SPITZER OBSERVATIONS OF HYDROGEN DEUTERIDE

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ABSTRACT

We report the detection of interstellar hydrogen deuteride (HD) toward the supernova remnant IC 443, and the tentative detection of HD toward the Herbig-Haro objects HH 54 and HH 7 and the star-forming region GGD 37 (Cep A West). Our detections are based upon spectral line mapping observations of the R(3) and R(4) rotational lines of HD, at rest wavelengths of 28.502 and 23.034 μm, respectively, obtained using the Infrared Spectrograph on board the Spitzer Space Telescope. The HD R(4)/R(3) line intensity ratio promises to be a valuable probe of the gas pressure in regions where it can be observed. The derived HD/H₂ abundance ratios are (1.19^{+0.35}_{-0.25}) × 10^{-3}, (1.80^{+0.54}_{-0.32}) × 10^{-3}, and (1.41^{+0.46}_{-0.33}) × 10^{-3}, respectively (68.3% confidence limits, based upon statistical errors alone) for IC 443 (clump C), HH 54, and HH 7. If HD is the only significant reservoir of gas-phase deuterium in these sources, the inferred HD/H₂ ratios are all consistent with a gas-phase elemental abundance [n_D/n_H]_gas ∼ 7.5 × 10^{-6}, a factor of 2–3 below the values obtained previously from observations of atomic deuterium in the Local Bubble and the Galactic halo. However, similarly low gas-phase deuterium abundances have been inferred previously for molecular gas clouds in the Orion region and in atomic clouds along sight lines within the Galactic disk to stars more distant than 500 pc from the Sun.

Subject headings: ISM: abundances — ISM: clouds — ISM: molecules — molecular processes

Online material: color figure

1 INTRODUCTION

With a cosmic abundance of more than 10^{-5}, deuterium is more common than all but a half-dozen heavy elements. The initial deuterium abundance was set by primordial nucleosynthesis (see, e.g., Schramm & Turner 1998), roughly 100 s after the Big Bang, and has been reduced by stellar nuclear reactions over the subsequent 13.7 Gyr. The primordial deuterium abundance revealed from intergalactic absorption components (e.g., Kirkman et al. 2003, who obtained [D/H] = 2.78^{+0.44}_{-0.30} × 10^{-3} toward Q1243+3047) is in good agreement with models for primordial nucleosynthesis, given the baryon densities derived independently from an analysis of the cosmic microwave background (e.g., Spergel et al. 2003). Thus, the distribution of deuterium in the Galaxy probes both stellar processing and the degree to which material is mixed efficiently within the interstellar medium. The abundance of interstellar deuterium has been measured primarily by ultra violet absorption-line observations of atomic deuterium within diffuse clouds (reviewed by Moos et al. 2002). Recent measurements of the Galactic deuterium abundance reveal significant variations [over the range ∼(0.7–2.2) × 10^{-3}] that are inconsistent with current predictions from Galactic chemical evolution models (e.g., Wood et al. 2004; Friedman et al. 2006; references therein); understanding the nature of these inconsistencies is critical to our understanding of chemical evolution within the Galaxy.

While deuterium has been extensively studied in atomic clouds, its abundance in molecular clouds is less certain. In diffuse molecular clouds, interstellar hydrogen deuteride (HD) has been widely observed by means of UV spectroscopy—starting over 30 years ago with the Copernicus satellite (reviewed by Spitzer & Jenkins 1975)—and is the most abundant D-bearing molecule. However, deriving the deuterium abundance from the HD column in diffuse clouds is difficult for several reasons: the chemistry is complex, HD contains only a trace amount of D, and the HD abundance is sensitive to the density and UV field in the cloud (Lacour et al. 2005; Le Petit et al. 2002).

In dense molecular clouds, by contrast, the observations are much fewer. Prior to the results reported here, detections of HD emissions had been reported toward just one cloud: the Orion molecular cloud (Wright et al. 1999; Howat et al. 2002; Bertoldi et al. 1999; the latter’s detection of HD from warm shocked gas had been anticipated theoretically by Tiemann (1996)). In addition, HD R(0) line absorption has been detected toward two far-IR continuum sources: Sgr B2 (Polehampton et al. 2002) and W49 (Caux et al. 2002). HD is not easily detected by infrared emission-line spectroscopy; its small dipole moment leads to relatively weak emission, and its large rotational constant places its pure rotational transitions at IR frequencies that are inaccessible from ground-based telescopes. On the other hand, a large number of other D-bearing molecules are readily detected with ground-based radio telescopes. Many molecules, such as methanol, show high levels of deuterium fractionation, in which the deuterated-to-nondeuterated abundance ratio can exceed the cosmic deuterium abundance by more than 4 orders of magnitude; several doubly and even triply deuterated species have been observed (Parise et al. 2004).

In this Letter, we report a detection of HD in shocked molecular gas within the supernova remnant IC 443, clump C, and tentative detections in three other sources—the Herbig-Haro objects HH 54 and HH 7, and the star-forming region GGD 37 (Cep A West)—all from observations with the Infrared Spectrometer (IRS) on the Spitzer Space Telescope. The observational results are discussed in § 2, and the implied gas
density and HD abundance are derived in § 3. The implications of the inferred HD abundance are discussed in § 4.

2. OBSERVATIONS AND RESULTS

Two pure rotational lines fall within the 19.5–37.2 μm wavelength range covered by the IRS Long-High module: the HD $R(3)$ and $R(4)$ transitions, at 28.502 and 23.034 μm respectively. Weak spectral features have been observed serendipitously at both wavelengths in several sources, as shown in Figure 1. The plotted spectra were obtained in spectral line mapping observations of IC 443C conducted in General Observer cycle 1 and of HH 54, HH 7, and GGD 37 carried out in IRAC and IRS Guaranteed Time Observation programs, along with observations with the Short-High module. In addition, IC 443C, HH 54, and HH 7 were observed in the Short-Low module, to provide complete spectral coverage from 5.2 to 37 μm so the H$_2$ S(0)–S(7) transitions and the fine-structure lines of [Fe ii], [Si i], [Ne ii], and [S i] could all be mapped. These other observations, especially those of the H$_2$ pure rotational transitions, tightly constrain the temperature and column density of the shocked gas, allowing a determination of the HD/H$_2$ abundance ratio.

Table 1 summarizes the measured $R(3)$ and $R(4)$ line intensities. At each of six positions—one each in IC 443C, HH 7, and GGD 37, and three in HH 54—we have obtained averages of all spectra observed within a circular region, the contributing spectra being weighted by a Gaussian taper (half-power beamwidth HPBW = 15″) from the center of each such region. The central positions are given in Table 1. Full details of the observations toward HH 7 and HH 54, as well as the data reduction methods we have developed, are given in Neufeld et al. (2006).

Searching the NIST database of atomic fine-structure lines—along with the JPL molecular line list—for alternative identifications of the 28.502 and 23.034 μm features, we found no plausible candidates besides HD. In particular, a large number of water rotational transitions lie in the wavelength region of interest, but the only such transitions within 1 spectral resolution element of 28.502 and 23.034 μm are very high lying transitions that would be accompanied by other, much stronger, transitions that are absent in the observed spectra. As a check upon the reality of the observed spectral features, we have constructed maps of their distribution. Figure 2 shows the map obtained toward IC 443C, which exhibits the highest column density of warm H$_2$ and the strongest 28.502 and 23.034 μm features. Here we compare maps of the 28.502 and 23.034 μm features with those of the H$_2$ S(2), which has an upper state energy $E_u/k = 1682$ K, similar to those of HD $R(3)$ and $R(4)$ ($E_u/k = 1271$ and 1895 K). A map of H$_2$ S(3)—for which $E_u/k = 2504$ K—is also shown. The agreement of the observed morphology in the four lines lends strong support to the identification of HD and eliminates the possibility that the 28.502 and 23.034 μm features are (previously unidentified) instrumental artifacts. In the other sources, the signal-to-noise ratio is insufficient to allow the distribution of the 28.502 and 23.034 μm features to be mapped reliably; accordingly, we conservatively describe the detection of HD in those sources as tentative.

3. HD ABUNDANCES OBTAINED WITH SPITZER

Using our IRS observations of the H$_2$ S(0)–S(7) transitions toward these sources, we can constrain the column density and temperature of the warm, shocked molecular hydrogen very well and thereby estimate the HD/H$_2$ abundance ratio. As described in Neufeld et al. (2006), we have fitted the H$_2$ rotational diagrams with a model that invokes two components: a warm component at temperature $T_w \sim 400$ K and a hot component at $T_h \sim 1000$ K. The temperatures and column densities of the warm and hot gas components are given in Table 1. Our analysis neglects the effects of subthermal excitation for the H$_2$ transitions that we have observed; while possibly important for the higher $J$ transitions of H$_2$ [i.e., S(6) and S(7)], such effects

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Footnote: 8 HD $R(0)$, $R(1)$, and $R(2)$ lie at wavelengths inaccessible to the Long-High module, while $R(5)$ and higher transitions are expected to be so weak that upper limits from Short-High observations would fail to provide useful constraints.
We thereby determined the resultant HD emission, given the dipole moment. We used a statistical equilibrium calculation in our excitation model. The critical densities for the components to the observed HD emissions were roughly equal and \(n = 10^9\) cm\(^{-3}\), which are negligible for the lower \(J\) HD transitions that probe most of the gas capable of producing HD \(R(3)\) and \(R(4)\) emissions.

Unlike the lower \(J\) states of HD, however, the HD level populations for \(J = 5\) and \(J = 4\) are expected to show departures from LTE, due to the presence of a small but nonzero dipole moment. We used a statistical equilibrium calculation to compute the HD level populations, adopting the collisional rate coefficients of Flower & Roueff (1999) for excitation by \(\text{H}_2\). We thereby determined the resultant HD emission, given the two-component model parameters derived from our fit to the \(\text{H}_2\) rotational diagram, and assuming (1) that HD is at the same kinetic temperature as \(\text{H}_2\); (2) that the HD abundance relative to \(\text{H}_2\), \(n(\text{HD})/n(\text{H}_2)\), is the same in both the warm (\(\sim 400\) K) and hot (\(\sim 1000\) K) gas components; and (3) that the warm and hot components have the same gas pressure, \(p = n(\text{H}_2)T\). Typically, the contributions made by the hot and warm components to the observed HD emissions were roughly equal in our excitation model. The critical densities for \(R(3)\) and \(R(4)\) — i.e., the densities at which the departure coefficients for \(J = 4\) and \(J = 5\) equal \(\frac{1}{2}\) — correspond to pressures \(\sim 2 \times 10^5\) and \(\sim 5 \times 10^7\) cm\(^{-3}\) K, respectively, so the \(R(4)/R(3)\) ratio is a useful density indicator for pressures in the \(10^7–10^8\) cm\(^{-3}\) K range. The \(R(4)/R(3)\) intensity ratios predicted for IC 443C are \(0.32, 0.40, 0.50, 0.61, 0.72,\) and \(0.82\), respectively, for \(\log [n(\text{H}_2)T/(1\ \text{cm}^2\text{K})] = 7.0, 7.2, 7.4, 7.6, 7.8,\) and \(8.0\).

We varied the gas pressure, \(p\), and the HD abundance relative to \(\text{H}_2\), \(n(\text{HD})/n(\text{H}_2)\), to obtain the best fit to the observed HD \(R(3)\) and \(R(4)\) line strengths. Because the HD transitions are optically thin, the HD line intensities scale linearly with \(n(\text{HD})/n(\text{H}_2)\). While our estimates of the gas pressure or density scale in inverse proportion to the assumed collisional rate coefficients, the derived HD abundance would be entirely unaffected by a (uniform) change in the adopted rate coefficients. Table 1 lists the best-fit \(p\) and \(n(\text{HD})/n(\text{H}_2)\) derived for each region.

In Figure 3, we show the confidence regions for the gas pressure and HD/\(\text{H}_2\) ratio: \(68.3\%\) and \(95.4\%\) confidence regions are shown for each of the five sources we observed, based upon the statistical errors on the HD \(R(3)\) and \(R(4)\) line fluxes and assuming the \(\text{H}_2\) column densities and temperatures (\(N_n, T_n\)) listed in Table 1. The confidence limits presented here are based solely upon the statistical errors in the measured line fluxes and do not include systematic uncertainties in the HD excitation model. Such uncertainties are hard to estimate quantitatively and include possible errors in the collisional rate coefficients and in the assignment that the warm and hot gas components share a common pressure. The derived HD abundances (although not the gas pressures) appear to be relatively insensitive to the assumed collisional rate coefficients. If the HD–\(\text{He}\) (Roueff & Zeippen 2000) or HD–\(\text{H}\) rate coefficients (Flower & Roueff 1999) are adopted in place of the HD–\(\text{H}_2\) rate coefficients, the best-fit HD abundances change by less than \(\sim 10\%\). On the other hand, if it is assumed that the warm and hot gas components share a common density rather than being in pressure equilibrium, the best-fit HD abundances increase by up to \(\sim 50\%\).

4. DISCUSSION

The signal-to-noise ratio is significantly better toward IC 443C, HH 54 FS, and HH 7, the only cases for which \(R(4)\) is detected at the 5 \(\sigma\) level. The best-fit gas pressures, found to lie in the range \((1.6–10) \times 10^8\) cm\(^{-3}\) K, correspond to gas densities in the range \((4–25) \times 10^5\) cm\(^{-3}\) for the warm gas component. These values are in reasonable agreement with those derived previously for these regions (see discussion of HH 7 and HH 54 in Neufeld et al. 2006; and of IC 443 by Snell et al. 2005.) The HD \(R(4)/R(3)\) intensity ratio promises to be a valuable probe of the gas pressure in regions where it can be observed.

Our analysis yields best estimates of (1.19\(^{+0.35}_{-0.24}\)) \(\times 10^{-3}\), (1.80\(^{+0.32}_{-0.35}\)) \(\times 10^{-3}\), and (1.41\(^{+0.46}_{-0.16}\)) \(\times 10^{-3}\) (68\% confidence intervals, respectively), for the HD abundance relative to \(\text{H}_2\) in IC 443C, HH 54 FS, and HH 7, but all three estimates are consistent (within the 68\% confidence intervals) with \(n(\text{HD})/n(\text{H}_2) = 1.5 \times 10^{-5}\). If HD accounts for all the deuterium in the gas phase,\(^a\) this would imply \(n(\text{HD})/n(\text{H}_2) = 7.5 \times 10^{-6}\), a value that is a factor of 2–3 below those inferred from atomic D absorption-line observations of the Local Bubble (\(n(\text{H}_2)/n(\text{H}_2) = (1.52 \pm 0.08) \times 10^{-5}\); Moos et al. 2002), atomic D absorption-line observations of the halo (\(n(\text{H}_2)/n(\text{H}_2) = (2.2 \pm 0.7) \times 10^{-5}\); Semenov et al. 2006).

\(^a\) In interpreting their observations of Orion, Bertoldi et al. argued that significant destruction of HD occurred in the shocked gas that they observed, as a result of the reaction \(\text{H} + \text{HD} \rightarrow \text{D} + \text{H}_2\) (Timmermann 1996), and applied a correction in deriving the gas-phase elemental abundance of HD. In the shocked regions that we have observed, however, the inferred shock velocities (\(\sim 10–20\) km s\(^{-1}\); Neufeld et al. 2006) are significantly smaller than those for the Orion shock; thus, the resultant atomic H abundance is expected to be much smaller and the extent of HD destruction negligible.
the gas-phase deuterium abundance, a possibility originally raised by Jura (1982). In this picture, material within the Local Bubble is anomalous because it has suffered recent grain destruction in shocks driven by stellar winds or supernovae. An observed correlation between the gas-phase abundances of deuterium and the refractory element titanium (Prochaska et al. 2005), and the possible detection of deuterated polycyclic aromatic hydrocarbons (Peeters et al. 2004), have been interpreted as supporting the importance of depletion. While our determination of the HD abundance in dense shocked clouds does not directly settle this debate, it does suggest that the gas-phase deuterium abundance in dense clouds differs little from that inferred for typical diffuse clouds along high-N\textsubscript{H} sight lines to distant stars within the Galactic disk.

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REFERENCES

Bertoldi, F., Timmermann, R., Rosenthal, D., Drapatz, S., & Wright, C. M. 1999, A&A, 346, 267
Caux, E., Ceccarelli, C., Pagani, L., Maret, S., Castets, A., & Pardo, J. R. 2002, A&A, 383, L9
Draine, B. T. 2003, in ASP Conf. Ser. 348, Astrophysics in the Far Ultraviolet, ed. G. Sonneborn, H. Moos, & B-G Andersson (San Francisco: ASP), 58
Friedman, S. D., Hebrard, G., Tripp, T. M., Chayer, P., & Sembach, K. R. 2006, ApJ, 638, 847
Hebrard, G., & Moos, H. W. 2003, ApJ, 599, 297
Hoopes, C. G., Sembach, K. R., Hebrard, G., Moos, H. W., & Knauth, D. C. 2003, ApJ, 586, 1094
Howat, S. K. R., Timmermann, R., Geballe, T. R., Bertoldi, F., & Mountain, C. M. 2002, ApJ, 566, 905
Jura, M. 1982, in Advances in Ultraviolet Astronomy, ed. Y. Kondo (NASA CP-2238) (Washington, NASA), 54
Kirkman, D., Tytler, D., Suzuki, N., O’Meara, J. M., & Lubin, D. 2003, ApJS, 149, 1
Lacour, S., et al. 2005, A&A, 430, 967
Le Petit, F., Roueff, E., & Le Bourlot, J. 2002, A&A, 390, 369
Moos, H. W., et al. 2002, ApJS, 140, 3
Neufeld, D. A., et al. 2006, in press (astro-ph/0606232)
Parise, B., Castets, A., Herbst, E., Caux, E., Ceccarelli, C., Mukhopadhyay, I., & Tielens, A. G. G. M. 2004, A&A, 416, 159
Peeters, E., Allamandola, J. L., Bauschlicher, C. W., Jr., Hudgins, D. M., Sandford, S. A., & Tielens, A. G. G. M. 2004, ApJ, 604, 252
Polehampton, E. T., Baluteau, J.-P., Ceccarelli, C., Swinyard, B. M., & Caux, E. 2002, A&A, 388, L44
Prochaska, J. X., Tripp, T. M., & Howk, J. C. 2005, ApJ, 620, L39
Roueff, E., & Zeippen, C. J. 2000, A&A, 416, 159
Sandford, S. A., & Tielens, A. G. G. M. 2004, A&A, 416, 159
Schramm, D. N., & Turner, M. S. 1998, Rev. Mod. Phys., 70, 303
Sembach, K. R., et al. 2004, ApJS, 150, 387
Snell, R. L., Hollenbach, D., Howe, J. E., Neufeld, D. A., Kaufman, M. J., Melnick, G. J., Bergin, E. A., & Wang, Z. 2005, ApJ, 620, 758
Spergel, D. N., et al. 2003, ApJS, 148, 175
Spitzer, L., Jr., & Jenkins, E. B. 1975, ARA&A, 13, 133
Timmermann, R. 1996, ApJ, 456, 631
Wood, B. E., Linsky, J. L., Hebrard, G., Williger, G. M., Moos, H. W., & Blair, W. P. 2004, ApJ, 609, 838
Wright, C. M., van Dishoeck, E. F., Cox, P., Sidher, S. D., & Kessler, M. F. 1999, ApJ, 515, L29