makes an appreciable contribution to $N(\text{D I})$. The longer lines of sight recently studied in the context of measuring $(\text{D/H})_g$ are shown in Fig. 1 as the solid symbols (Hoopes et al. 2003; Wood et al. 2004; Hébrard et al. 2005; Williger et al. 2005). These lines of sight have H_2 column densities near the lower end of the observed range at their measured $N(\text{H I})$, but can hardly be said to be atypical and have F_{H_2} in the range 3–22%.

As noted by Savage et al. (1977) and Rachford et al. (2002) the H_2 column density-weighted mean kinetic temperature in H_2-bearing gas is 70–80 K, implying that it is not very dense unless it is highly over-pressured. That is, for values of the mean thermal pressure $\langle p/k \rangle = 2 \times 10^3$ cm^{-3} K (Jenkins & Tripp 2001; Jenkins 2002), the inferred density $p/k/75$ K $= 30$ cm^{-3} is not large. Equilibrium models of H_2-formation in the diffuse ISM have absolutely no need for high densities or anything beyond typical values of p/k in order to reproduce the run of $N(H_2)$ with $N(\text{H})$, as illustrated in Fig. 8 of Liszt & Lucas (2000). Thus the H_2 seen along diffuse and translucent lines of sight is not obviously sequestered into dense knots having $f_{H_2} \approx 1$, within which it might possibly be assumed that all of the H and D is in the form of H_2 and HD. In any case direct measurement shows that the deuterium remains mostly in atomic form even in H_2-bearing regions, as we now discuss.

Figure 2 summarizes available measurements of $N(\text{HD})$ from the recent comprehensive treatment of Lacour et al. (2005) and the D/H studies noted above. The typical HD/H_2 ratio is somewhat larger than had previously been believed (Liszt 2003) following an upward revision of older results, but in general $1.5 \times 10^{-6} < N(\text{HD})/N(H_2) < 5 \times 10^{-6}$. In a gas with the same fractions of D- and H-nuclei in molecular form, $N(\text{HD})/N(H_2) = 2(\text{D/H})_g \approx 1.5{-}3.0 \times 10^{-5}$ depending on whether the distant (lower) or nearer $(\text{D/H})_g$ ratio is relevant.

The HD observed in diffuse gas arises from prompt gas-phase fractionation of H_2 formed slowly on grains (Black & Dalgarno 1973; Jura 1974; Le Petit et al. 2002; Liszt 2003)

Table 1. Abundance ratios and log column densities[1].

Source	N(H I)	N(D I)	$N(H_2)$	N(HD)	N'(D I)[6]	N(D I)/N(H I) 10^{-5}	N(D)/N(H) 10^{-5}
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)
HD 191877[2]	21.05(0.05)	15.94(0.08)	19.7–20.0	14.47	14.7–15.4	$0.78^{+.26}_{-.13}$	0.68–0.74
HD 195965[2]	20.95(0.03)	15.88(0.07)	19.7–20.0	14.38	14.7–15.4	$0.85^{+.17}_{-.12}$	0.72–0.79
JL 9[3]	20.78(0.05)	15.78(0.06)	19.25(0.02)	[13.43–13.95]	14.3–14.7	1.00 ± 0.19	0.95–0.96
LS1274[3]	20.98(0.04)	15.86(0.09)	19.10(0.02)	[13.28–13.80]	14.1–14.6	0.76 ± 0.18	0.74–0.75
HD 90087[4]	21.17(0.05)	16.16(0.12)	19.92(0.02)	14.52(0.06)	15.0–15.3	0.98 ± 0.19	0.88
PG0038+199[5]	20.41(0.04)	15.75(0.04)	19.33(0.02)	13.95(0.05)	14.4–14.7	$2.19^{+.30}_{-.27}$	$1.91^{+.26}_{-.24}$

[1] Figures in parenthesis are approximate 1σ errors, see original references for more precise values; [2] data from Hoopes et al. (2003); [3] data from Wood et al. (2004); [4] data from Hébrard et al. (2005) who quote $(D/H)_g = N$(D I)/N(H I) but also measured N(D)/N(H); [5] data from Williger et al. (2005) who quote $(D/H)_g = N$(D)/N(H); [6] lower bound for the likely D I contribution from H_2-bearing gas $N'(\mathrm{D\ I}) = 2N(H_2) \times (D/H)_g - N(\mathrm{HD})$.

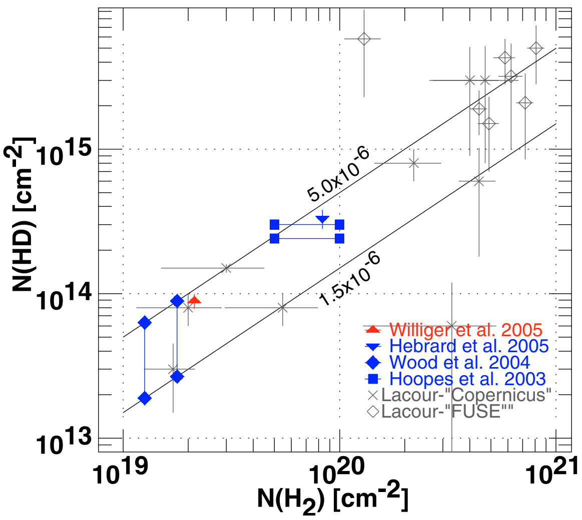

Fig. 2. Measurements of H_2 and HD. Values derived by Lacour et al. (2005) along new ("FUSE") and previously-studied ("Copernicus") lines of sight are shown as grayed symbols. The HD-measurements and H_2-estimates of Hoopes et al. (2003) are shown as solid rectangles. The likely ranges of N(HD) given the values of $N(H_2)$ along two lines of sight studied by Wood et al. (2004) are shown as filled, connected diamonds.

and in principle the fraction of D in HD could be smaller or larger than the fraction of H in H_2 in the H_2-bearing region (the latter for $f_{H_2} < 1$ of course). Observationally, however, the fraction of deuterium in HD is always small enough that most of the deuterium in the H_2-bearing region remains in the form of D I: in Fig. 2, $N(\mathrm{HD})/N(H_2) \lesssim 0.5 \times 10^{-5} < 2\ (D/H)_g = 1.5–3.0 \times 10^{-5}$. Conservation of nuclei then requires that $N(\mathrm{D\ I})/N(\mathrm{H\ I}) \approx (D/H)_g/(1 - f_{H_2}) > (D/H)_g$ in the H_2-bearing regions, which is discussed further in Sect. 3.

In Fig. 2 we have included the measurements of N(HD) and estimates $N(H_2) = 0.5–1.0 \times 10^{20}$ cm^{-2} for the two long lines of sight with D I/H I ratios measured by Hoopes et al. (2003): they appear to be typical in the HD-H_2 plane, as they were when comparing H_2 and H I (Fig. 1). The deuterium column expected to be associated with these H_2 column densities varies from a minimum of $2 \times 0.75 \times 10^{-5} \times 5 \times 10^{19}/f_{H_2}$ cm^{-2} assuming the lower value of $N(H_2)$ and $(D/H)_g = 0.75 \times 10^{-5}$, to a value four times larger for the larger $N(H_2)$ and $(D/H)_g$ typical of nearer gas (despite the long line of sight one does not know where the H_2-bearing gas is, if indeed it is highly localized). That is, $N(\mathrm{D}) = 0.75/f_{H_2}–3.0/f_{H_2} \times 10^{15}$ cm^{-2} for the H_2-bearing gas compared to measured values of $N(\mathrm{HD}) = 0.24–0.30 \times 10^{15}$ cm^{-2} and D I column densities $N(\mathrm{D\ I}) = 8–9 \times 10^{15}$ cm^{-2}. The implication is that the deuterium in the H_2-bearing gas has contributed meaningfully to the observed N(D I), so that the hydrogen column density in the H_2-bearing gas should also be included when the D/H ratio is calculated.

The range of N(HD) expected for the two sources observed by Wood et al. (2004) is illustrated in Fig. 2 but Table 1 contains a quantitative estimate of the effects considered here and forms the basis for our continued discussion. Columns 2–4 repeat the measurements and estimates of N(H I), N(D I) and $N(H_2)$ from the original references. For N(HD) in Col. 5 the table shows the measurements of Hoopes et al. (2003), Hébrard et al. (2005) and Williger et al. (2005) and in square brackets, estimates $N(\mathrm{HD}) = 1.5–5.0 \times 10^{-6}\ N(H_2)$ based on the results shown in Fig. 2. The quantity $N'(\mathrm{D\ I}) = 2N(H_2) \times (D/H)_g/f_{H_2} - N(\mathrm{HD})$, tabulated in column 6 for $f_{H_2} = 1$, is an estimate of the least amount of D I in the H_2-bearing gas, which can be compared with the measured N(D I) but is not used to estimate $(D/H)_g$. Column 7 repeats the values N(D I)/N(H I) of the original references (but quoting 1σ errors); in all references except Williger et al. (2005) the values in Col. 7 were taken equal to $(D/H)_g$. Column 8 shows the values $(D/H)_g = N(\mathrm{D})/N(\mathrm{H})$ calculated with the values tabulated, including the contributions N(HD) and $2N(H_2)$ to the total deuterium and hydrogen gas columns.

Comparing Cols. 7 and 8 in Table 1 one sees that the estimated bias is quite perceptible – 5–15% lower values for $(D/H)_g$ in most cases – and for HD 195965, perhaps even slightly beyond the 1σ range of the original measurement. As noted above, the overall H_2-fractions range from 3% to 22%. The ratios N(HD)/N(D I) are somewhat smaller, 0.2%–3%: therefore even taking the ratio N(D I)/N(H), neglecting N(HD), is a much better approximation to $(D/H)_g$ than is N(D I)/N(H I).

3. Summary and discussion

We showed that deuterium remains mostly in atomic form even in H_2-bearing regions, and, therefore, that measured values of N(D I) contain a non-neglible contribution from H_2-bearing gas whenever the fraction of hydrogen nuclei in H_2 is non-negligible. Along six longer lines of sight with recently-measured gas-phase D/H ratios $(D/H)_g$ and overall molecular fractions F_{H_2} = 3%–22%, we estimated that the true $(D/H)_g$ are lower than reported $(D/H)_g = N(\mathrm{D\ I})/N(\mathrm{H\ I})$ by as much as 15%, which in one case exceeds the 1σ error of measurement.

The effects demonstrated here for lines of sight having overall H_2-fractions which are low to moderate at the given N(H I) are unlikely to be negligible whenever $N(\mathrm{H\,I}) > 4 \times 10^{20}$ cm^{-2} and should be considered whenever $N(\mathrm{HI}) > 1.4 \times 10^{20}$ cm^{-2} (Fig. 1). To reckon the distances over which such H I columns will accumulate, note that lines of sight chosen for *uv* absorption tend to have lower than average mean densities, for instance see the discussion of biases against H_2-bearing gas in the original *Copernicus* H_2 survey of Savage et al. (1977): they found $\langle F_{H_2} \rangle = 0.17$, representing a possible 15% bias in measurements of $(D/H)_g$ at a sample mean density 0.35 cm^{-3}. At this density, $N(\mathrm{H\,I}) = 10^{20}$ cm^{-2} corresponds to a distance of 93 pc.

The lines of sight chosen for studies of the D/H ratio have had lower mean densities yet, 0.08 cm^{-3}, 0.04 cm^{-3}, and 0.19 cm^{-3} for sample distances of <10 pc, 10–100 pc and >100 pc, respectively, for the data tabulated by Wood et al. (2004). Thus, the use of short and/or low-density lines of sight has generally protected *uv* absorption studies of the interstellar D/H ratio from the influence of H_2-bearing gas until quite recently. However, when higher H_2-fractions are encountered their contribution must not be dismissed.

One detail of the inferred predominance of D I in diffuse H_2-bearing regions is that $N(\mathrm{D\,I})/N(\mathrm{H\,I}) \approx (D/H)_g/(1 - f_{H_2}) > (D/H)_g$ where f_{H_2} is the local molecular fraction: this is an unavoidable consequence of conservation of nuclei. Clearly, a generally-applicable value for $(D/H)_g$ can not be inferred from $N(\mathrm{D\,I})/N(\mathrm{H\,I})$ found in the contributions of H_2-bearing regions. Moreover, along lines of sight having multiple kinematic components this fractionation of the atomic gas is capable of displacing the velocity centroids of H I and D I gas columns. Wood et al. (2004) found such a shift toward JL 9.

We stress that the ratio $n(\mathrm{HD})/n(H_2)$ is determined in situ by ionization balance and resulting chemical fractionation in diffuse gas, (Black & Dalgarno 1973; Le Petit et al. 2002), because possible differences in the proton density exceed by far the factor of two variations in local $(D/H)_g$: $N(\mathrm{HD})$ does not reflect the rate of formation of HD on grains because essentially all of that HD is promptly photodissociated. The variability in $N(\mathrm{HD})/N(H_2)$ seen in Fig. 2 could also cause displacements between HD and H_2 velocity centroids when kinematic substructure is present along a single line of sight. Velocity shifts have already been noted in two cases (Wood et al. 2004; Hébrard et al. 2005). Last we note that it is common to measure O I column densities when studying $(D/H)_g$ and occasionally to infer or check $(D/H)_g$ from measured $N(\mathrm{D\,I})/N(\mathrm{O\,I})$ and an assumed a value for $(O/H)_g$, as the latter is seen to vary relatively little (Moos et al. 2002; Cartledge et al. 2004). Oxygen remains as O I in diffuse H_2-bearing gas and $N(\mathrm{D\,I})/N(\mathrm{O\,I})$ ratios do not suffer from the strongest of the effects discussed here (see Fig. 4 of Cartledge et al. 2004). However, when H_2-bearing gas is present, asserting $(O/H)_g = N(\mathrm{O\,I})/N(\mathrm{H\,I})$ incurs the same degree of bias as $(D/H)_g = N(\mathrm{D\,I})/N(\mathrm{H\,I})$.

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