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THE UPPER LIMIT FOR CH_4 IN THE PROTOSTELLAR DISK TOWARD HL TAURI

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ABSTRACT

We used high-resolution infrared spectra of the heavily embedded T Tauri star HL Tau to search for evidence of absorption due to the *R*0, *R*1, and *R*2 gas-phase CH_4 ν_3 lines near 3.3 μm. From this, we report a 3 σ upper limit of 1.3×10^{15} cm^{-2} for the CH_4 gas column density toward HL Tau. Our results are compared to those found for CO gas toward this source and to the recent model for chemistry in the inner (10 AU) disks around T Tauri stars by Markwick et al. We find that the upper limit of methane ice+gas column density toward HL Tau, when compared to CO, is somewhat lower than but consistent with that measured toward other interstellar sources (~1%) but that it is much lower than that predicted in the Markwick et al. model and much less than the CH_4/CO ratio (10%–80%) found in cometary volatiles. This has important implications for the processing of interstellar material and its incorporation into planetary bodies.

Subject headings: infrared: ISM — ISM: abundances — ISM: molecules

1. INTRODUCTION

HL Tau is a heavily embedded, low-mass, young stellar object (YSO) located in the Taurus molecular cloud at a distance of ~140 pc (Elias 1978). Bright submillimeter emission suggests the presence of a massive (~0.1 $M_\odot$) disk of circumstellar material surrounding the central star (Sargent 1989; Beckwith et al. 1990). The bulk of the disk material is thought to reside within a radius of less than 200 AU (Sargent & Beckwith 1991).

There have been very few studies of the chemistry of the inner, planet-forming regions of disks around young stars. Most submillimeter/millimeter studies do not have the spatial resolution to investigate the inner regions of protostellar disks where planet formation may occur. With the advent of instruments capable of providing both high spatial and spectral resolution in the infrared, such as NIRSPEC at the W. M. Keck Observatory, studies of such disks are now possible. Also, with arrays such as the Atacama Large Millimeter Array and the Submillimeter Array coming on line in the near future, now is the ideal time to study the chemistry in disks around young stars.

Methane is a symmetric tetrahedral hydrocarbon. It lacks a permanent dipole moment and hence has no pure rotational lines. For this reason, it cannot be observed at radio wavelengths. It also does not fluoresce efficiently at visible or UV wavelengths. In order to determine CH_4 column densities in disks around young stars, we must rely on observations of rovibrational transitions in the infrared. Methane has been studied in the solid and gas phase around massive YSOs via the ν_4 band (Boogert et al. 1997, 1998) as well as via the ν_3 band in the comae of Oort Cloud comets (Gibb et al. 2003). For this study, we searched for the ν_3 lines near 3.3 μm.

We present high-resolution, near-infrared observations of the 3026–3050 cm^{-1} region toward HL Tau. We searched for but did not detect methane ν_3 absorption or emission lines toward this source. We show that the upper limit for the total column density of CH_4 (gas+ice), compared to CO, is not inconsistent with values determined along the lines of sight to massive YSOs. However, our upper limit for the methane/CO column density ratio is significantly lower than that predicted by the model of Markwick et al. (2002), which predicts chemical abundances of several key species in the inner 10 AU of the protostellar disk surrounding a T Tauri star. It is also more than order of magnitude less than that observed in Oort Cloud comets, implying a mechanism to produce or selectively retain CH_4 on icy dust mantles in the early protoplanetary disk.

2. OBSERVATIONS AND DATA REDUCTION

Observations were performed using the high-dispersion, cryogenic echelle spectrometer NIRSPEC at the 10 m W. M. Keck Observatory on Mauna Kea, Hawaii (McLean et al. 1998). The data were acquired on 2002 March 23 with good seeing and a low atmospheric water burden. We achieved 20 minutes on-source. A spectral resolving power of ~25,000 was obtained using the 3 pixel (0″.43) wide slit. Data processing included using a series of flats and darks to remove systematic effects from the grating setting. Systematically hot and dead pixels and cosmic-ray hits were then removed, and the data were resampled to align the spectral and spatial dimensions along rows and columns, respectively (DiSanti et al. 2001; Brittain et al. 2003).

Observations were taken in an observing sequence ABBA where the telescope was nodded a small distance (15″) along the slit in the north-south direction. Combining the scans as $\{A - B - B + A\}/2$ canceled the telluric emission to first order. Atmospheric models were obtained using the Spectral Synthesis Program (SSP; Kunde & Maguire 1974) that accesses the HITRAN 2000 molecular spectroscopic database (Rothman et al. 2003). We used these SSP models to assign the wavelength scales to the extracted spectra and to determine column burdens for the absorbing species in the Earth's atmosphere, primarily water and methane in the spectral region covered in this study. The atmospheric model is then binned to the resolution of the spectrum, normalized, and scaled to the continuum level. We

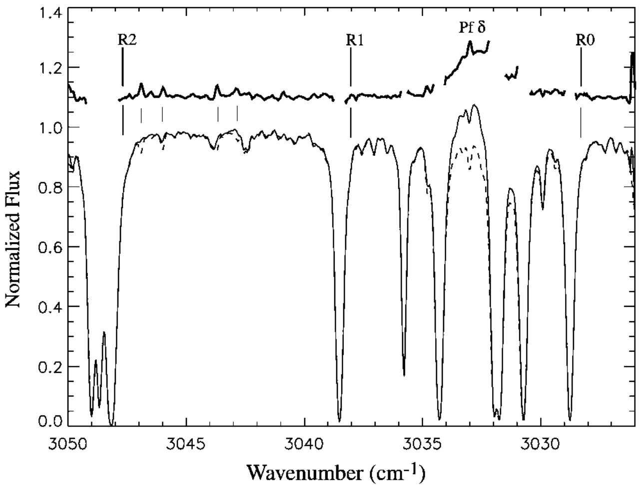

FIG. 1.—Spectrum of HL Tau. The dashed line is the atmospheric transmittance model. The solid line at the top is the ratio between the spectrum and the atmospheric transmittance model. The gaps are where the transmittance is less than 50%. The expected Doppler-shifted positions of the CH_4 *R*0, *R*1, and *R*2 lines are indicated. Poorly fitted telluric ozone lines are indicated with tick marks. There is no indication of CH_4 absorption or emission present. The strong emission feature near 3033 cm^{-1} is due to the Pfδ line of hydrogen.

then divided the atmospheric model from the observation to reveal the residual spectrum of HL Tau.

The resulting spectrum is plotted in Figure 1. The residual is plotted at the top. The expected Doppler-shifted line positions of the CH_4 ν_3 *R*0, *R*1, and *R*2 lines, determined from the CO absorption-line positions to be 48 ± 1 km s^{-1} (Brittain et al. 2004), are indicated on the plot. The strong, broad emission feature near 3033 cm^{-1} is the Pfδ line of hydrogen. Excess residual between 3043 and 3047 cm^{-1} (indicated by the short ticks in Fig. 1) is a result of the atmospheric model not adequately fitting the ozone absorption lines in this spectral region. We note that the ozone lines in other parts of the spectrum do reproduce the data very well (i.e., those from 3026 to 3040 cm^{-1}) and conclude that the few lines that are poorly fitted, which do not correspond to the positions of expected methane lines, should not affect the detectability of methane in this study.

3. RESULTS

3.1. *Methane Gas*

We determined the upper limits to equivalent widths of the CH_4 *R*0, *R*1, and *R*2 lines based on the signal-to-noise ratio of our data, taking into account the atmospheric transmittance at each line position. For the purpose of this work, we assume that the CH_4 gas will be absorbing in the same region of the disk as the CO gas. We assume an unresolved Gaussian line shape and a rotational temperature of 100 K, consistent with the CO absorption lines (Brittain et al. 2004). The equivalent width for a Gaussian is by definition

$$W_\nu = 1.0645 \frac{\Delta I}{I_0} \Delta\tilde{\nu} \text{ cm}^{-1}, \quad (1)$$

where $\Delta I/I_0$ is the depth of the line as a fraction of the fitted continuum level and $\Delta\tilde{\nu}$ is its full width at half-peak, expressed in units of cm^{-1}. From this, an upper limit for the column density for each line is determined using

$$N = \left(\frac{m_e c^2}{\pi e^2}\right) \frac{W_{\tilde{\nu}}}{f}, \quad (2)$$

where the oscillator strength $f = cm_e A/8\pi^2 e^2 \tilde{\nu}^2$ and A is the Einstein A-value. The 3 σ upper limits for each line are reported in Table 1.

The total column density for CH_4 absorption was then calculated by assuming a Boltzmann distribution at a temperature of 100 K. From this, the fractional population for each transition is given by

$$F(T) = (2J + 1) g_{A,E,F} e^{(-1.439 E_l/T)}/Q(T), \quad (3)$$

where Q is the partition function at temperature T (assumed to be 100 K) and E_l is the lower state energy (in units of cm^{-1}). CH_4 has three noncombining spin species labeled *A*, *E*, and *F*, each with a statistical weight that is the product of $(2J + 1)$ and 5, 2, and 3, respectively. The rotational partition function is given for each spin species by Fox (1970). In addition, many CH_4 lines are superpositions of unresolved multiple transitions. This is unimportant for *R*0 and *R*1, which are pure *A* and *F* transitions, respectively. *R*2, however, is comprised of an *E* and an *F* transition, unresolved by NIRSPEC. For this line, we summed over the two contributing lines. The total column density upper limits are reported in Table 1.

Using this methodology, we determined a 3 σ upper limit for the total column density of CH_4 gas absorption of 1.3×10^{15} cm^{-2} toward HL Tau from the strongest (*R*2) line. The *R*0 and *R*1 lines are somewhat less constraining, giving $N_{tot} < 4.2 \times 10^{15}$ cm^{-2}. Gas-phase CO absorption has also been observed toward this source (Brittain et al. 2004). Figure 2 shows two sample CO spectra. Both broad emission lines (from hot CO very close to the star) and narrow absorption lines (for both ^{12}CO and ^{13}CO) are visible and result from colder gas along the line of sight. We compare our methane results to those for CO. CO and CH_4 are both expected to be primarily in the gas phase at the temperatures of interest (although, as noted below, it is possible that some methane could be trapped in icy grain mantles), so it is reasonable to assume that they coexist in the same region of the disk. The column density of

TABLE 1
UPPER LIMITS FOR CH_4[a]

Line	ν_{rest} (cm^{-1})	Atmospheric Transmittance (%)	W_ν (cm^{-1})	A (s^{-1})	N_{line} (cm^{-2})	$F(T)$	N_{tot} (cm^{-2})
*R*0	3028.75	85	<3.38(−3)	126.27	<1.9(14)	0.0435	<4.3(15)
*R*1	3038.50	85	<2.96(−3)	75.182	<2.7(14)	0.0673	<4.1(15)
*R*2[b]	3048.16	77	<3.31(−3)	127.46	<1.8(14)	0.138	<1.3(15)

[a] The 3 σ upper limits are reported.
[b] The *R*2 line is comprised of two unresolved components. The quantities reported are for the sum of both components.

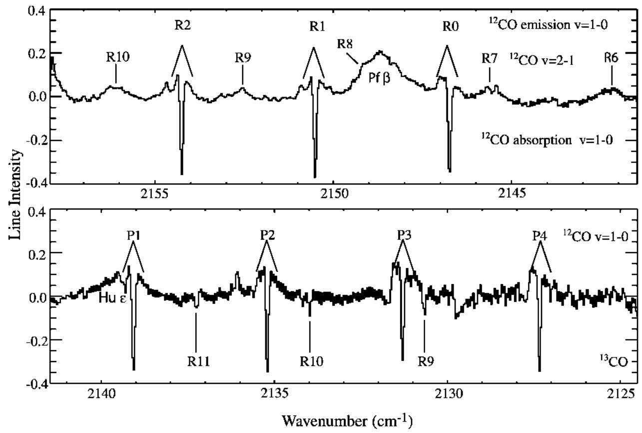

FIG. 2.—CO absorption and emission spectrum of HL Tau from Brittain et al. (2004). The broad emission features (labeled above the spectra) result from hot (∼1500 K) CO gas near the star. The narrow absorption features of both ^{12}CO and ^{13}CO (labeled below the spectra) are superposed on these emission features. They have a lower T_{rot} (∼100 K), indicating colder gas along the line of sight. Also shown are the broad hydrogen Pfβ and Huϵ emission lines.

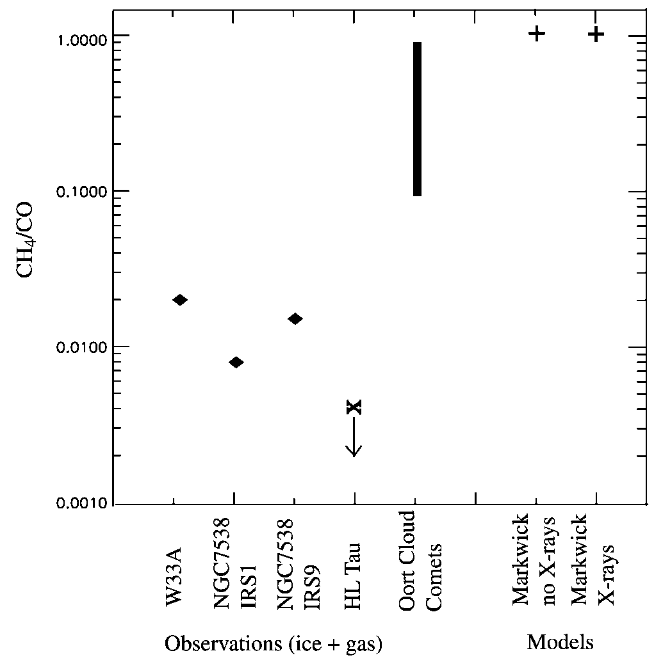

FIG. 3.—Plot showing gas+ice CH_4/CO ratios for various physical environments in the ISM, comets, and the Markwick et al. (2002) chemical model. This shows that the upper limit for HL Tau is not inconsistent with the range of interstellar values obtained by observations toward massive YSOs. However, our upper limit is much lower than that for comets or the Markwick et al. (2002) model.

CO absorption was found to be $(7.1 \pm 0.3) \times 10^{18}$ cm^{-2} with a rotational temperature of ∼100 K. When we compare this to our 3 σ upper limit for CH_4 gas absorption toward this source, an upper limit of gaseous $N(CH_4)/N(CO) < 0.02\%$ is determined.

This result is substantially lower than the few measured interstellar CH_4/CO ratios (Boogert et al. 1997, 1998) shown in Figure 3. These objects, for which methane has been studied in absorption in both the gas and solid phase, are massive, embedded YSOs. The CH_4/CO ratios were calculated from the combined solid-phase+gas-phase column densities along the lines of sight. Although volatile species do vary, sometimes dramatically, from one line of sight to another, the CH_4/CO ratio is fairly consistent among the few sources studied to date. We therefore consider it reasonable to expect that the initial CH_4/CO ratio in the infalling material (ice and gas) to be on the order of 1%. While our upper limit on gas-phase CH_4/CO is significantly less than the values toward YSOs, we point out that those studies include ice column densities as well.

We also searched for CH_4 emission, using the methodology outlined in Brittain et al. (2004) to determine column density upper limits. We assumed that any emission would result from 1500 K gas close to the star, as found for CO. Our 3 σ upper limit for the effective hot CH_4 gas abundance (relative to CO) is less than 4.5%. As this is not nearly as well constrained as the absorption, we do not discuss it further but point out that future studies should also search for evidence of CH_4 emission.

3.2. *Methane Ice*

H_2O ice has been observed toward HL Tau (van de Bult et al. 1985). Its profile shows evidence of partial annealing. When compared to laboratory spectra, it is found to be consistent with ice that has been heated to ∼80–100 K. In the interstellar medium (ISM), CH_4 is thought to form via H-atom addition reactions to C, analogous to the formation method for H_2O (Boogert et al. 1998). CH_4 is thought to form alongside H_2O and is then trapped in the ice where its sublimation is suppressed (Hiraoka et al. 1998). Studies of CH_4 toward massive YSOs are consistent with this interpretation since gas-phase CH_4 absorption in the sources in which it has been detected are all consistent with warm (∼70–100 K) gas. If CH_4 were not trapped, it would evaporate at a much lower temperature, and line ratios consistent with T_{rot} as low as ∼30 K would be expected. Hence, it is possible that some CH_4 toward this source may yet be trapped in the icy dust grain mantle. The H_2O-ice column density toward HL Tau is $\sim 1.4 \times 10^{18}$ cm^{-2} (Tegler et al. 1995). If we assume that the abundance of CH_4 ice is up to ∼2% relative to water (consistent with the values/upper limits determined for other YSOs), then there could be at most 2.8×10^{16} cm^{-2} CH_4 in the ice. CO ice has not been detected toward HL Tau, and Tegler et al. (1995) derive an upper limit of 1×10^{16} cm^{-2}. This would bring our maximum possible (ice+gas) CH_4/CO ratio to ∼0.4%, which is somewhat lower than but still consistent with observations of massive YSOs.

4. MODEL DISCUSSION

Using our derived rotational temperature of ∼100 K for the CO absorption lines (Brittain et al. 2004), the inferred temperature for the water ice absorption (∼80–100 K), and comparing to disk models, we can estimate the region of the disk from which most of the absorption occurs. Chiang et al. (2001) used spectral energy distributions to model temperature profiles in disks surrounding T Tauri stars. According to their Figure 5, 100 K material corresponds to distances of ∼1–10 AU from the parent star (depending on the vertical height in the disk). This is the same region modeled by Markwick et al. (2002), who investigated the chemistry in the inner (1–10 AU) region of the protoplanetary disk around a T Tauri star (corresponding to midplane temperatures of ∼60–700 K). For this reason, we compare our results to this model.

Markwick et al. (2002) based their chemical model on that by Willacy et al. (1998) and investigated cases including and excluding X-ray ionization. They took into account a vertical temperature profile and the effect of adsorption of several key species, including CH_4, onto an icy grain mantle. They determined column densities for many species, including CH_4 and CO, at 1, 5, and 10 AU. In all cases, the CH_4 and CO column densities were comparable, resulting in $CH_4/CO \sim 1$ (shown as a plus sign in Fig. 3). This is more than 2 orders of magnitude greater than our estimated upper limit for the total gas+ice CH_4/CO column density ratio toward HL Tau.

This discrepancy may be due in part to model assumptions. The chemical model of Willacy et al. (1998) assumed that elements were initially atomic at 100 AU. They also ran a dark cloud model to determine the initial composition and found the results for both models to be similar for most species, including CH_4. However, the initial abundance of CH_4 was likely overestimated in these models since, as pointed out by Willacy & Langer (2000), starting with atomic C and a high H/H_2 ratio results in an efficient production of CH_4 that disagrees with observational constraints. They suggested modifications that reduce production of CH_4 by a factor of 10. It is not clear whether or not this reduced input will entirely compensate for the factor of greater than 100 difference between the results of Markwick et al. (2002) and our upper limit for HL Tau. We suggest that additional modeling of the inner regions of protostellar disks is needed as well as additional searches for CH_4 in disks around other young stars to see whether our result is general or specific to HL Tau. In particular, it would be valuable to search for methane gas toward sources that have lost most of their icy grain mantle material, ensuring that any methane would reside in the gas.

As an interesting comparison, Figure 3 also shows the range of CH_4/CO values for eight Oort Cloud comets from Gibb et al. (2003). Oort Cloud comets are thought to have formed in the giant planet region (5–40 AU) of the protoplanetary disk before being gravitationally scattered into the Oort Cloud. CH_4 and CO both vary by over an order of magnitude in the comet population (when compared to water), but CH_4/CO (0.1–0.8) is much higher than that toward HL Tau or massive YSOs. Clearly there was some mechanism for either producing methane in the solar disk or selectively maintaining it on icy dust mantles during the comet formation process, assuming that the solar nebula was similar in composition to star-forming regions today. For example, if CH_4 was trapped in a polar (water-dominated) ice matrix and if the grains were never heated enough to evaporate the polar mantle, then methane could have been retained. However, CO ice exists predominantly in the more volatile apolar mantle, which requires much lower temperatures (~30 K) to evaporate. Hence, there is a range of temperatures (~30–90 K) at which CO would evaporate but at which methane could be retained on the icy grain mantles. This is one possible mechanism that could explain an enhancement of the CH_4/CO ratio in comets.

5. CONCLUSION

We derive a very low (<0.02%) 3 σ upper limit for the CH_4/CO gas ratio in the disk surrounding the T Tauri star HL Tau. If we assume that methane ice could be trapped in the icy mantles of dust grains, then our upper limit of 0.4% is somewhat lower than but not inconsistent with the total (ice+gas) CH_4/CO determined toward other star-forming regions (Boogert et al. 1997, 1998). This low abundance suggests that gas-phase reactions have not significantly enhanced the methane column density toward this T Tauri object.

It is important to ascertain whether or not this is also the case for disks around other T Tauri stars. This result shows the need for improved models of the disk chemistry in the inner regions surrounding T Tauri stars and for further observations to search for minor volatile constituents in these poorly studied regions. It also shows the necessity of studying both disks around young stars and comets, the most pristine solar system bodies, to understand chemical evolution through the planet formation process. It is hoped that by increasing the sample of well-studied comets and disks around young stars, we can bridge the gap in chemical evolution from infall through planet formation.

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