DISCOVERY OF INTERSTELLAR ACETYLENE

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ABSTRACT

Absorption by interstellar acetylene (C_2H_2) has been detected in the spectra of three infrared sources embedded in molecular clouds. One or more lines in the 13.7 μ m v_5 vibration-rotation band were detected toward GL 2591, W3 IRS 5, and OMC-1 IRc2. The observations require C_2H_2 abundances $\sim 3 \times 10^{-4}$ to 10^{-3} of CO. Such abundances can be explained by models in which the molecular clouds are chemically unevolved or in which gas phase abundances have been enhanced by recent evaporation of grain mantles.

Subject headings: interstellar: abundances — interstellar: molecules — stars: pre-main-sequence —

infrared: spectra

I. INTRODUCTION

The chemical composition of interstellar clouds has been a subject of extensive study since the discovery of the first polyatomic molecules 20 years ago. More than 70 species have now been detected, almost all through their microwave and millimeter-wave rotational emission lines. However, several molecules, notably CH_4 , C_2H_2 , and other symmetric hydrocarbons, are predicted to be quite abundant, but have not been observed at millimeter wavelengths because their symmetry forbids dipole rotational transitions. In contrast, these molecules do have permitted infrared vibration-rotation transitions. Infrared transitions of methane (CH_4) and acetylene (C_2H_2) have been seen in absorption in circumstellar shells, but have not been reported from interstellar clouds. Absorption by interstellar CH_4 has been searched for by Knacke *et al.* (1982), but not detected.

We realized that, although it is predicted to be somewhat less abundant than CH₄, C₂H₂ could be significantly easier to detect. Unlike CH_4 , C_2H_2 is a linear molecule, so has its population distributed among a small number of rotational states. In addition, there is relatively little interference by telluric C_2H_2 . We chose to search for absorption by lines in the v_5 vibration-rotation band of C_2H_2 at 13.7 μ m. The v_5 band is the strongest vibration-rotation band of C₂H₂ and is stronger than any band of CH₄. In addition, it falls at a wavelength accessible to a new multichannel echelle spectrometer which is more sensitive to weak absorption lines than previously used instruments. Although the atmospheric transmission near 13.7 μm is severely affected by CO₂ lines, there are C₂H₂ lines at wavelengths with adequate transparency. The v_5 vibration is the symmetric bending mode of the linear C_2H_2 $(H-C \equiv C-H)$ molecule. The v₅ band has P(J' = J - 1), Q(J' = J), and R(J' = J + 1) branches, with 3:1 statistical weight alternations favoring odd-J lines [J(J')] is the rotational quantum number of the lower (upper) vibrational state]. The Q-branch, which contains half the opacity of the band in the case of a bending mode of a linear molecule, is particularly interesting observationally as many rotational states can be observed in a narrow spectral region. See Herzberg (1945, pp. 384–388) for an energy level diagram and a discussion of the spectrum of C_2H_2 .

In this Letter we report the detection of interstellar C_2H_2 in absorption toward three infrared sources embedded in molecular clouds, GL 2591, W3 IRS 5, and OMC-1 IRc2. The sources were chosen on the basis of previous CO absorption line studies, and for OMC-1, the interesting chemistry of the region.

II. OBSERVATIONS

The observations were made with a cryogenic echelle spectrograph (Lacy *et al.* 1987) on the NASA IRTF 3 m telescope on the nights of 1988 October 13–16. The instrument measures 64 point spectra at 10 positions along a slit. For these observations, the slit length was 4", the slit width was 1", and the spectral resolution was ~ $0.05 \text{ cm}^{-1} (\lambda/15,000 \text{ or } 20 \text{ km s}^{-1})$. The system NEFD was ~10 Jy (1 σ in 1 s).

Three spectral intervals of ~0.9 cm⁻¹ were observed, centered at 729.3 cm⁻¹ [including the $v_5 = 0-1 Q(1)-Q(10)$ lines of C_2H_2], 743.4 cm⁻¹ [the R(5) line], and 755.2 cm⁻¹ [the R(10) line]. Four sources were observed: GL 2591 at R(10), W3 IRS 5 and OMC-1 IRc2 in all three intervals, and OMC-1 IRc4 in the Q-branch interval. Integration times were typically 1 hr. Mu Cephei and Alpha Tauri were used as comparison stars to remove variations in instrumental response and atmospheric absorption. A check was made for intrinsic spectral features in μ Cep and α Tau by comparing them to α Aur; no stellar features were apparent.

III. RESULTS

The spectra of the R(5) line, R(10) line, and Q-branch are shown in Figures 1–3, respectively. In each figure the top two spectra are raw spectra of α Tau and OMC-1 IRc2. Below

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LACY ET AL.



FIG. 1.—Spectra of the $v_5 R(5)$ line of C_2H_2 at 743.26 cm⁻¹. The top two are observed spectra. Below them are ratioed spectra and fits to the ratios. FIG. 2.—Spectra of the $v_5 R(10)$ line of C_2H_2 at 755.01 cm⁻¹

them are divided spectra and fits to the divided spectra. In Figure 3, a spectrum of narrow-line gas is also plotted to show the line positions in the Q-branch. As the features in the undivided spectra were caused both by the instrument and the atmosphere, no corrections for differing air mass were made before dividing by the comparison star. In all cases, the source



FIG. 3.—Spectra of the $v_5 Q$ -branch of C_2H_2 . The Doppler scale is referred to the Q(1) line at 729.17 cm⁻¹. The bottom spectrum shows the structure of the Q-branch from Q(10) on the left to Q(1). Note the intensity enhancement of the odd-J lines.

and the comparison star were observed at air masses which agreed to within 0.2. Several atmospheric features are nearly opaque (the peak transmission near 729 cm⁻¹ is <30%, the minimum <2%). The noise in the divided spectra increases markedly near such features, particularly in cases where there are slight wavelength shifts between source and comparison star spectra. In regions of relatively constant atmospheric transmission the SNR is $\gtrsim 100$. Near strong atmospheric lines it is ~10 times worse.

Several arguments support our identification of the observed lines with C_2H_2 . First, it is extremely unlikely that another molecule could have a *Q*-branch and two lines coincident with those observed. Second, the unusual strength of the v_5 band and the linear nature of C_2H_2 means that nearly any other molecule would have to be much more abundant than C_2H_2 to account for the observed absorption.

The divided spectra were fitted with Gaussian absorption lines on sloping continua, with the positions, depths, and widths of the lines, and levels and slopes of the continua as free parameters. (For two of the spectra, a quadratic fit to the continuum was required.) In the Q-branch region, the model included lines from Q(1) to Q(12), with the relative strengths based on a thermal distribution of the rotational populations. For OMC-1 IRc2, two temperature components were required to produce a good fit to the data. Column densities in the observed rotational states were derived using the line strengths of Varanasi, Giver, and Valero (1983). The derived parameters are given in Table 1.

It is very difficult to determine the uncertainties in the C_2H_2 parameters, as they result primarily from systematic errors in the correction for atmospheric transmission and instrumental response variations. For the R(5) and R(10) spectra, the lines are in regions of relatively constant instrumental and atmospheric transmission, so are not terribly sensitive to differences in air mass or wavelength shifts between the source and comparison star. Attempts were made to correct for such differences, and it was possible to improve the appearance of the divided spectra in the regions of strong atmospheric absorp-

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	TABLE	1	
Derived Parameters			
Parameter	GL 2591	W3 IRS 5	OMC-1 IRc2
	R(5)		
$v_{LSR} (km s^{-1}) \dots m_{v_v} (km s^{-1})^b \dots m_{v_v} (cm^{-1})^c \dots m_{v_v} (cm^{-2})^d$	 	 <4 × 10 ⁻² <4 × 10 ¹⁴	-35^{a} 43 3.0×10^{-2} 3.2×10^{15}
<i>N</i> j (chi)	 R(10)	<4×10	5.5 × 10
(lens a = 1)		Nr	
$ \begin{aligned} v_{\text{LSR}} & (\text{km s}^{-1}) & \dots \\ \Delta v & (\text{km s}^{-1})^{\text{b}} & \dots \\ w_{v} & (\text{cm}^{-1})^{\text{c}} & \dots \\ N_{J} & (\text{cm}^{-2})^{\text{d}} & \dots \end{aligned} $	$ \begin{array}{r} -20 \\ 25 \\ 2.6 \times 10^{-3} \\ 3.1 \times 10^{14} \end{array} $	$< 3 \times 10^{-3}$ < 4 × 10 ¹⁴	$-6401.4 \times 10^{-2}1.7 \times 10^{15}$
	Q		
$w_{v} (cm^{-1})^{e} \dots N_{J=1-10} (cm^{-2})^{e} \dots T(K) \dots V_{LSR} (km s^{-1}) \dots \Delta v (km s^{-1})^{b} \dots \dots$	··· ··· ···	$ \begin{array}{r} < 4.8 \times 10^{-2} \\ < 3.3 \times 10^{15} \\ 68 \\ -10 \\ 34 \end{array} $	$\begin{array}{c} 0.13\\ 9.0\times10^{15}\\ 25; > 300^{\rm f}\\ -9; \ -9^{\rm f}\\ 13; \ 90^{\rm f} \end{array}$
	Total		
$N_{C_{2H_2}}(cm^{-2})^{g}$	>1.2 × 10 ^{16 h}	<4.2 × 10 ¹⁵	$3.1 \times 10^{15};$ > 1.5×10^{16}
N _{co} C ₂ H ₂ /CO	1.2×10^{19} i > 1 $\times 10^{-3}$	$1.3 \times 10^{19 \text{ j}}$ < 3 × 10 ⁻⁴	$> 1.3 \times 10^{19}$ k $\sim 10^{-3}$

^a Wavelength calibration very uncertain.

^b Observed FWHM; not corrected for instrumental resolution.

 $w_v = \int \tau \, dv.$

^d $N_J = (6.9 \times 10^{16})[(2J + 1)/(J + 2)]w_v$ for *R*-branch lines.

 $N_J = (6.9 \times 10^{16}) W_v$ for Q-branch lines.

^f Fitted by eye.

⁸ $N_{\text{total}} = Q_r e^{E_J kT} N_J / [g_I (2J + 1)]$, where $Q_r \approx 2kT/hcB$, and $g_I = 3$ for J odd, $g_I = 1$ for J even.

^h Assuming same temperature as CO (Mitchell *et al.* 1989).

ⁱ For the gas components contributing to the C_2H_2 R(10) line; Mitchell *et al.* 1989.

^j Mitchell 1989.

^k Geballe and Wade 1985 and Scoville et al. 1983.

tion, but in most cases the derived C_2H_2 parameters were not significantly affected ($\leq 30\%$). The Q-branch spectra were much more affected by atmospheric absorption, as the deepest atmospheric absorption is coincident with the Q(1) line. The spectrum of W3 IRS 5 is particularly suspect as two features appear in the corrected spectrum which coincide with atmospheric H₂O lines. There is no evidence of uncorrected H₂O absorption in OMC 1 IRc2, and we feel confident in the reality of the Q-branch detection there. The apparent structure within the Q-branch, attributed by the fitting program to individual Q-branch lines, is much less certain, however.

Additional uncertainties arise from the likelihood of unresolved structure within the lines. Gas from the observed sources probably has linewidths significantly less than our resolution. If the absorption by this gas is saturated, the column densities would be underestimated. Alternatively, gas near the stars may emit significantly in the C_2H_2 lines or reemit the absorbed radiation. Either effect could fill in the absorption lines, again causing column densities to be underestimated. Including all uncertainties, we estimate that the derived C_2H_2 column densities may be in error by as much as a factor of 2.

For the purpose of determining the abundance of C_2H_2 relative to other molecules we compare the C_2H_2 column densities to previously determined CO column densities, derived from absorption-line studies near 4.7 μ m wavelength. As those observations sample the same lines of sight as the C_2H_2 observations, the comparison should be reasonably reliable, although the possibility of different distributions of C_2H_2 and CO along the line of sight should be kept in mind.

a) GL 2591

Only the R(10) line was observed toward GL 2591 (Fig. 2). Mitchell et al. (1989) observed CO vibrational absorption toward this source at 4.7 μ m wavelength and found several gas components at different temperatures and velocities. They found two gas components at $v_{LSR} = -11$ km s⁻¹, one with T = 38 K and $N_{CO} = 7.2 \times 10^{18}$ cm⁻², the other with T = 1000 K and $N_{CO} = 5.6 \times 10^{18}$ cm⁻². A third component was found at $v_{LSR} = -28$ km s⁻¹, with T = 200 K and $N_{CO} = 6.6 \times 10^{18}$ cm⁻². As the C₂H₂ absorption is centered at -20km s⁻¹, it seems likely that it is due to blended absorptions by the 200 K and the 1000 K gas. The 38 K gas would not contribute noticeably to the R(10) line. If we assume that the C_2H_2/CO abundance ratio is the same in the 200 K and 1000 K gas, we can derive the column density of C_2H_2 in the ground vibrational state for these two components; $N_{C_2H_2} = 1.2$ $\times 10^{16}$ cm⁻², and C₂H₂/CO = 1.0 $\times 10^{-3}$. If the 1000 K C_2H_2 is in vibrational LTE, the total C_2H_2 abundance in this gas is 7.4 times that in the ground vibrational state. If only the infrared inactive vibrational modes are in LTE, the total abundance is 3.1 times that in the ground state. As the excited state populations depend strongly on the rather uncertain 1000 K value, we choose not to correct for them, but the derived C_2H_2/CO ratio should be considered a lower limit.

b) W3 IRS 5

The R(5), R(10), and Q-branch regions were observed toward W3 IRS 5 [R(5) and Q-branch spectra are shown in Figs. 1 and 3]. The R-branch lines were not detected, a result consistent with the observed Q-branch depth. The Q-branch was fitted with $N_{C_2H_2} = 4 \times 10^{15}$ cm⁻², T = 68 K, and $\Delta v = 34$ km s⁻¹ (FWHM). We note, however, that the fit to the Q-branch is not particularly good, and the two strongest absorptions are coincident with telluric H₂O lines. As some part of the apparent Q-branch absorption may be due to uncorrected H₂O absorption, the derived $N_{C_2H_2}$ will be considered to be an upper limit.

Mitchell (1989) observed CO absorption toward W3 IRS 5, and found two dominant gas components, one with $N_{\rm CO} = 6.5 \times 10^{18}$ cm⁻² and T = 50 K, the other with $N_{\rm CO} = 7 \times 10^{18}$ cm⁻² and T = 470 K. Comparing the total $N_{\rm CO}$ to our C_2H_2 upper limit gives $C_2H_2/CO < 3 \times 10^{-4}$. A fit was also made to the C_2H_2 spectrum including the two temperature components seen in CO. These results were not significantly changed.

c) OMC-1 IRc2

Absorptions due to the C_2H_2 R(5) and R(10) lines and the Q-branch were detected toward OMC-1 IRc2 (Figs. 1-3). The Q-branch spectrum shows evidence for two gas components: cold narrow-line gas with $T \approx 25$ K and $\Delta v < 20$ km s⁻¹, and hot broad-line gas with T > 300 K and $\Delta v > 50$ km s⁻¹. The column density in J = 1-10, derived from the equivalent width of the measured region of the Q-branch, is 9×10^{15} cm⁻². The C₂H₂ column density summed over all rotational levels must be several times larger, depending on the temperature of the hot gas. The R(5) and R(10) absorption lines indicate a factor of ~1.5-2 times more than C_2H_2 than derived from the Qbranch. Because of the much better atmospheric transmission for the R-branch lines and their lower optical depths, the conclusions from the R-branch lines should probably be given more weight than those from the Q-branch. In addition, the region around IRc2 is known to be complicated, with substan-

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L46

tial extinction variations. Small pointing differences could easily account for the discrepancies between the different lines.

One CO absorption line [12 CO v = 1-0 R(2)] has been observed toward IRc2 by Geballe and Wade (1985). They find the line to have essentially the same depth, width, and velocity as that seen toward the nearby Becklin-Neugebauer (BN) object, and suggest that similar gas lies along the lines of sight to IRc2 and BN. Given the large column of C_2H_2 toward IRc2, the larger extinction toward IRc2 than BN, and the likelihood of saturation of the ¹²CO line, it is perhaps best to simply take N_{co} toward BN as a lower limit to that toward IRc2. Scoville *et al.* (1983) give $N_{\rm CO} = 1.3 \times 10^{19}$ cm⁻² toward BN, suggesting $C_2H_2/CO \approx 10^{-3}$ toward IRc2. Note, however, that this ratio is very uncertain, as both column densities are lower limits.

The region of the Q-branch was also observed toward IRc4, \sim 7" SW of IRc2. The light from IRc4 is seen through much less extinction than is IRc2. Consistent with expectations, Qbranch absorption was not detected, with a limit about onethird that seen toward IRc2.

IV. COMPARISON WITH MODELS

The published models of molecular cloud chemistry predict widely varying C_2H_2 abundances, with C_2H_2/CO ranging from 10^{-6} to 10^{-1} . In the three sources in which we detected C_2H_2 absorption, we find $C_2H_2/CO \approx 3 \times 10^{-4}$ to 10^{-3} .

Early attempts to understand the chemistry of molecular clouds concentrated on two basic models, dominated by either ion-molecule reactions in the gas phase or neutral-neutral reactions on grain surfaces. In both cases, equilibrium abundances were calculated. An example of the first type of model is described by Viala (1986). Although he calculated quite high C_2H_2 abundances in diffuse clouds ($A_v = 1$), he and others have consistently predicted very little C_2H_2 (~10⁻⁶ of CO) in dense clouds like those we observed. In contrast, Allen and Robinson (1977) investigated the effects of grain-surface reactions on molecular cloud chemistry by making a model including only these reactions. They predicted much more C₂H₂ $(\sim 10^{-2} \text{ to } 10^{-1} \text{ of CO})$ than we observe.

Recently, several authors have discussed variations on the original models, including time dependent chemistry and the combined effects of gas-phase and grain-surface reactions. The newer models agree much better with our observations than do the earlier ones. Millar and Nejad (1985) and Herbst and Leung (1986) calculate time-dependent models in which initially atomic gas clouds evolve chemically at constant density and temperature. They both find that abundances of complex molecules, including C_2H_2 , peak at ~10⁵ yr into the calculation, and then fall to the equilibrium abundances. Herbst and Leung calculate a peak C_2H_2/CO ratio of 3×10^{-3} for a dense dark cloud, falling to 2.5×10^{-5} after $\sim 10^7$ yr. Millar and Nejad find about 4 times higher abundances, apparently due to different assumed reaction rates for unmeasured reactions, especially those in which oxygen atoms breakdown hydrocarbon chains (Millar, Leung, and Herbst 1987). Our observed C_2H_2/CO ratios are intermediate between the peak and steady state predictions of both models, suggesting chemical ages of molecular clouds $\sim 10^6$ yr. This chemical age is considerably less than the $\gtrsim 10^7$ yr cloud ages based on other arguments (e.g., Bash, Green, and Peters 1977; Leisawitz, Bash, and Thaddeus 1989).

A means of producing chemically unevolved molecular abundances in a cloud much older than 10⁶ yr has been suggested by Brown, Charnley, and Millar (1988; see also Blake et al. 1987). They combine gas-phase and grain-surface reactions, but make rather different assumptions about grain-surface reactions from those of Allen and Robinson (1977). Brown et al. assume that the primary effect of dust grains is to allow molecules to freeze out and that the only reactions that occur in the molecular mantles formed on grains are reactions which add H to C, N, O and their hydrides to form CH₄, NH₃, and H₂O. They find that the freeze-out time scale is $\sim 10^6$ yr, resulting in mantle abundances like those in the gas phase at this time, when complex molecules are near their peak abundances. They then suggest that if at some later time a region of the molecular cloud is heated by the formation of a star, the grain mantles evaporate, resulting in gas phase abundances characteristic of chemically unevolved molecular clouds. They predict $C_2H_2/CO \sim 10^{-2}$ after evaporation of the mantles. This ratio is larger than we observe, but depends on the assumptions made about gas-phase reactions, the freeze-out time scale, and the fraction of the gas which is frozen.

The Brown et al. model and the similar model of Blake et al. (1987) seem particularly appropriate in the present context, in that we necessarily observe gas near embedded stars. In addition, they were motivated by a desire to explain the Orion "hot core" abundances, observed near IRc2. If such a model is the correct explanation for the hot core abundances, our observations of moderately abundant C₂H₂ in W3 and GL 2591 suggest they also have unusual molecular abundances.

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