Ground-based detection of a vibration-rotation line of HD in Orion

T. R. Geballe[a], S. K. Ramsay Howat[b], R. Timmermann[c], F. Bertoldi[d],
C.M. Mountain[a]

Gemini Preprint #81

a. Gemini Observatory, Hilo, HI 96720, USA
b. Astronomical Technology Centre, Royal Observatory, Blackford Hill, Edinburgh, EH9 3HJ Scotland
c. Universität zu Köln, Physikalisches Institut, Zülpicher Strasse 77, Cologne, D-50937, Germany
d. Max Planck Institut für Radioastronomie, Auf dem Hügel 69, Bonn, D-53121, Germany

Ground-based detection of a vibration-rotation line of HD in Orion

T. R. Geballe[a,*], S. K. Ramsay Howat[b], R. Timmermann[c], F. Bertoldi[d], C. M. Mountain[a]

[a] *Gemini Observatory, Hilo, HI 96720, USA*

[b] *Astronomical Technology Centre, Royal Observatory, Blackford Hill, Edinburgh, EH9 3HJ Scotland*

[c] *Universität zu Köln, Physikalisches Institut, Zülpicher Strasse 77, Cologne, D-50937, Germany*

[d] *Max Planck Institut für Radioastronomie, Auf dem Hügel 69, Bonn, D-53121, Germany*

Abstract

The $v = 1$–0 R(5) line of HD at 2.46 μm has been detected at the position of brightest line emission of shocked H_2 in the Orion Molecular Cloud. The flux in this HD line, when compared to that of the previously detected HD 0–0 R(5) line at 112 μm, suggests that, like the v=1 levels of H_2, the v=1 levels of HD are populated in LTE, despite their much higher rates of spontaneous emission compared to H_2. The higher than expected population of vibrationally excited HD may be due to chemical coupling of HD to H_2 via the reactive collisions HD + H $\leftrightarrow$ H_2 + D in the shocked gas. The deuterium abundance implied by the strengths of these lines relative to those of H_2 is $(5.1\pm1.9) \times 10^{-6}$.

*Corresponding author. Gemini Observatory, Hilo, HI 96720, USA. Tel. +1-808-974-2519; fax +1-808-935-9650

Email address: tgeballe@gemini.edu; fax: 1-808-935-9650 (T. R. Geballe)

To be published in a special issue of Planetary and Space Science: Proceedings of the conference, "Deuterium in the Universe," held at Meudon Observatory, 25-27 June 2001

1. Introduction

Until recently, observations of the deuterium abundance in the interstellar medium have been restricted almost entirely to ultraviolet and millimeter wavebands. Both wavebands have limitations: UV observations probe only regions of low extinction; millimeter measurements are uncertain because of the inaccurately known degree of chemical fractionation. In addition, analyses of measurements in both bands are plagued by uncertainties in the corrections for line saturation (in the non-deuterated species).

Recently, two pure rotational lines of HD were detected by the spectrometers on the Infrared Space Observatory (ISO), toward the Orion star forming region OMC-1, offering new opportunities for determining [D]/[H]. Wright et al. (1999) used the Long Wavelength Spectrometer (LWS) to detect the pure rotational R(0) J=1–0 transition at 112 μm toward the Orion Bar. Bertoldi et al. (1999) detected the pure rotational R(5) (v=0, J=6–5) line at H_2 Peak 1, the brightest position of shocked line emission in the OMC-1 outflow, with the Short Wavelength Spectrometer (SWS). Both measurements have led to new estimates of [D]/[H] in Orion, Wright et al. finding $(1.0 \pm 0.3) \times 10^{-5}$ and Bertoldi et al. obtaining $(7.6 \pm 2.9) \times 10^{-6}$.

Both of these estimates have large uncertainties, stemming only in part from the low signal-to-noise ratios of the line detections. One source of uncertainty is the value of [HD]/[H] in the warm partially dissociated gas produced by C-shocks, where the exothermic reaction, HD + H + 418K $\rightarrow$ H_2 + D, selectively depletes HD. Bertoldi et al. (1999) estimate that the depletion factor at Peak 1 is 1.67 for gas in the range of temperatures where most of the HD $v = 0$ R(5) line emission occurs. The second is the lack of information about the populations of other energy levels. This is a serious problem at Peak 1, because (1) the post-shock gas has a wide range of temperatures, and (2) HD radiatively relaxes much more rapidly than H_2, so that its v=0 J=6 level, which is 2,636 K above ground, might not be in LTE, unlike H_2 lines of similar excitation.

The value of [D]/[H] given by Bertoldi et al. (1999) includes both the correction for depletion and an adjustment factor of 1.5, their estimate of the factor by which the population of v=0, J=6 falls below that for LTE. This factor, which is highly uncertain, could be tested if other transitions of HD were detected. One possible source of additional information is the fundamental vibration-rotation band of HD, which should be excited into emission by collisions in the post-shock gas. The fundamental band occurs at the long wavelength edge of the 2 μm window and short wavelength edge of the 3 μm window, where telluric absorption, mostly by H_2O, is severe. However, the v=1-0 R(5) line of HD at 2.459 μm is accessible from a dry, high altitude sites such as Mauna Kea. The upper level of this line is 7,747 K above ground (Herzberg 1950; Essenwanger & Gush 1984), and hence the intensity ratio of it to the 0-0 R(5) line observed by ISO can provide valuable information concerning the excitation of HD. The 1-0 Q(5) line of H_2 is nearby at 2.455 μm, so its strength can be easily compared to the HD line.

2. Observations and Results

A search for the 1-0 R(5) line of HD was conducted on UT 1999 January 20 at the United Kingdom Infrared Telescope (UKIRT), using the 1–5 μm spectrometer CGS4 (Mountain et al. 1990). CGS4's echelle was used with a slit of width 0.82 arcsec oriented east-west across OMC-1 Peak 1 for a total of 40 minutes of exposure time; an equal amount of time was spent on blank sky 5' east. The resolution was 16 km s^{-1}. The spectrum of the star HR 2007, measured with the same instrumental configuration, was used to flux- and wavelength-calibrate (using telluric absorption lines) the spectrum at Peak 1.

The resulting spectrum of a 0.82×7.28 arcsec^2 strip at Peak 1 is shown in Fig. 1. The spectrum is dominated by the 1-0 Q(5) line of H_2, but the 1-0 R(5) of HD is clearly detected at about 1/700th the strength of the H_2 line, roughly as predicted by Hartquist et al. (1982). The HD line is at the predicted wavelength to within 0.0001 μm. Its intensity distribution, which is similar to that of the Q(5) line along the slit, solidifies the identification. The profiles of the two lines do not appear identical, but are the same to within the noise.

3. Analysis

3.1 Beam dilution

To determine the excitation parameters of the HD at Peak 1, it is necessary to compare the two line fluxes. The 0-0 R(5) line was measured by the SWS in an aperture of 380 arcsec^2, centered on Peak 1, whereas the 1-0 R(5) line was observed at UKIRT through a 6 arcsec^2 aperture on the brightest part of Peak 1. From the H_2 Q(5) line, which was observed both by the SWS in a large aperture (Rozenshtein 2000) and UKIRT in the small aperture, we conclude that the observed HD 1-0 R(5) surface brightness must be decreased by a factor of (2.1$\pm$0.4) to properly compare it with the average surface brightness of the pure rotational HD line measured in the larger aperture.

3.2 Column densities

The surface brightness of an optically thin vibration-rotation line can be converted into a column density via N(v,J) = $(4\pi/\mathrm{hc})$ $(\mathrm{I}\lambda/\mathrm{A})10^{0.4A_\lambda})$, where I is the observed line intensity, A is the Einstein coefficient, and A_λ is the extinction. Bertoldi et al. (1999) found an HD column density in the v=0, J=6 level, N(0,6), of (3.0$\pm$1.1) $\times$ 10^{14} cm^{-2} at Peak 1. After correcting for the difference in surface brightnesses as described above, the 1-0 R(5) line yields a column density N(1,6) = (5.1$\pm$1.3) $\times$ 10^{12} cm^{-2} averaged over the large beam. This is a factor of 60 lower than the column density in the v=0, J=6 level, demonstrating that most of the HD is not vibrationally excited. However, as shown in Fig. 2, the two populations match the relative populations of H_2 levels (Rosenthal, Bertoldi, & Drapatz 2000; Bertoldi et al.) of similar energies. This is somewhat surprising, as one might have expected that the higher HD levels would have a sub-thermal excitation, due to their much higher radiative transition rates (60 times higher when comparing the rate for HD(1,6), 5×10^{-5} s^{-1}, with that for H_2(1,4), which has the same excitation energy). Thus one might have predicted that the population of the higher energy level of HD would fall far below the H_2 curve. We return to the discussion of HD excitation below.

4. Deuterium abundance

Assuming that the lower energy states of HD are populated in LTE (i.e., in the same way as the levels of H_2, as suggested by Fig. 2), and after correcting for the depletion of HD, we find [D]/[H] = $(5.1 \pm 1.9) \times 10^{-6}$, where the uncertainty does not include the uncertainty in the depletion. This abundance ratio is 1.5 times lower than that given by Bertoldi et al. (1999), who had corrected for their assumed non-LTE level population by that factor in addition to correcting for depletion. The abundance is the lowest yet determined for deuterium. However, within the uncertainties the value is consistent with the recent value of $7.4^{+1.9}_{-1.3} \times 10^{-6}$ derived by Jenkins et al. (1999) toward δ Orionis. We note that Jenkins et al. and Sonneborn et al. (2000) find that the deuterium abundance varies significantly along different lines of sight.

5. Excitation of HD

The excitation of the HD (0,6) and (1,6) levels appears to mimic that of similarly excited levels of H_2. If this is generally true for HD, then there must be a way of maintaining HD level populations in the spite of their radiative transition rates, which are substantially higher than those of H_2. While it is believed that H_2 levels are in LTE as a result of standard collisional relaxation with H_2 and H, post-shock densities would need to be considerably higher than 10^7 cm^{-3} in order for simple inelastic collisions to maintain HD in or near LTE.

We have already noted the exchange reaction, HD + H $\leftrightarrow$ H_2 + D, which tends to deplete HD in the warm, partially dissociated post-shock gas of OMC-1. Our analysis of this reaction, which has been studied previously by Rozenshtein et al. (1985), Zhang & Miller (1989), Gray & Balint-Kurti (1998), and Timmermann (1996), indicates that at Peak 1 *the fraction of vibrationally excited HD, HD*, is significantly enhanced by this reaction.* Details of our analysis are provided in Ramsay Howat et al. (2002). To summarize, we find the following.

- H_2(v=0) + D $\rightarrow$ HD* + H is the dominant channel for "chemically" exciting HD vibrationally, with a rate coefficient of 1.24×10^{-12} cm^{-3} s^{-1}. Vibrationally excited H_2 has an order of magnitude higher rate coefficient for production of HD*, but only a very small fraction of H_2 is vibrationally excited (see below).

- The formation of HD* is faster than its relaxation to the ground vibrational state when $n(\mathrm{H_2}) > 4 \times 10^7[n(\mathrm{HD})/n(\mathrm{D})][n(\mathrm{HD^*})/n(\mathrm{HD})]$ cm^{-3}. The deuterium fraction, $n(\mathrm{D})/n(\mathrm{HD})$ is determined by detailed balance of the HD–H_2 exchange reaction, and the above equation simplifies to $n(\mathrm{H}) > 2 \times 10^7\ [n(\mathrm{HD^*})/n(\mathrm{HD})]\ \mathrm{e}^{418/T(K)}$.

- The ratio $n(\mathrm{HD^*})/n(\mathrm{HD})$ varies greatly over the range of post-shock temperatures where line emission occurs. For a reasonable assumption of 0.01 for the mean value of this ratio, the abundance of HD* is dominated by reactive collisions if $n(\mathrm{H}) > 2 \times 10^5$ cm^{-3}.

In the post-shock gas $n(\mathrm{H})$ is believed to be well in excess of 10^5 cm^{-3}. Thus, we tentatively conclude that at Peak 1 partially dissociative shocks strongly couple the excitation of HD to H_2. Because of the much larger abundance of H_2, the HD effectively becomes part of the H_2 level system.

To further test the importance of this excitation mechanism, detections of additional lines of HD are needed, in order to determine if the populations of their upper levels also fall on the H_2 curve in Fig. 2.

Acknowledgements

This program was observed as part of the UKIRT Service Programme. We thank the staff of UKIRT for its support. The United Kingdom Infrared Telescope is operated by the Joint Astronomy Centre on behalf of the U.K. Particle Physics and Astronomy Research Council. We also thank J. Black and D. Flower for helpful discussions.

References

Bertoldi, F., Timmermann, R., Rosenthal, D., Drapatz, S., & Wright, C. M. 1999. A&A, 346, 267.

Essenwanger, P. & Gush H.P. 1984, Can. J Phys., 62, 1680.

Gray, J.K & Balint-Kurti, G.G. 1998, J Chem. Phys., 108 (3), 950.

Hartquist, T.W. 1982, in Galactic and Extragalactic Infrared Spectroscopy, ESA SP 192, 45.

Herzberg, G. 1950. In Molecular Physics and Molecular Structure. Vol. I (New York: Van Nostrand Reinhold).

Jenkins, E.B., et al. 1999, ApJ, 520, 182.

Mountain, C. M., Robertson, D. J., Lee, T. J., & Wade, R. 1990, SPIE, 1235, 25.

Ramsay Howat, S.K., Timmermann, R., Geballe, T.R., Bertoldi, F., & Mountain, C.M. 2002. ApJ, in press.

Rosenthal, D., Bertoldi, F., & Drapatz, S. 2000. A&A, 356, 705.

Rozenshtein, V.B., Gershenzon, Yu. M., Ivanov, A. V., Il'in, S. D., Kucheryavii, S. I., & Umanskii, S. Ya. 1985. Chem Phys. Lett., 121, 89.

Sonneborn, G., Tripp, T. M., Jenkins, E. B., Sofia, U. J., Vidal Madjar, A., & Wozniak, P. R. 2000. ApJ, 545, 277.

Timmermann, R. 1996, ApJ, 456, 631.

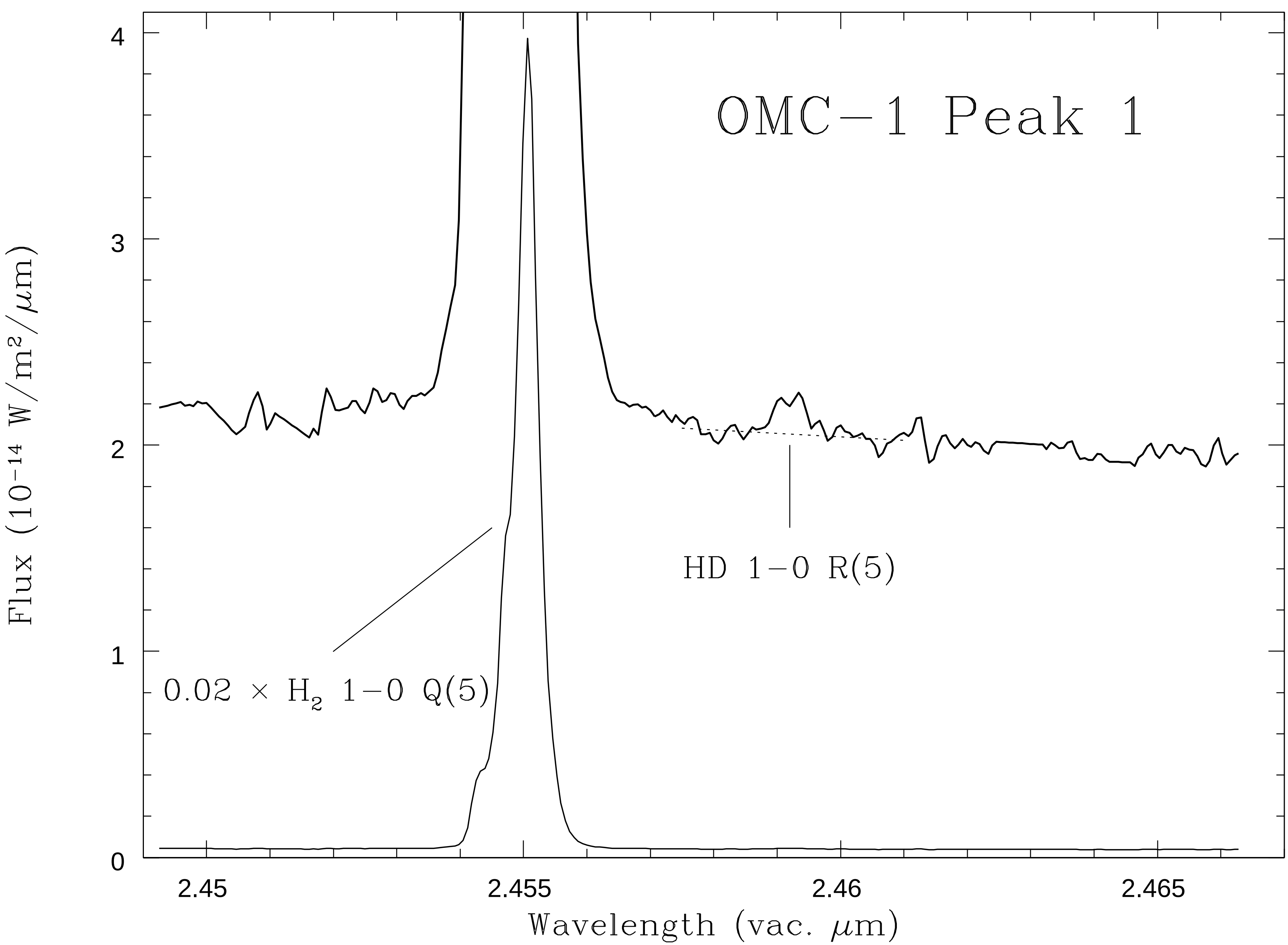
Wright, C.M., van Dishoeck, E. F., Cox, P., Sidher, S., & Kessler, M. F. 1999, ApJ, 515, L29.

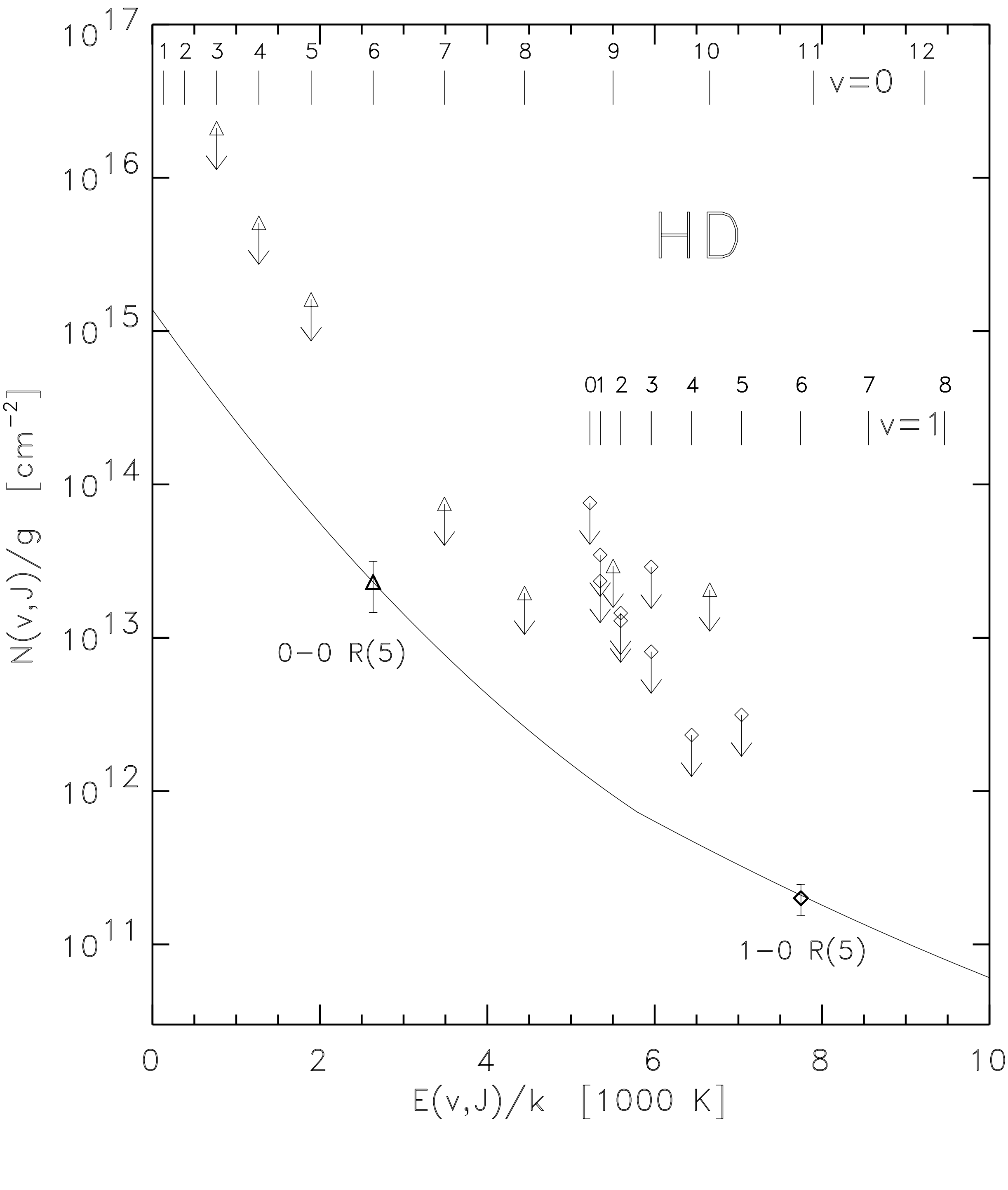
Zhang, J. Z. H., & Miller, W. H. 1989. J Chem. Phys., 91 (3), 1528.

Figure Captions

Figure 1 - Spectrum of a 0.82"×7.28" (NS x EW) area of at the center of OMC-1 Peak 1 near 2.46 μm. The H_2 and HD lines are indicated. The assumed continuum, used to estimate the flux in the HD line, is shown by the dashed line.

Figure 2 - HD excitation diagram, with column densities plotted versus energy of upper level. Triangles are pure rotational transitions; diamonds are vibration-rotation transitions. Most measurements are upper limits. The curve is the fit to the H_2 excitation diagram, scaled to pass through the HD 0-0 R(5) point.


OMC−1 Peak 1
HD 1−0 R(5)
0.02 × H2 1−0 Q(5)
Flux (10-14 W/m2/μm)
Wavelength (vac. μm)
0
1
2
3
4
2.45
2.455
2.46
2.465



HD
v=0
1 2 3 4 5 6 7 8 9 10 11 12
v=1
01 2 3 4 5 6 7 8
0–0 R(5)
1–0 R(5)
N(v,J)/g [cm^{-2}]
E(v,J)/k [1000 K]