HOT ORGANIC MOLECULES TOWARD A YOUNG LOW-MASS STAR: A LOOK AT INNER DISK CHEMISTRY

F. Lahuis, 1,2 E. F. van Dishoeck, 1 A. C. A. Boogert, 3 K. M. Pontoppidan, 1,4 G. A. Blake, 4 C. P. Dullemmond, 5 N. J. Evans II, 6 M. R. Hogerheide, 1 J. K. Jørgensen, 7 J. E. Kessler-Silacci, 6 and C. Knez 6

Received 2005 August 18; accepted 2005 November 28; published 2005 December 28

Abstract

Spitzer Space Telescope spectra of the low-mass young stellar object (YSO) IRS 46 ($L_{bol} \approx 0.6 L_{\odot}$) in Ophiuchus reveal strong vibration-rotation absorption bands of gaseous C$_2$H$_2$, HCN, and CO$_2$. This is the only source out of a sample of ~100 YSOs that shows these features, and this is the first time that they are seen in the spectrum of a solar-mass YSO. Analysis of the Spitzer data combined with Keck L- and M-band spectra reveals excitation temperatures of $\geq 350$ K and abundances of $10^{-6}$ to $10^{-5}$ with respect to H$_2$, orders of magnitude higher than those found in cold clouds. In spite of this high abundance, the HCN $J = 4-3$ line is barely detected with the James Clerk Maxwell Telescope (JCMT), indicating a source diameter less than 13 AU. The (sub)millimeter continuum emission and the absence of scattered light in near-infrared images limit the mass and temperature of any remnant collapsing envelope to less than 0.01 $M_{\odot}$ and 100 K, respectively. This excludes a hot-core–type region as found in high-mass YSOs. The most plausible origin of this hot gas rich in organic molecules is in the inner ($< 6$ AU) region of the disk around IRS 46, either the disk itself or a disk wind. A nearly edge-on two-dimensional disk model fits the spectral energy distribution (SED) and gives a column of dense warm gas along the line of sight that is consistent with the absorption data. These data illustrate the unique potential of high-resolution infrared spectroscopy to probe the organic chemistry, gas temperatures, and gas kinematics in the planet-forming zones close to a young star.

Subject headings: infrared: ISM — ISM: individual (IRS 46) — ISM: jets and outflows — ISM: molecules — planetary systems: protoplanetary disks — stars: formation

1. INTRODUCTION

The presence of gas-rich disks around young stars is well established observationally and theoretically (see review by Geaves 2005), but comparatively little is known about their chemical structure. A good understanding of the chemistry is important since a fraction of the gases and solids in protoplanetary disks will end up in future solar systems where they may form the basis for prebiotic species (see reviews by Ehrenfreund & Charnley 2000 and Markwick & Charnley 2004). Virtually all observational studies of molecules other than CO have been limited to the outer regions, where simple organic molecules such as HCO$^+$, CN, HCN, and H$_2$CO have been detected at millimeter wavelengths (e.g., Dutrey et al. 1997; Kastner et al. 1997; Qi et al. 2003; Thi et al. 2004). Because of beam dilution, these observations cannot probe radii $< 50$ AU from the star, which is the relevant zone for planet formation. High-resolution infrared (IR) spectroscopy has found CO emission from the warm dense gas in the inner disk region (Najita et al. 2003; Brittain et al. 2003; Blake & Boogert 2004), but H$_2$O is the only molecule besides CO and H$_2$ that has been convincingly detected (Carr et al. 2004).

Models of inner disk chemistry initially focused on our own primitive solar nebula (see review by Prinn 1993) but now also consider exosolar systems. They have grown considerably in sophistication, including nonequilibrium chemistry, gas-solid interactions, radial and vertical mixing, and the effects of UV radiation and X-rays from the central star on the gas temperature and molecular abundances (e.g., Markwick et al. 2002; Gail et al. 2004; Glassgold et al. 2004; Gorti & Hollenbach 2004). Large concentrations of organic molecules like C$_2$H$_2$ and HCN are predicted in some of these models in the inner few AU, but no observational tests have been possible to date.

The sensitive Infrared Spectrograph (IRS) on board the Spitzer Space Telescope opens a new window to study molecules in disks through IR pencil-beam line-of-sight absorption spectroscopy. The Spitzer c2d Legacy program “From Molecular Cores to Planet-forming Disks” (Evans et al. 2003) is collecting a coherent sample of IRS spectra of low-mass YSOs in five nearby star-forming regions. To date more than 100 Class I and Class II sources have been observed. Of these only one source, IRS 46, shows strong gas-phase absorption bands of hot molecules. These gas-phase bands have previously been seen only toward deeply embedded high-mass YSOs, where they have been associated with the inner ($\sim 1000$ AU) warm dense regions of the spherical envelopes, also known as “hot cores” (Carr et al. 1995; Lahuis & van Dishoeck 2000; Boonman et al. 2003). The sources studied with Spitzer have factors of $10^4$ to $10^5$ lower luminosity, thus limiting the maximum temperatures and amount of warm gas in the envelope.

IRS 46, also known as YLW 16b and GY 274, is part of the Ophiuchus cloud at a distance of $\sim 125$ pc (de Geus et al. 1989). It is classified as a Class I source, i.e., a protostar with a compact accretion disk embedded in a more extended and collapsing envelope, based on its near- and mid-IR colors (André & Montmerle 1994) with $L_{bol} \approx 0.6 L_{\odot}$ (Bontemps et al. 2001). However, the complete SED is also consistent with a Class II source viewed nearly edge-on, i.e., a pre–main-sequence star with a disk but without a significant collapsing envelope (see § 4). It is similar...
High-resolution L- and M-band spectra ($R \approx 25,000$) were obtained with NIRSPEC at the Keck II telescope$^8$ to provide kinematic information and confirmation of the Spitzer HCN detection through the CO $v = 1\rightarrow 0$ 4.7 $\mu$m and HCN $v_1 = 1\rightarrow 0$ 3.0 $\mu$m stretching mode rovibrational bands (see Fig. 3). The $^{13}$CO absorption lines are unresolved at the quiescent cloud velocity of $V_{\rm LSR} \approx 4$ km s$^{-1}$. However, the resolved $^{12}$CO ($\Delta V \approx 30$ km s$^{-1}$) and HCN ($\Delta V \approx 20$ km s$^{-1}$) absorption lines are observed to be shifted, at $V_{\rm LSR} \approx -20$ km s$^{-1}$. Of these no counterpart is observed in the HCN $J = 4\rightarrow 3$ and CO $J = 3\rightarrow 2$ JCMT spectra. We associate the HCN, CH$_3$, CO$_2$ absorptions seen in the Spitzer spectra with the blueshifted components.

3. ANALYSIS

The Spitzer spectra are analyzed using a pure absorption model assuming local thermodynamic equilibrium (LTE) excitation of the levels at a single temperature. The adopted method is described in detail in Lahuis & van Dishoeck (2000) and Boonman et al. (2003), and includes references to the molecular parameters and data used in the model. The main fit parameters are the average temperature and integrated column-density of the gas.

$^8$ The W. M. Keck Observatory is operated as a scientific partnership among Caltech, the University of California, and NASA and is made possible by the W. M. Keck Foundation.

---

$^9$ The JCMT is operated by the JAC in Hilo, Hawaii on behalf of PPARC (UK), NRC (Canada), and NWO (Netherlands).
With cm sorption in the latter two determinations, all estimates are consistent with respect to both H$_2$ and CO, is up to 4 orders of magnitude larger than that found in cold interstellar clouds. The 9.7 $\mu$m band responds to assuming a conversion factor: $n(CO)/(n(H_2)+n(CO))$ corresponding to an H$_2$ abundance of (all gas-phase carbon in CO), as required to thermalize HCN and C$_2$H$_2$.

Therefore, $b$ is taken to range from 2 to 12 km s$^{-1}$. The best fits to the C$_2$H$_2$ $\nu_3$, HCN $\nu_1$, and CO$_2$ $\nu_3$, bands observed in the IRS spectrum give $T_{\text{ex}}$ of $\sim 700, 400, 300$ K and column densities of 3, 5, and $10 \times 10^{16}$ cm$^{-2}$, respectively, for $b \approx 5$ km s$^{-1}$. The uncertainty in $b$ results in an uncertainty of 25% in these values. The blueshifted CO $\nu_1 = 1$–0 absorption band gives $T_{\text{ex}} = 400 \pm 100$ K and $N = (2 \pm 1) \times 10^{14}$ cm$^{-2}$ corresponding to a minimum H$_2$ column density of $1 \times 10^{22}$ cm$^{-2}$ assuming a CO abundance of $2 \times 10^{-4}$ (all gas-phase carbon in CO), as appropriate for warm dense gas. The 9.7 $\mu$m silicate depth corresponds to $N_{\text{H}_2} = 3 \times 10^{23}$ cm$^{-2}$ assuming a conversion factor: $N_{\text{H}_2} = 3.5 \times 10^{17}$ cm$^{-2}$ (see Draine 2003). X-ray observations give $N_{\text{H}_2} = 11(\pm 7) \times 10^{17}$ cm$^{-2}$ (Inamishi et al. 2001). Assuming most hydrogen is in H$_2$ and allowing for some foreground absorption in the latter two determinations, all estimates are consistent with $N(H_2) = 1 \times 10^{23}$ cm$^{-2}$ within a factor of 2. The resulting abundance estimates are 3, 5, and $10 \times 10^{-4}$ for C$_2$H$_2$, HCN, and CO$_2$, respectively. The density of the gas is at least $10^9$ cm$^{-3}$, required to thermalize HCN and C$_2$H$_2$.

Additional constraints can be obtained from a combined analysis of the HCN $\nu_1$ and $\nu_3$ bands (Fig. 3). Assuming the same excitation temperature for both bands, the required column density to fit the $\nu_1$ band is higher by a factor of 4 than that found from the $\nu_3$ band. This suggests that geometrical effects and emission filling in the absorption may play an important role (see Boonman et al. 2003). One possibility is that the absorbing region is smaller than the continuum-emitting region, the size of which may depend on wavelength. Similar increases may be expected for C$_2$H$_2$ and CO$_2$. Thus, the above cited abundances are lower limits. The inferred HCN abundance, with respect to both H$_2$ and CO, is up to 4 orders of magnitude larger than that found in cold interstellar clouds.

4. DISCUSSION

Where does this hot gas rich in organic molecules reside? The first clue comes from the HCN submillimeter JCMT spectrum. For a HCN column density of $>10^{17}$ cm$^{-2}$ derived from the IR data, the $J = 4$–3 pure rotational line is highly optically thick. Thus, $T_{\text{mb}}$ is expected to be close to the excitation temperature of $\sim 400$ K if the emission would fill the beam. Although a weak emission line is observed at $V_{\text{LSR}} = 4$ km s$^{-1}$, the broad $-20$ km s$^{-1}$ component is not detected with a $3 \sigma$ limit of 0.02 K in a 1 km s$^{-1}$ bin. This gives a beam dilution $>2 \times 10^4$ that, for the JCMT beam size of $15''$, implies a source diameter for the hot gas of $<0\prime\prime11$ or 13 AU diameter at the distance of Ophiuchus. A similar limit follows from the lack of a blue wing on the CO $J = 3$–2 line.

The second clue comes from the high temperatures and densities of the molecular gas. In general, temperatures of a few hundred kelvins are found in YSO environments only in the innermost part of envelopes or in the inner disks. The velocity of the hot gas provides a final clue. The radial velocity of IRS 46 is unknown, and it is possible that IRS 46 itself is at a velocity of $-20$ km s$^{-1}$ (Doppmann et al. 2005). More likely, however, IRS 46 is close to the nominal cloud velocity of 4.4 km s$^{-1}$, and the hot gas is blueshifted by $\sim 25$ km s$^{-1}$.

Based on these arguments, three possibilities are considered for the location of this hot gas: (1) the inner layer of any remnant collapsing envelope on scales $\leq 100$ AU around IRS 46; (2) the inner $\leq 10$ AU regions of a nearly edge-on disk; and (3) dense hot gas at the footpoint of a wind launched from the inner disk. The first two options are examined through radiative transfer models to constrain the physical parameters of the source environment.

To explore the first option, a spherically symmetric model with a power-law density distribution was constructed by reproducing the Submillimeter Common-User Bolometric Array continuum map and the SED of IRS 46 from mid-IR to submillimeter wavelengths following Jørgensen et al. (2002). This model has two severe problems: to reproduce the mid-IR continuum emission, the temperature in the innermost envelope cannot exceed roughly 100 K, and an $-0.01$ M$_\odot$ envelope (estimated from the submillimeter continuum data) produces a significant scattering nebula at near-IR wavelengths that is not observed in VLT-ISAAC images (Pontoppidan et al. 2005). The envelope model also cannot explain the line widths and velocities unless IRS 46 itself is at $-20$ km s$^{-1}$. Thus, most of the IR and submillimeter continuum emission must arise from the disk around IRS 46.

To investigate the second option, the physical structure of the IRS 46 disk was constrained from the observed SED in a manner similar to CRBR 2422.8$-$3423 (Pontoppidan et al. 2005) using the two-dimensional axisymmetric Monte Carlo radiative transfer code of Dullemond & Dominik (2004). Figure 4 shows the temperature and density structure of the hot inner part of the nearly edge-on self-shadowed flaring disk, and Figure 1 shows the best-fitting SED. There is some degeneracy in the parameters of the best-fitting model (see the discussion in Pontoppidan et al. 2005), but spatially resolved data are needed to further constrain the fits. The fit to the silicate feature is sensitive to the assumed opacities, emission from the outer disk, and the presence of foreground absorption; these uncertainties have little impact on the part of the disk model relevant to this work, i.e., the dense inner disk region.

The main continuum contribution from the disk at 3–14 $\mu$m comes from the puffed up inner rim and inner rim wall on the far side of the star. In the disk model, the integrated column of dense gas ($>10^9$ cm$^{-2}$) toward these areas is in the range $(1-2) \times 10^{22}$ cm$^{-2}$, with average temperatures of 300–1500 K. This is consistent with the H$_2$ column density and temperatures derived from the observations (see § 3). Indeed, more generally, the observed temperatures are consistent with disk models that explicitly calculate the gas temperature in the inner disk. The
gas temperatures may be even higher than the dust temperatures in the upper layers (Glassgold et al. 2004; Gorti & Hollenbach 2004). The velocity-broadened CO and HCN profiles (Fig. 3) could result from absorption in the Keplerian inner rim at 0.1 AU ($V_{\text{sh}} \approx 70 \text{ km s}^{-1}$ for a 0.5 $M_\odot$ star). If IRS 46 is at the cloud velocity of $+4 \text{ km s}^{-1}$, the blueshifted absorption implies a deviation from Keplerian rotation in the disk plane, for example, as the result of a close binary. A near edge-on disk explanation is consistent with a detection toward only one in a hundred objects, since a very small fraction of sources should have the right orientation.

A blueshifted velocity may also indicate that the observed absorption features originate in a wind emanating from the inner disk. Possibilities include a magnetocentrifugal wind (either an X-wind launched within 0.1 AU or a disk wind launched farther out), a photoevaporative flow, or a stellar wind interacting with the upper layer and entraining molecular material (see, e.g., Eisloffel et al. 2000). For the gas to be seen in absorption, it must be comparable in size to the inner disk region responsible for the 14 μm background, i.e., a few AU in radius. For a smaller region the background continuum will dominate, whereas for a much larger region line emission from the warm molecular gas will fill in or dominate the absorption. For a few AU region, the mass-loss rate would be of order $10^{-7}$ to $10^{-5} M_\odot$ yr$^{-1}$, assuming a density of $\geq 10^5$ cm$^{-3}$, a total H$_\text{2}$ column of $10^{22}$ cm$^{-2}$, and a flow velocity of $\sim 25$ km s$^{-1}$. IRS 46 does not show strong accretion signatures, and so a higher flow rate seems unlikely. Quantitative predictions in terms of velocities, column densities, densities, and temperatures of the molecular gas are needed to distinguish between the above models.

Regardless of the precise origin in the disk or disk wind, the high inferred excitation temperatures of 400–900 K and high abundances of HCN and C$_2$H$_2$ of $10^{-6}$ to $10^{-5}$ are characteristic of high-temperature chemistry. Hot chemistry in general is dominated by evaporation of the molecules from the grains with subsequent gas-phase processing. At high temperatures, the hydrocarbon and nitrogen chemistries are enhanced as much of the oxygen is converted into water by neutral-neutral reactions. The abundances of molecules such as C$_x$H$_y$, CH$_4$, and HCN can be increased by orders of magnitude (e.g., Doty et al. 2002; Rodgers & Charnley 2003), while at the same time the formation of CO$_2$ is reduced since its primary formation route through OH is blocked. Interestingly, CO$_2$ has a lower excitation temperature in our observations. The most recent models of inner disk chemistry predict enhanced abundances of HCN and C$_2$H$_2$. In particular, Markwick et al. (2002) give HCN, C$_2$H$_2$, and CO$_2$ abundances of $10^{-6}$ to $10^{-5}$ in the inner 1 AU of a protoplanetary disk, in good agreement with the abundances found in this work.

In summary, we present the first detection of gaseous molecular absorption bands with Spitzer toward a solar-mass YSO. These bands offer direct, unique probes of hot organic chemistry in its immediate environment. In addition, they provide independent constraints on the gas temperatures and velocity patterns. The most plausible scenario is that the absorption originates from the inner few AU of the circumstellar disk, perhaps at the footpoint of a disk wind. Further work, both observationally and theoretically, is required to prove this, including a determination of the velocity of IRS 46 itself and monitoring of the infrared lines at high spectral resolution to check for time variability of the radial velocity and/or absorbing column along the line of sight. This detection offers prospects for future high spectral and spatial resolution mid-infrared and submillimeter searches for these and other organic molecules in emission in more face-on disks.

We are grateful to J. Carr and J. Najita for useful discussions and to R. Tilanus for carrying out the JCMT observations. Astrochemistry in Leiden is supported by a Spinoza grant from NWO. Support for this work, part of the Spitzer Legacy Science Program, was provided by NASA through contracts 1224608, 1250779, and 1256316 issued by the Jet Propulsion Laboratory, California Institute of Technology, under NASA contract 1407.

REFERENCES

André, P., & Montmerle, T. 1994, ApJ, 420, 837
Blake, G. A., & Boogert, A. C. A. 2004, ApJ, 606, L73
Bontemps, S., et al. 2001, A&A, 372, 173
Boonman, A. S. M., van Dishoeck, E. F., Lahuis, F., & Doty, S. D. 2003, A&A, 399, 1063
Brittain, S. D., Rettig, T. W., Simon, T., Kulesa, C., DiSanti, M. A., & Dello Russo, N. 2003, ApJ, 588, 535
Carr, J. S., Evans, N. J., Lacy, J. H., & Zhou, S. 1995, ApJ, 450, 667
Carr, J. S., Tokunaga, A. T., & Najita, J. 2004, ApJ, 603, 213
de Geus, E. J., de Zeeuw, P. T., & Lub, J. 1989, A&A, 216, 44
Doppmann, G. W., Greene, T. P., Covey, K. R., & Lada, C. J. 2005, AJ, 130, 1145
Doty, S. D., van Dishoeck, E. F., van der Tak, F. F. S., & Boonman, A. M. S. 2002, A&A, 389, 446
Draine, B. T. 2003, ARA&A, 41, 241
Dullemond, C. P., & Dominik, C. 2004, A&A, 417, 159
Dutrey, A., Guilloteau, S., & Güell, M. 1997, A&A, 317, L55
Ehrenfreund, P., & Charnley, S. B. 2000, ARA&A, 38, 427
Eisloffel, J., Mundt, R., Ray, T. P., & Rodríguez, L. F. 2000, in Protostars and Planets IV, ed. V. Mannings, A. P. Boss, & S. S. Russell (Tucson: Univ. Arizona Press), 815
Evans, N. J., et al. 2003, PASP, 115, 965
Gail, H.-P. 2002, A&A, 390, 253
Glassgold, A. E., Najita, J., & Igea, J. 2004, ApJ, 615, 972
Gorti, U., & Hollenbach, D. 2004, ApJ, 613, 424
Greaves, J. S. 2005, Science, 307, 68
Ilgner, M., Henning, Th., Markwick, A. J., & Millar, T. J. 2004, A&A, 415, 643
Inamishi, K., Koyama, K., & Tsuboi, Y. 2001, ApJ, 557, 747
Jørgensen, J. K., Schöier, F. L., & van Dishoeck, E. F. 2002, A&A, 389, 908
Kastner, J. H., Zuckerman, B., Weintraub, D. A., & Forveille, T. 1997, Science, 277, 67
Kessler-Silacci, J. E., et al. 2005, ApJ, in press (astro-ph/0511092)
Lahuis, F., & van Dishoeck, E. F. 2000, A&A, 355, 699
Markwick, A. J., & Charnley, S. B. 2004, in ASL3 305, Astrobiology: Future Perspectives, ed. P. Ehrenfreund et al. (Dordrecht: Kluwer), 33
Markwick, A. J., Ilgner, M., Millar, T. J., & Henning, Th. 2002, A&A, 385, 632
Najita, J., Carr, J. S., & Mathieu, R. D. 2003, ApJ, 589, 931
Pontoppidan, K. M., Dullemond, C. P., van Dishoeck, E. F., Blake, G. A., Boogert, A. C. A., Evans, N. J., Kessler-Silacci, J. E., & Lahuis, F. 2005, ApJ, 622, 463
Pontoppidan, K. M., et al. 2003, A&A, 408, 981
Prinn, R. G. 1993, in Protostars and Planets III, ed. J. H. Levy & J. I. Lunine (Tucson: Univ. Arizona Press), 1005
Qi, C., Kessler, J. E., Koerner, D. W., & Sargent, A. I., & Blake, G. A. 2003, ApJ, 597, 986
Ridge, N. A., et al. 2006, AJ, submitted
Rodgers, S. D., & Charnley, S. B. 2003, ApJ, 585, 355
Thi, W.-F., van Zadelhoff, G.-J., & van Dishoeck, E. F. 2004, A&A, 425, 955