

## INTERSTELLAR ABSORPTION LINES TOWARD NGC 2264 AND AFGL 2591: ABUNDANCES OF H<sub>2</sub>, H<sub>3</sub><sup>+</sup>, AND CO

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### ABSTRACT

High-resolution infrared spectra of NGC 2264 IRS reveal interstellar absorption lines of CO near 2.3  $\mu\text{m}$  wavelength and provide upper limits on the strengths of lines of H<sub>2</sub> at 2.12 and 2.22  $\mu\text{m}$  and of H<sub>3</sub><sup>+</sup> at 3.72  $\mu\text{m}$ . Toward NGC 2264, the interstellar CO exhibits a uniform rotational excitation temperature,  $T_{\text{rot}} = 28^{+6}_{-4}$  K for levels  $J = 0-6$  and has a total column density  $N(\text{CO}) = (5.0 \pm 1.2) \times 10^{18} \text{ cm}^{-2}$ . The true abundance of CO is  $N(\text{CO})/N(\text{H}_2) > 5 \times 10^{-5}$  if the hydrogen is thermalized at  $T = 28$  K, and the abundance of H<sub>3</sub><sup>+</sup> is less than  $3 \times 10^{-4}$  times that of CO. Similar spectra of AFGL 2591 provide an upper limit on the column density of H<sub>3</sub><sup>+</sup> of  $5 \times 10^{15} \text{ cm}^{-2}$ . These limits on H<sub>3</sub><sup>+</sup> and measurements of CO and H<sub>2</sub> are in harmony with theoretical expectations if the clouds are exposed to cosmic-ray ionization rates of the order of  $10^{-16} \text{ s}^{-1}$  or less. The limit for NGC 2264 is particularly interesting in relation to the tentative identification of H<sub>2</sub>D<sup>+</sup> in submillimeter emission in that direction. If the H<sub>2</sub>D<sup>+</sup> detection is real, then our limit on H<sub>3</sub><sup>+</sup> implies  $\text{H}_2\text{D}^+/\text{H}_3^+ > 0.05$ .

*Subject headings:* clusters: open — infrared: spectra — interstellar: abundances — interstellar: molecules — molecular processes

### I. INTRODUCTION

Interstellar clouds are now known to contain more than 70 different molecular species. Molecules regulate some aspects of cloud structure and evolution and provide diagnostic probes of physical conditions, composition, and chemical history of clouds. Elaborate theories of interstellar chemistry have been developed to account for the observed abundances and distributions of atoms and molecules. Comparison of observation and theory requires accurately determined abundances. The interpretation of radiofrequency emission lines is often complicated by saturation effects and by uncertain corrections for excitation of unobserved energy levels. Worse, many species of interest entirely lack allowed radiofrequency transitions. High-resolution infrared absorption spectroscopy can overcome some of these limitations and complement data on emission lines. Two species are particularly worthy of note in this regard. The most abundant interstellar molecule, H<sub>2</sub>, has not yet been observed directly in thick, quiescent molecular clouds. The molecular ion, H<sub>3</sub><sup>+</sup>, which is central to all theories of ion-molecule chemistry and which is thought to control deuterium fractionation in many species, has also eluded detection. In this work, we discuss sensitive searches for an infrared line of H<sub>3</sub><sup>+</sup> toward the highly obscured sources NGC 2264 IRS and AFGL 2591. For the former, the same measurements yield direct limits on the column densities of H<sub>2</sub> and provide infor-

mation on the abundance and excitation of CO. Our limits on H<sub>3</sub><sup>+</sup> can be compared with results of a recent infrared measurement of CO at  $\lambda 4.6 \mu\text{m}$  toward AFGL 2591 by Mitchell *et al.* (1989).

H<sub>3</sub><sup>+</sup> was long ago predicted to be a constituent of the interstellar medium (Martin, McDaniel, and Meeks 1961; Stecher and Williams 1969, 1970). Estimates of its abundance and discussions of its effects on interstellar chemistry date back to the work of Herbst and Kemperer (1973) and Watson (1976). The H<sub>3</sub><sup>+</sup> abundance in dense molecular clouds has been discussed recently by Lepp, Dalgarno, and Sternberg (1987). According to most theories of interstellar ion-molecule chemistry, the abundance of H<sub>3</sub><sup>+</sup> is governed by the rate of ionization of H<sub>2</sub> by penetrating cosmic rays and by the rates with which H<sub>3</sub><sup>+</sup> reacts destructively with electrons and with various neutral atoms and molecules. Although the rate of destruction of cold (i.e., ground-state) H<sub>3</sub><sup>+</sup> through dissociative electron capture remains controversial (Smith and Adams 1984; Michels and Hobbs 1984; Macdonald, Biondi, and Johnsen 1984; Hus *et al.* 1988; Amano 1988; Adams and Smith 1989), its removal in dense molecular clouds is dominated by reactions with abundant neutrals like CO and O and is fairly well understood (e.g., Marquette, Rebrion, and Rowe 1989). Thus, the abundance of H<sub>3</sub><sup>+</sup> may provide an excellent probe of the cosmic-ray ionization.

Oka (1981) pointed out that H<sub>3</sub><sup>+</sup> might be observable in the interstellar medium through lines of its  $\nu_2$  vibration-rotation band measured in absorption toward highly obscured infrared stars. Oka presented a weak limit on the column density of H<sub>3</sub><sup>+</sup>

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toward Orion BN. More recently, Geballe and Oka (1989) have measured upper limits on  $H_3^+$  toward several infrared sources. Geballe and Oka have concentrated on searches for a line from the  $(J''K'') = (10)$  level and have presented a single upper limit for the  $\tilde{\nu} = 2457 \text{ cm}^{-1}$  line that arises in the (11) state. The  $(JK) = (11)$  level is the lowest level of the para modification of  $H_3^+$  and is the very lowest rotational level of the molecule (see Fig. 1 of Pan and Oka 1986 for an energy level diagram). The lowest level of the ortho modification,  $(JK) = (10)$ , lies  $22.83 \text{ cm}^{-1}$  (32.8 K in temperature units) above the ground level. The (11) level is expected to be the most populous level at low temperature ( $T < 50 \text{ K}$ , see below). In the  $\nu_2$  fundamental band of  $H_3^+$ , there are four potential interstellar absorption lines that arise in (11) and two lines that originate in (10). The observations presented here are of the  $2691 \text{ cm}^{-1}$  line that arises in the (11) ground level. This transition was selected because the atmospheric transmission is good, and a narrow-band blocking filter is readily available at that frequency. Owing to its symmetrical structure,  $H_3^+$  lacks an allowed pure rotational spectrum, although it does have very weak, distortion-induced dipole transitions (Pan and Oka 1986; Miller and Tennyson 1988).

In contrast, the deuterated form of the ion,  $H_2D^+$ , has a large permanent dipole moment and strong rotational transitions. Phillips *et al.* (1985) have reported the possible detection of the  $1_{10}-1_{11}$  transition of  $H_2D^+$  at  $372.4213 \text{ GHz}$  in emission toward NGC 2264. This observation suggests that the corresponding column density of  $H_3^+$  could easily be  $N(H_3^+) \approx 10^{14} \text{ cm}^{-2}$  or larger, depending on the excitation of  $H_2D^+$ . This provided the main motivation to search for absorption lines toward the bright infrared source NGC 2264 IRS, also known as Allen's star (Allen 1972) and as AFGL 989.

One of the brightest (at  $\lambda \approx 3-5 \mu\text{m}$ ) of all deeply embedded infrared sources is AFGL 2591. Mitchell *et al.* (1989) have recently reported observations of interstellar CO absorption lines in the  $4.6 \mu\text{m}$  spectrum of this source at a resolution of approximately  $8 \text{ km s}^{-1}$ . The lines of  $^{12}\text{CO}$  are heavily saturated. The corresponding lines of  $^{13}\text{CO}$  are at worst lightly saturated and reveal the presence of two velocity components. The component identified with the quiescent molecular cloud also contains highly excited  $^{13}\text{CO}$  with a rotational excitation temperature  $T_{\text{rot}} \approx 1000 \text{ K}$  and vibrationally excited  $^{12}\text{CO}$  ( $v = 1$ ).

## II. OBSERVATIONS AND ANALYSIS

AFGL 2591 and NGC 2264 IRS were observed with the Fourier Transform Spectrometer (FTS) at the coudé focus of the 4 m telescope of Kitt Peak National Observatory on 1986 August 18–20 and 1988 December 16–19, respectively. In both instances, the unapodized resolution was  $0.02 \text{ cm}^{-1}$ , which corresponds to a resolution in Doppler velocity of  $2.2 \text{ km s}^{-1}$  at  $\tilde{\nu} = 2691 \text{ cm}^{-1}$  ( $H_3^+$ ) and  $1.4 \text{ km s}^{-1}$  at  $\tilde{\nu} = 4264 \text{ cm}^{-1}$  (CO). The instrument is described by Hall *et al.* (1979). It is a two-beam interferometer which can be configured with a dichroic beamsplitter in order to record two bandpasses simultaneously with two pairs of InSb detectors. The two bandpasses in these measurements were isolated with a cold K band filter ( $\tilde{\nu} = 4100-5000 \text{ cm}^{-1}$ ) and a temperature-tuned interference filter (OCLI N03796,  $\tilde{\nu} \approx 2691 \text{ cm}^{-1}$ ) with a width of approximately  $8 \text{ cm}^{-1}$ . The sum of outputs from the two beams is a photometric signal, while their difference is the interferometric signal. The ratio of difference signal to sum signal is recorded as the interferogram, and it automatically compensates for seeing fluctuations and guiding errors. In practice, only the K

band contributed significantly to the sum signal. Both infrared sources are invisible to the guiding camera, hence guiding was accomplished by monitoring the photometric signal. Total integration times were 8.1 and 17.2 hr on AFGL 2591 and NGC 2264, respectively. In total, eight nights have been allocated for the observation of NGC 2264, although the telescope dome could be opened on only three of those nights owing to inclement weather.

Each interferogram (eight for AFGL 2591 and 12 for NGC 2264) was transformed using the standard NOAO procedures. Similar interferograms of higher signal-to-noise (S/N) ratio were recorded and transformed for the comparison sources Sirius, CW Leo (=IRC + 10°216), and Mars. Telluric absorption was removed by ratioing of the source and comparison spectra. The ratioed spectra were combined and the lines and noise were measured. Unfortunately, Mars could not be used as a comparison for the K band measurements of NGC 2264, because the CO in the atmosphere of Mars and in the interstellar medium toward NGC 2264 happened to have identical apparent Doppler velocities in December 1988. The final spectra of NGC 2264 are displayed in Figures 1 and 2. Interstellar absorption lines were measured by least-squares fits of Gaussian functions to the combined, ratioed spectra. The equivalent width of a line is

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

where  $\Delta I/I_0 = (I_0 - I)/I_0$  is the amplitude of the line as a fraction of the fitted continuum level in the vicinity of the line and  $\Delta \tilde{\nu}$  is its full width at half-peak in  $\text{cm}^{-1}$ . The measured line parameters for NGC 2264 are listed in Table 1. Uncertainties in measured equivalent widths are determined from the fitting errors in the Gaussian parameters and are quoted at the level of one standard deviation ( $1 \sigma$ ). That the centers of strong telluric lines lie accurately at zero intensity suggests that errors due to continuum placement are negligible in these spectra, which have peak S/N  $\approx 10$ . Where no interstellar lines are apparent, uncertainties correspond to fluctuations about a linear continuum in the vicinity of the expected line position. All upper limits are quoted as  $3 \sigma$  limits for lines of width equal to the resolution.

An unsaturated line has an equivalent width

$$W_{\tilde{\nu}} = \frac{\pi e^2}{mc^2} N_l f = 8.853 \times 10^{-13} N_l f \text{ cm}^{-1}, \quad (2)$$

where  $N_l$  is the column density in the lower state in  $\text{cm}^{-2}$  and  $f$  is the absorption oscillator strength of the line. The CO (2, 0) lines are slightly saturated, so that column densities were determined from curve-of-growth analyses with Doppler broadening parameters inferred from the measured line widths as described below.

Frequencies of the CO lines are from Pollock *et al.* (1983), and oscillator strengths are from Chackerian and Tipping (1983). The oscillator strengths adopted here are approximately 17% larger than those based on the theoretical work of Kirby-Docken and Liu (1978) and tabulated by Black and Willner (1984). The line frequencies for  $H_2$  are based on the work of Bragg, Brault, and Smith (1982), and the oscillator strengths are derived from the transition probabilities of Turner, Kirby-Docken, and Dalgarno (1977). For  $H_3^+$  the frequency of the  $\nu_2(J'G'U') - (J''K'') = (21-1) - (11)$  line mea-

INTERSTELLAR H<sub>2</sub>, H<sub>3</sub><sup>+</sup>, AND CO

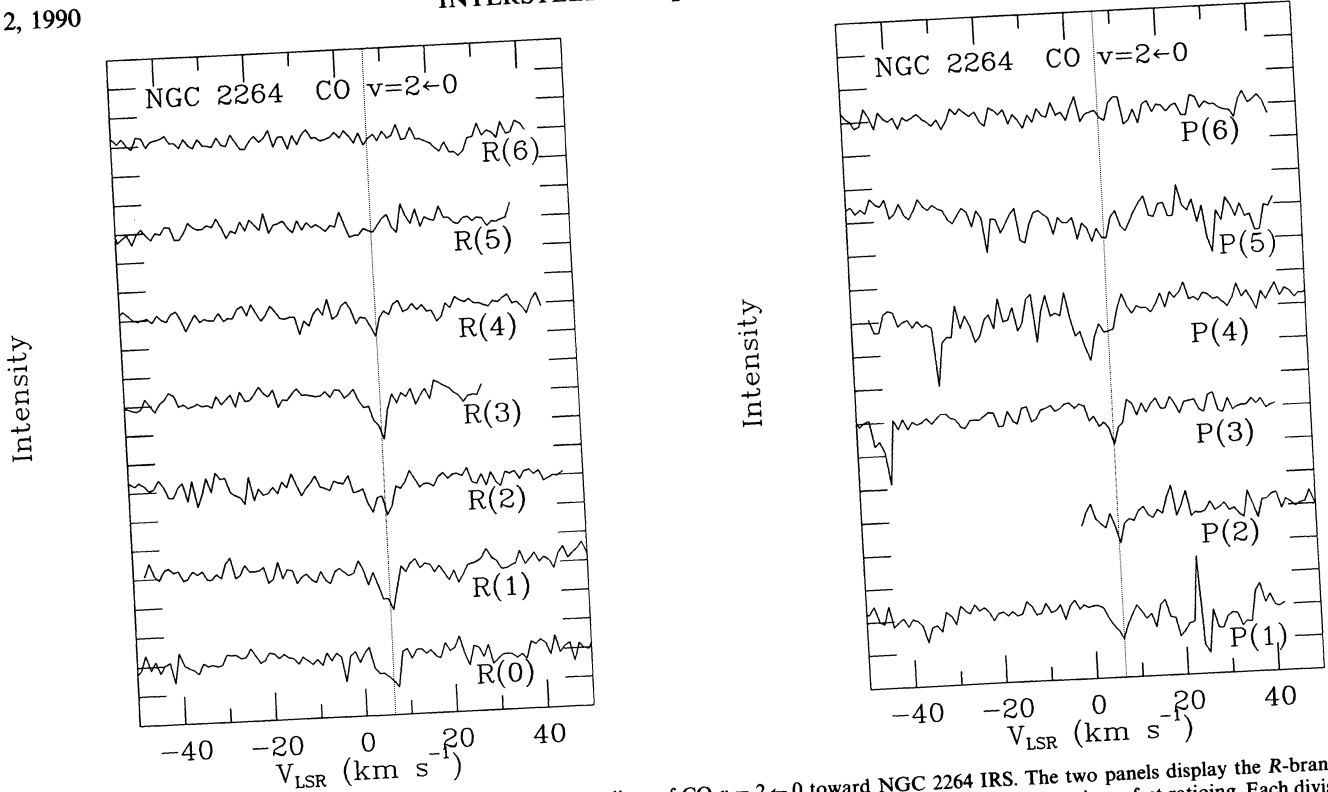


FIG. 1.—Summed spectra in the vicinities of interstellar absorption lines of CO  $v = 2 \leftarrow 0$  toward NGC 2264 IRS. The two panels display the R-branch and P-branch lines separately. Atmospheric features have been divided out, although some large excursions in the noise result from imperfect ratioing. Each division on the vertical scale is 0.5 in relative intensity, and the mean continuum level of each segment of spectrum lies at 1.0 on this scale. The vertical dotted line marks the mean radial velocity,  $V_{\text{LSR}} = 6.4 \text{ km s}^{-1}$ , of the measured absorption lines.

measured by Majewski *et al.* (1987) is identical to that published previously by Oka (1981). The absorption oscillator strength has been derived from the transition probability computed by Miller and Tennyson (1988). Note that the entries in Table 2 of Miller and Tennyson which are labelled  $A_{if}$  are actually  $(2J' + 1)A_{if}$ , where  $J'$  is the angular momentum quantum number

of the upper state ( $v_2 = 1$ ) and  $A_{if}$  is the spontaneous transition probability in  $\text{s}^{-1}$  (S. Miller 1989, private communication). The H<sub>3</sub><sup>+</sup> oscillator strengths in Table 2 of Black and van Dishoeck (1989) should therefore all be divided by the factor  $(2J' + 1)$ . Both  $f$  and  $A_{if}$  are consistent with a dipole transition matrix element of 0.16 D for the  $v_2$  fundamen-

TABLE 1  
OBSERVED LINES: NGC 2264 IRS

Species	Transition	$\tilde{\nu}^a$ ( $\text{cm}^{-1}$ )	$f$	$W_\nu$ ( $\text{cm}^{-1}$ )	$\Delta V^b$ ( $\text{km s}^{-1}$ )	$V_{\text{LSR}}$ ( $\text{km s}^{-1}$ )
CO	(2, 0) R(0)	4263.837197	8.78 (-8)	$0.026 \pm 0.009$	$\leq 2.9$	+6.9
	(2, 0) R(1)	4267.542065	5.89 (-8)	$0.040 \pm 0.008$	$3.7 \pm 0.7$	+6.2
	(2, 0) P(1)	4256.217139	2.89 (-8)	$0.019 \pm 0.011$	$4.4 \pm 2.1$	+6.5
	(2, 0) R(2)	4271.176630	5.33 (-8)	$0.047 \pm 0.012$	$6.1 \pm 1.1^c$	+5.8 <sup>e</sup>
	(2, 0) P(2)	4252.302244	3.45 (-8)	$0.027 \pm 0.012$	$2.0 \pm 0.7$	+7.0
	(2, 0) R(3)	4274.740746	5.11 (-8)	$0.035 \pm 0.007$	$2.6 \pm 0.5$	+6.4
	(2, 0) P(3)	4248.317632	3.67 (-8)	$0.024 \pm 0.009$	$3.2 \pm 1.9$	+6.1
	(2, 0) R(4)	4278.234264	5.00 (-8)	$0.020 \pm 0.007$	$1.5 \pm 0.3$	+6.2
	(2, 0) P(4)	4244.263453	3.79 (-8)	$0.022 \pm 0.015$	$3.1 \pm 1.5$	+6.7
	(2, 0) R(5)	4281.657040	4.94 (-8)	$0.012 \pm 0.009$	...	...
	(2, 0) P(5)	4240.139851	3.85 (-8)	$\leq 0.019$	...	...
	(2, 0) R(6)	4285.008925	4.90 (-8)	$0.004 \pm 0.008$	...	...
	(2, 0) P(6)	4235.946976	3.89 (-8)	$\leq 0.007$	...	...
	(2, 0) R(7)	4288.289774	4.89 (-8)	$\leq 0.010$	...	...
H <sub>2</sub>	(1, 0) S(0)	4497.8391	9.37 (-14)	$< 0.0092$	...	...
	(1, 0) S(1)	4712.9054	5.46 (-14)	$< 0.0125$	...	...
H <sub>3</sub> <sup>+</sup>	$v_2 2_{1,-1} - 1_1$	2691.444	1.78 (-5)	$\leq 0.014$	...	...

<sup>a</sup> All line positions are vacuum values at rest. Uncertainties in measured properties are 1  $\sigma$ ; upper limits are 3  $\sigma$ .  
<sup>b</sup> Entries in this column are the FWHM corrected for instrumental broadening.  
<sup>c</sup> Interference by a telluric feature.

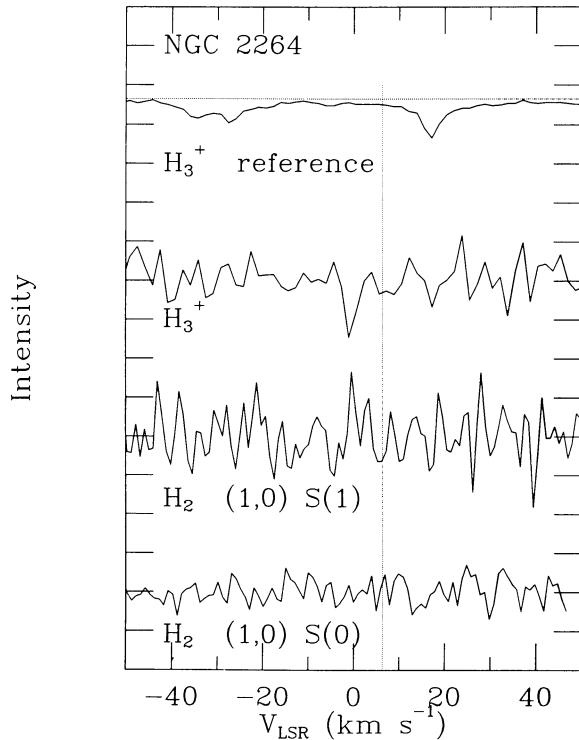


FIG. 2.—Spectra around the expected position of interstellar lines of  $H_2$  and  $H_3^+$  in NGC 2264 IRS. The top spectrum is the atmospheric reference spectrum in the vicinity of the  $H_3^+$  line at  $2691.444 \text{ cm}^{-1}$ . The second spectrum is that of NGC 2264 IRS around the expected position of the  $H_3^+$  line after the atmospheric reference has been divided out. The lowest two spectra are of the regions around the  $H_2(1,0) S(1)$  and  $S(0)$  lines after ratioing. All spectra are on a common scale of radial velocity, and the vertical dotted line indicates the mean velocity measured for the CO lines,  $V_{\text{LSR}} = 6.4 \text{ km s}^{-1}$ . Each division on the vertical scale is 0.5 in relative intensity, and the mean continuum levels of the three lowest spectra lie at 1.0 on this scale. The mean continuum level of the top spectrum is shown as a horizontal dotted line.

tal band. The adopted molecular data are summarized in Table 1.

### III. RESULTS

#### a) NGC 2264

The final ratioed spectra in the vicinities of several CO lines are shown in Figure 1. Spectra in the vicinities of the  $H_2(1,0) S(1)$ ,  $H_2(1,0) S(0)$ , and  $H_3^+ v_2(J'G'U') - (J''K'') = (21-1) - (11)$  lines are shown in Figure 2. Expected positions of the interstellar features at the same radial velocities as the measured CO lines are indicated.

CO absorption lines arising in  $J = 0-4$  are clearly present. The measured equivalent widths  $W_v$ , the line widths  $\Delta V$ , and radial velocities with respect to the local standard of rest  $V_{\text{LSR}}$ , are listed in Table 1. The mean line width (FWHM) after correction for instrumental broadening  $\Delta V = 2.9 \pm 1.0 \text{ km s}^{-1}$  and the corresponding Doppler broadening parameter is  $b = 1.75 \pm 0.60 \text{ km s}^{-1}$ . The strongest, most highly saturated lines have central optical depths

$$\tau_0 = 1.497 \times 10^{-7} \frac{N_J f}{\bar{v} b} \approx 1.0 - 1.6 ; \quad (3)$$

therefore, the corrections for saturation are at worst a factor of 2 in derived column density. We derive column densities from  $W_v$  using single-component curves of growth for  $b = 1.75 \pm 0.6$

TABLE 2  
NGC 2264 IRS: DERIVED PROPERTIES

Species	Level	Line	$\log N_J$ ( $\text{cm}^{-2}$ )	$N_J$ ( $\text{cm}^{-2}$ )
CO	$J = 0$	R(0)	$17.63 \pm 0.20$	4.3 (17)
		R(1)	$18.11 \pm 0.19$	...
	$J = 1$	P(1)	$17.88 \pm 0.34$	...
		mean	$18.05 \pm 0.17$	1.1 (18)
		R(2)	$18.31 \pm 0.31$	...
	$J = 2$	P(2)	$18.05 \pm 0.25$	...
		mean	$18.17 \pm 0.20$	1.5 (18)
		R(3)	$18.07 \pm 0.15$	...
	$J = 3$	P(3)	$17.98 \pm 0.20$	...
		mean	$18.04 \pm 0.12$	1.1 (18)
		R(4)	$17.74 \pm 0.17$	...
	$J = 4$	P(4)	$17.86 \pm 0.37$	...
		mean	$17.76 \pm 0.15$	5.8 (17)
		R(5)	$17.35 \pm 0.42$	...
	$J = 5$	P(5)	$< 17.75$	...
mean		...	2.3 (17)	
R(6)		$16.9_{-\infty}^{+0.6}$	...	
$J = 6$	P(6)	$< 17.28$	...	
	mean	...	8.5 (16)	
	R(7)	$< 17.36$	$< 2.3$ (17)	
Total			5.0 (18)	
$H_2$	$J = 0$	S(0)	...	$< 1.1$ (23)
	$J = 1$	S(1)	...	$< 2.6$ (23)
	$J = 1^a$	...	...	$< 2.2$ (21)
	Total <sup>a</sup>			$< 1.1$ (23)
$H_3^+$	$J_K = 1_1$	...	...	$\leq 8.9$ (14)
	Total <sup>a</sup>			$\leq 1.4$ (15)

<sup>a</sup> Assuming that the rotational excitation temperature is the same as that measured for CO,  $T_{\text{rot}} = 28.0 \text{ K}$ .

$\text{km s}^{-1}$  and tabulate the results in Table 2. The uncertainties in column density  $N_J$  combine the measurement errors and the effects of the uncertainty in  $b$ . The total column density of CO is

$$N(\text{CO}) = \sum_{J=0}^6 N_J = (5.0 \pm 1.2) \times 10^{18} \text{ cm}^{-2}.$$

Figure 3 shows the dependence of column density in level  $J$

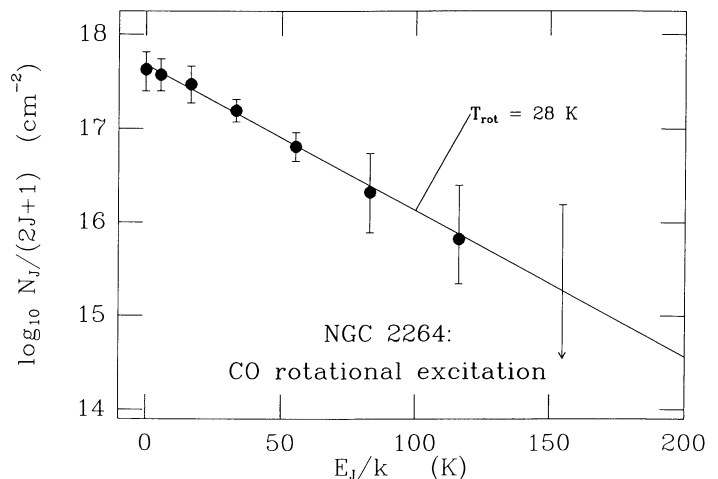


FIG. 3.—Excitation diagram for CO toward NGC 2264. The column density in level  $J$ ,  $N_J$ , divided by the statistical weight of the level, is plotted on a logarithmic scale vs. the excitation energy of level  $J$ ,  $E_J/k$  in K, where  $E_0 = 0.0$  for level  $J = 0$ . The solid line is the expected behavior for thermal excitation at a temperature  $T_{\text{rot}} = 28 \text{ K}$ .



upon the excitation energy of the level. The slope of the best-fit straight line yields a uniform rotational excitation temperature  $T_{\text{rot}} = 28 \pm 4$  K. In all that follows, we adopt this as the true excitation temperature of CO and equate it with the kinetic temperature of the absorbing gas. The populations in  $J > 6$  contribute less than 1% to the total column density at  $T = 28$  K.

We find no evidence of a hotter component of CO nor of any high-velocity gas like that detected in the much stronger (1, 0) lines of CO at  $\lambda 4.6 \mu\text{m}$  toward AFGL 2591 and Orion OMC-1 (Geballe and Wade 1985; Scoville *et al.* 1983; Mitchell *et al.* 1989). A column density of  $10^{17} \text{ cm}^{-2}$  in hot, disturbed CO could easily be hidden in the noise of our spectra, however. The signal-to-noise ratio of our data is too low to place any useful constraints on the strengths of  $^{13}\text{CO } v = 2 \leftarrow 0$  lines.

The derived column densities and line widths of CO imply large line-center optical depths in the pure rotational lines at millimeter wavelengths:  $\tau_0 \approx 45, 133, 184,$  and  $165$  for the  $J = 1-0, 2-1, 3-2,$  and  $4-3$  lines, respectively. This means that a uniform thermal distribution for  $J = 0$  to  $5$  at the kinetic temperature is readily maintained by rotational line trapping even at rather low densities. A 10 level statistical equilibrium calculation shows that the current infrared measurements place only a weak limit,  $n(\text{H}_2) > 300 \text{ cm}^{-3}$ , on the density of the absorbing gas. This is limited by the uncertainty in the relative column density in  $J = 5$ . In the future, measurements like these, but with much higher signal-to-noise, could be used to determine densities based on the value of  $J$  at which the level population begins to deviate from that expected for uniform excitation (see Fig. 3).

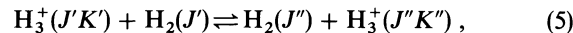
We searched unsuccessfully for absorption lines of the (1, 0) vibration-rotation band of H<sub>2</sub>. Although these are forbidden electric quadrupole transitions, the large abundance of H<sub>2</sub> may make them detectable. If the level populations of H<sub>2</sub> are thermalized by reactive, ortho-para interchange collisions (Dalgarno, Black, and Weisheit 1973) at low temperature,  $T \leq 100$  K, then the expected equivalent width of a weak (1, 0) S(0) line is

$$W_v = 0.0083 \left[ \frac{N(\text{H}_2)}{10^{23} \text{ cm}^{-2}} \right] \left[ \frac{1}{1 + 9 \exp(-170.5/T)} \right] \text{ cm}^{-1}. \quad (4)$$

Our (3  $\sigma$ ) upper limit on (1, 0) S(0) implies a column density of H<sub>2</sub> in  $J = 0$  of  $N_0 < 1.1 \times 10^{23} \text{ cm}^{-2}$ . The limit on the (1, 0) S(1) line is poorer, and no useful limit on (1, 0) Q(1) is possible. It is likely that the  $J = 0$  and 1 level populations are thermalized at  $T = 28$  K by reactive collisions with H<sup>+</sup> and H<sub>3</sub><sup>+</sup>. In this case, the direct limit on H<sub>2</sub> toward NGC 2264 IRS is  $N(\text{H}_2) < 1.1 \times 10^{23} \text{ cm}^{-2}$ , an amount that would be expected for a visual extinction  $A_V < 126$  mag, if the gas-to-extinction ratio has a typical interstellar value (Savage *et al.* 1977). If we assume that all molecules are distributed uniformly along the absorbing column, then the derived fractional abundance is  $\text{CO}/\text{H}_2 > 4.6 \times 10^{-5}$ . This implies that more than 6% of a solar carbon abundance is in the form of CO.

In the H<sub>3</sub><sup>+</sup> spectrum (Fig. 2), there is a "feature" at  $\tilde{\nu} = 2691.366 \text{ cm}^{-1}$  which has  $\Delta V = 3 \text{ km s}^{-1}$  and  $W_v = 0.014 \pm 0.004 \text{ cm}^{-1}$ . The 3  $\sigma$  uncertainty in equivalent width per resolution element is  $0.013 \text{ cm}^{-1}$ . The radial velocity of this "feature" is  $V_{\text{LSR}} = -0.7 \text{ km s}^{-1}$ , which differs substantially from that of the observed CO lines and from the velocities of any molecular features observed at radio frequencies. Thus we

do not believe that H<sub>3</sub><sup>+</sup> is present and quote an upper limit of  $W_v < 0.014 \text{ cm}^{-1}$ . The limit on column density in the (J, K) = (1, 1) level of H<sub>3</sub><sup>+</sup> is  $N(1, 1) < 8.9 \times 10^{14} \text{ cm}^{-2}$ . As suggested by Oka (1981) and discussed further by Black and van Dishoeck (1989) and Geballe and Oka (1989), it is likely that rapid proton-interchange reactions



equilibrate the populations of the lowest rotational levels at the kinetic temperature of the gas. In this case, the excitation at low temperatures ( $T \leq 100$  K) is given by  $n(1, 0)/n(1, 1) = 2 \exp(-32.8/T)$ , and the corresponding limit on the total column density of H<sub>3</sub><sup>+</sup> at  $T = 28$  K is  $N(\text{H}_3^+) < 1.4 \times 10^{15} \text{ cm}^{-2}$ . The column-averaged abundance limit with respect to CO is  $\text{H}_3^+/\text{CO} < 2.8 \times 10^{-4}$ . This abundance ratio ignores any possible contribution to the H<sub>3</sub><sup>+</sup> from the much hotter infrared "photosphere" of the background source itself.

#### b) AFGL 2591

The spectrum of AFGL 2591 in the vicinity of the H<sub>3</sub><sup>+</sup> 2691.444  $\text{cm}^{-1}$  line is displayed in Figure 4. Also shown is the spectrum of the comparison star, Sirius, which indicates how well the atmospheric features can be divided out. No interstellar feature is evident. The upper limit on equivalent width is  $W_v < 0.0063 \text{ cm}^{-1}$  (3  $\sigma$ ) and the corresponding upper limit on column density in the (J, K) = (1, 1) level is  $N(1, 1) < 4.0 \times 10^{14} \text{ cm}^{-2}$ . If H<sub>3</sub><sup>+</sup> is thermalized at the temperature of the cold, quiescent CO toward AFGL 2591,  $T = 38$  K (Mitchell *et al.* 1989; see § IVb), then the limit on the total column density of cold H<sub>3</sub><sup>+</sup> is  $N(\text{H}_3^+) < 7.4 \times 10^{14} \text{ cm}^{-2}$ . Alternatively, if we simply combine our limit on the (1, 1) level with that of Geballe and Oka (1989) for the (1, 0) level, then the upper limit on cold H<sub>3</sub><sup>+</sup> toward AFGL 2591 is  $N(\text{H}_3^+) < 5.1 \times 10^{14} \text{ cm}^{-2}$  (rescaled to the 3  $\sigma$  level of confidence and adjusted for a consistent set of oscillator strengths). We adopt the latter, more restrictive limit in the discussion which follows. For rotational populations in equilibrium at any  $T < 50$  K, the (1, 1)

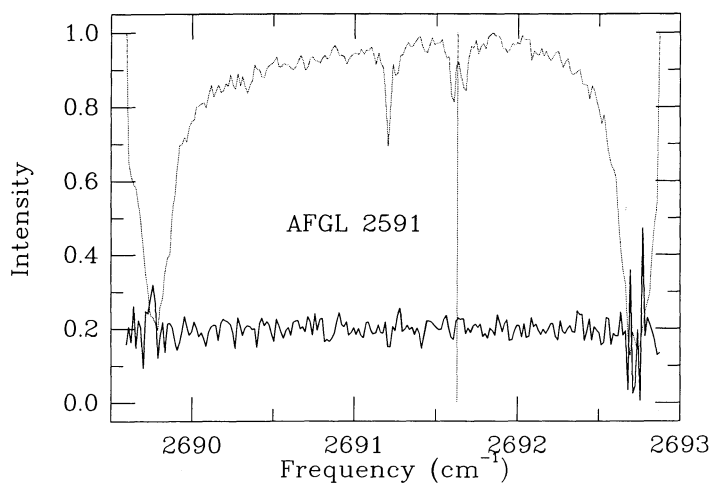


FIG. 4.—Spectra near the H<sub>3</sub><sup>+</sup> line at 2691.444  $\text{cm}^{-1}$  (rest) for AFGL 2591 and Sirius. The dark, solid curve with a mean continuum level at a relative intensity of 0.2 is the summed spectrum of AFGL 2591 after division by the spectrum of Sirius. The light, dotted curve shows the spectrum of Sirius in the same region and illustrates the locations of atmospheric absorption features. For reference, the three narrow features in the spectrum of Sirius at 2691.21, 2691.60, and 2691.67  $\text{cm}^{-1}$  have equivalent widths of 0.0105, 0.0060, and 0.0064  $\text{cm}^{-1}$ , respectively.

and (1, 0) levels account for more than 95% of the total abundance.

The spectral energy distribution of AFGL 2591 is much steeper than that of NGC 2264 IRS in the 2–4  $\mu\text{m}$  wavelength region. Consequently, our spectra in the K band yield  $S/N \approx 1$  and do not permit any sensible limits to be placed on the CO  $v = 2 \leftarrow 0$  and  $\text{H}_2 v = 1 \leftarrow 0$  absorption lines.

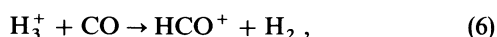
### c) Other Sources

It has been suggested previously on chemical grounds that classical diffuse interstellar clouds may harbor column densities of  $\text{H}_3^+$  as large as those in thick, dense molecular clouds (van Dishoeck and Black 1986). Accordingly, some data were obtained for  $\zeta$  Per,  $\zeta$  Oph, and Cyg OB2 No. 12. Owing to problems with weather, the integration times on these sources were limited, and  $S/N$  ratios in the spectra near 3.7  $\mu\text{m}$  wavelength were too low to provide useful limits on  $\text{H}_3^+$ .

The high-resolution spectra of NGC 2024 IRS 2 discussed by Black and Willner (1984) yielded information on CO and  $\text{H}_2$  absorption in the 2  $\mu\text{m}$  region but were of inadequate  $S/N$  to constrain the  $\text{H}_3^+$  line strength at 3.7  $\mu\text{m}$ . Drossart *et al.* (1989) have recently suggested that interstellar  $\text{H}_3^+$  might be detectable through lines of the  $2\nu_2$  band in the  $\lambda \approx 2 \mu\text{m}$  region. Thus we have reexamined the older data on NGC 2024 IRS 2 for evidence of these  $\text{H}_3^+$  lines. Three potential interstellar absorption lines of this band lie at  $\tilde{\nu} = 4907.869$ , 4968.162, and 5094.212  $\text{cm}^{-1}$ , and their absorption oscillator strengths are  $f = 9.65 \times 10^{-6}$ ,  $9.41 \times 10^{-6}$ , and  $8.76 \times 10^{-6}$ , respectively (Watson *et al.* 1990). The first and third of these lines arise in the (1, 0) rotational level, and the second arises in the (1, 1) level. All three of these lines lie in a region of poor atmospheric transmission, and only for the 4908  $\text{cm}^{-1}$  line was the  $S/N$  ratio as high as 3 in the combined spectra of NGC 2024 IRS 2. We find a nominal upper limit of  $W_\nu < 0.016 \text{ cm}^{-1}$  ( $3\sigma$ ) for the 4908  $\text{cm}^{-1}$  line, which implies a column density of  $\text{H}_3^+$  (1, 0) of  $N(1, 0) < 1.9 \times 10^{15} \text{ cm}^{-2}$ . This is a weaker limit by a factor of 11 than that derived by Geballe and Oka (1989) from measurements of the  $\nu_2$  line at 2529.724  $\text{cm}^{-1}$ . The analysis of CO  $v = 2 \leftarrow 0$  lines in this source gave a temperature  $T \approx T_{\text{rot}} = 44 \text{ K}$  (Black and Willner 1984). Thus if  $\text{H}_3^+$  is thermalized at the same temperature as the observed CO, our upper limit on total column density is  $N(\text{H}_3^+) < 3.9 \times 10^{15} \text{ cm}^{-2}$ . The corresponding limit of Geballe and Oka (1989) is  $N(\text{H}_3^+) < 3.5 \times 10^{14} \text{ cm}^{-2}$ . In obtaining this result, we have rescaled the limit on equivalent width of Geballe and Oka to  $3\sigma$  ( $W_\nu < 0.0045 \text{ cm}^{-1}$ ) for consistency with our quoted limits and have adopted an oscillator strength  $f = 3.02 \times 10^{-5}$  (Miller and Tennyson 1988, adjusted as indicated in § II) for the line at 2529.724  $\text{cm}^{-1}$ .

## IV. DISCUSSION

The molecular ion,  $\text{H}_3^+$ , has been thought for some time to play a pivotal role in interstellar chemistry (Herbst and Klemperer 1973). Cosmic-ray ionization of the most abundant molecule,  $\text{H}_2$ , forms  $\text{H}_2^+$ , which reacts rapidly with another  $\text{H}_2$  to form  $\text{H}_3^+$ . In regions of low ionization, the removal of  $\text{H}_3^+$  is controlled primarily by reactions with the most abundant carbon- and oxygen-containing species, typically O, CO,  $\text{O}_2$ ,  $\text{H}_2\text{O}$ , etc. Deep inside molecular clouds, the reaction



is one of the principal sinks of  $\text{H}_3^+$  and competes with  $\text{H}^+$  in removing the otherwise nearly indestructible CO molecule.

This reaction does not usually cause a net loss of CO, however, because the product  $\text{HCO}^+$  tends to reform CO with high efficiency. Thus the chemistries of  $\text{H}_2$ ,  $\text{H}_3^+$ , and CO are closely coupled. It is fortunate, then, that high-resolution infrared absorption spectroscopy provides a means of sampling the abundances and excitation of all three species at the same time for exactly the same absorbing column of interstellar gas. In principle, the measurements of the rotational population distribution of CO yield values of temperature and limits on densities in these absorbing clouds, so that these important parameters in a chemical analysis can also be determined. These considerations strictly apply provided that the interstellar molecules can be distinguished from circumstellar absorbers within the stratified atmosphere of the “background” infrared source. In the following section, we discuss the current absorption-line results.

### a) NGC 2264

The abundance and excitation of CO are rather well constrained by the infrared observations presented here. The rotational excitation temperature of CO,  $T_{\text{rot}} = 28 \text{ K}$ , is in harmony with the kinetic temperature  $T = 25\text{--}28 \text{ K}$  inferred from the CO  $J = 1\text{--}0$ ,  $J = 2\text{--}1$ , and  $J = 4\text{--}3$  rotational emission lines and the  $\text{NH}_3$  (1, 1) and (2, 2) inversion transitions by Krügel *et al.* (1987). Moreover, the measured width of the  $\text{C}^{18}\text{O}$   $J = 1\text{--}0$  line,  $\Delta V = 3.0 \text{ km s}^{-1}$ , agrees well with our value for the infrared lines of  $\Delta V = 2.9 \pm 1.0 \text{ km s}^{-1}$ , as does the observed range of radial velocities,  $V_{\text{LSR}} \approx 5\text{--}8 \text{ km s}^{-1}$ , with our result,  $V_{\text{LSR}} = +6.4 \pm 0.4 \text{ km s}^{-1}$ . Krügel *et al.* cannot use the very saturated emission lines to determine a column density of  $^{12}\text{C}^{16}\text{O}$  directly, but their measurements of  $^{12}\text{C}^{18}\text{O}$  indicate  $N(\text{C}^{18}\text{O}) \approx 1.8 \times 10^{16} \text{ cm}^{-2}$  in the direction of NGC 2264 IRS. If the usual isotopic abundance ratio of  $^{16}\text{O}/^{18}\text{O} \approx 500$  applies to carbon monoxide, as would be expected in such a thick molecular cloud, then their inferred column densities are no more than twice as large as ours. Our measurements apply only to a column in the foreground of the infrared source, while the emission-line observations sample material surrounding the source and averaged over the 21”–30” beams of the antennae. Our limit on the column density of  $\text{H}_2$  is consistent with estimates of the extinction  $A_V \approx 100 \text{ mag}$  and column density  $N(\text{H}_2) \approx 10^{23} \text{ cm}^{-2}$  that are based on the  $\lambda 350 \mu\text{m}$  continuum observations of Chini, Krügel, and Kreysa (1986) as discussed by Krügel *et al.* (1987). Chini, Krügel and Kreysa have interpreted the near-infrared flux measurements in terms of a dense disk viewed face-on and a dilute envelope of dust with a total  $A_V = 19 \text{ mag}$  to the embedded star. This amount of extinction would imply only  $N(\text{H}_2) \approx 1.5 \times 10^{22} \text{ cm}^{-2}$  for a normal interstellar gas/extinction ratio. If this were the case,  $N(\text{CO})/N(\text{H}_2) \approx 3 \times 10^{-4}$ , and 35% of a solar abundance of carbon would be in the form of gas-phase CO. The 9.7  $\mu\text{m}$  silicate absorption feature provides an independent estimate of the extinction to the infrared source. According to Merrill, Russell, and Soifer (1976) and Willner *et al.* (1982), the silicate optical depth  $\tau_{9.7} = 2.4$ , and the corresponding visual extinctions are  $A_V = 19$  to 34 mag for extinction curves for stars at the Galactic center and for Cyg OB2 No. 12, respectively. Again, this implies hydrogen column densities in the range  $N(\text{H}_2) = 0.5 N_{\text{H}} = 8 \times 10^{20} A_V = 1.5\text{--}2.7 \times 10^{22} \text{ cm}^{-2}$ .

Krügel *et al.* (1987) estimate a hydrogen density of  $n(\text{H}_2) \approx 5 \times 10^4 \text{ cm}^{-3}$  on average from emission-line data, with local values exceeding  $10^5 \text{ cm}^{-3}$  in condensations. More recently, Krügel *et al.* (1989) have reported the detection of CO  $J = 7\text{--}6$

toward NGC 2264 IRS with  $T_A^* = 7$  K and  $\Delta V = 8$  km s<sup>-1</sup>. Although Krügel *et al.* (1989) urge caution in interpreting such measurements for which the telescope efficiency and absolute calibration may be poorly known, we find from a multilevel excitation calculation that a CO  $J = 7-6$  line with  $T_R = 8.7$  K and  $\Delta V = 8$  km s<sup>-1</sup> arises when  $T = 28$  K,  $N(\text{CO}) = 5.0 \times 10^{18}$  cm<sup>-2</sup>, and  $n(\text{H}_2) = 5 \times 10^4$  cm<sup>-3</sup>. Thus we expect the density in a narrow column along the line of sight to be similar, and we adopt a mean density of  $n(\text{H}_2) = 5 \times 10^4$  cm<sup>-3</sup> in the following discussion. The thickness of a uniform absorbing column with our adopted properties is  $L \approx N(\text{H}_2)/n(\text{H}_2) < 2.2 \times 10^{18}$  cm.

According to equation (23) of Black and van Dishoeck (1989), the concentration of H<sub>3</sub><sup>+</sup> in steady state in a molecular cloud is expected to be

$$n(\text{H}_3^+) \approx \frac{0.9\zeta_0 n(\text{H}_2)}{k_{\text{DR}} n(e) + 8 \times 10^{-10} n(\text{O}) + 1.7 \times 10^{-9} n(\text{CO}) + \dots}, \quad (7)$$

where  $n(i)$  is the concentration in cm<sup>-3</sup> of species  $i$ ,  $k_{\text{DR}}$  is the rate coefficient of dissociative recombination of H<sub>3</sub><sup>+</sup>, and  $\zeta_0$  is the ionization rate per hydrogen nucleus due to penetrating cosmic rays. The reaction of H<sub>3</sub><sup>+</sup> with CO alone is always a lower bound on the removal of the ion, and the observations discussed above supply upper bounds on the thickness of the absorbing column  $L$  and the H<sub>2</sub>/CO ratio; therefore, the theoretically predicted column density of H<sub>3</sub><sup>+</sup> is

$$N(\text{H}_3^+) \leq 5.3 \times 10^8 \zeta_0 \frac{Ln(\text{H}_2)}{n(\text{CO})} \\ \leq 2.6 \times 10^{14} \left( \frac{\zeta_0}{10^{-17} \text{ s}^{-1}} \right) \left( \frac{L}{2.2 \times 10^{18} \text{ cm}} \right) \text{ cm}^{-2}. \quad (8)$$

This expectation is consistent with the observed limit provided that the ionization rate is  $\zeta_0 < 5 \times 10^{-17}$  s<sup>-1</sup>. For comparison, ionization rates this large and larger have been inferred for diffuse interstellar clouds from detailed model analyses of the observed abundances of OH and HD (van Dishoeck and Black 1986). If the H<sub>2</sub> column density were as low as  $N(\text{H}_2) \approx 1.5 \times 10^{22}$  cm<sup>-2</sup>, then the constraint on the cosmic-ray ionization rate would be relaxed to  $\zeta_0 < 3 \times 10^{-15}$  s<sup>-1</sup>.

Alternatively, the H<sub>3</sub><sup>+</sup> abundance can be described in relation to those of O and OH as pointed out by Lepp, Dalgarno, and Sternberg (1987). In their formulation, one expects

$$N(\text{H}_3^+) = 0.1N(\text{OH}) + 1.1 \times 10^{13} \left[ 10^{-4} \frac{n(\text{H}_2)}{n(\text{O})} \right] \\ \times \left( \frac{\zeta_0}{10^{-17} \text{ s}^{-1}} \right) \left( \frac{L}{2.2 \times 10^{18} \text{ cm}} \right) \text{ cm}^{-2}, \quad (9)$$

in a uniform, cold molecular cloud. The OH column density toward NGC 2264 IRS is not well determined. Measurements of the 1667 MHz emission line of OH in this direction (Lang and Willson 1980) imply  $N(\text{OH}) \approx 1-10 \times 10^{15}$  cm<sup>-2</sup> for OH excitation temperatures  $T_{\text{ex}} = 3.7-10$  K and background brightness temperatures  $T_{\text{bg}} = 2.7-4$  K. Thus our adopted upper limit,  $N(\text{H}_3^+) \leq 1.4 \times 10^{15}$  cm<sup>-2</sup>, is consistent with the chemical model of Lepp, Dalgarno, and Sternberg (1987), provided that

$$\left[ 10^{-4} \frac{n(\text{H}_2)}{n(\text{O})} \right] \left( \frac{\zeta_0}{10^{-17} \text{ s}^{-1}} \right) \left( \frac{L}{2.2 \times 10^{18} \text{ cm}} \right) < 10^2. \quad (10)$$

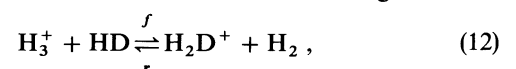
Our motivation for observing NGC 2264 was the report of a possible detection of the H<sub>2</sub>D<sup>+</sup> 1<sub>10-11</sub> line at 372 GHz in this direction (Phillips *et al.* 1985). Armed with a well-determined temperature and an estimated density for this cloud, we reexamine the excitation of H<sub>2</sub>D<sup>+</sup>. The equations of statistical equilibrium and radiative transfer are solved in a mean escape probability treatment for the lowest 11 rotational levels of H<sub>2</sub>D<sup>+</sup>. The  $T_{\text{bg}} = 2.7$  K cosmic background radiation is included. Energy levels and transition probabilities of H<sub>2</sub>D<sup>+</sup> were computed from the spectroscopic constants of Amano (1985) with a dipole moment  $\mu_a = 0.6364$  D that is consistent with the ab initio calculations of Miller, Tennyson, and Sutcliffe (1989). Our transition probabilities are in harmony with those of Miller, Tennyson, and Sutcliffe (1989) after allowance is made an error in their Table 6, namely in the transition probability for the 1<sub>01-000</sub> transition, which is a factor of 3 times too large (S. Miller 1989, private communication). We include additional transitions not tabulated by Miller, Tennyson, and Sutcliffe. The adopted transition probabilities are approximately 12% larger than those published by Khersonskii, Varshalovich, and Opendak (1987). Rates of rotationally inelastic H<sub>2</sub>-H<sub>2</sub>D<sup>+</sup> collisions are taken to have values  $q_{ul} = 10^{-10} S_{ul}$  cm<sup>3</sup> s<sup>-1</sup>, where  $S_{ul}$  is the line strength of the corresponding radiative transition from upper state  $u$  to lower state  $l$  in D<sup>2</sup>. The corresponding upward rates are computed according to detailed balance. These collision rates are very similar in magnitude to those for H<sub>2</sub>-HCO<sup>+</sup> collisions (Monteiro 1985). We assume that reactive collisional transitions between ortho and para states,



all have downward rate coefficients  $q_{ul}(\text{o/p}) = 10^{-10}$  cm<sup>3</sup> s<sup>-1</sup> (but see Herbst 1982 for a more detailed discussion).

The observation of H<sub>2</sub>D<sup>+</sup> (Phillips *et al.* 1985) gave an intensity  $T_A^* = 0.23$  K and a width  $\Delta V = 3.8$  km s<sup>-1</sup> for the 372 GHz line. At a kinetic temperature of  $T = 28$  K, the excitation model predicts that a perfect antenna would measure a Rayleigh-Jeans radiation temperature  $T_R = 0.23$  K from an extended source of column densities  $N(\text{H}_2\text{D}^+) = 1.2 \times 10^{15}$ ,  $1.25 \times 10^{14}$ , and  $3.3 \times 10^{13}$  cm<sup>-2</sup> at respective densities of  $n(\text{H}_2) = 10^4$ ,  $10^5$ , and  $10^6$  cm<sup>-3</sup>. The required column density of H<sub>2</sub>D<sup>+</sup> in the high-density limit (thermalized populations) is  $1.7 \times 10^{13}$  cm<sup>-2</sup>, in fair agreement with the "thermal" value quoted by Phillips *et al.* (1985). At our adopted value of the mean density,  $n(\text{H}_2) = 5 \times 10^4$  cm<sup>-3</sup>, the derived column density of H<sub>2</sub>D<sup>+</sup> is  $2.3 \times 10^{14}$  cm<sup>-2</sup>. This result is, of course, as uncertain as the unknown collision rates and is also limited by uncertainty about the coupling of the telescope beam to the emission. If the ortho/para interchange rates were 5 times larger than those adopted here, the estimated column density would be diminished by a factor of 3 to  $7.7 \times 10^{13}$  cm<sup>-2</sup> at  $n(\text{H}_2) = 5 \times 10^4$  cm<sup>-3</sup>. We find that inclusion of the thermal radiation at submillimeter wavelengths from NGC 2264 IRS itself has only a small ( $\approx 10\%$ ) effect on the calculated intensity of the 1<sub>10-11</sub> line, although we predict that some of the transitions at higher frequencies will appear weakly in absorption against it.

If we take seriously the inferred column density of H<sub>2</sub>D<sup>+</sup>, then the ratio H<sub>2</sub>D<sup>+</sup>/H<sub>3</sub><sup>+</sup> > 0.05 is found to be extremely high. If this abundance ratio were governed simply by the balance between the forward and reverse rates of the exchange reaction

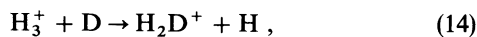




then one would expect

$$\frac{n(\text{H}_2\text{D}^+)}{n(\text{H}_3^+)} \approx \frac{n(\text{HD})}{n(\text{H}_2)} \frac{k_f}{k_r}. \quad (13)$$

According to the nonequilibrium phase-space calculation of Herbst (1982), the ratio of forward and reverse rate coefficients in reaction (12) is  $k_f/k_r \approx 400$  at  $T = 28$  K. The ion abundance ratio implied by observations would then require an uncomfortably large value of the ratio  $\text{HD}/\text{H}_2 > 10^{-4}$ . The additional source of  $\text{H}_2\text{D}^+$  from atomic D,



probably alters this argument by no more than a factor of 2 in a dense cloud (Dalgarno and Lepp 1984). Even if the  $\text{H}_2\text{D}^+$  372 GHz line emission is thermalized, the inferred ratio  $\text{H}_2\text{D}^+/\text{H}_3^+ \geq 0.01$  is barely consistent with a typical interstellar deuterium abundance of  $[\text{D}/\text{H}] = 1.5 \times 10^{-5}$  by number of nuclei. The abundance of  $\text{DCO}^+$  relative to that of  $\text{HCO}^+$  is directly related to the  $\text{H}_2\text{D}^+/\text{H}_3^+$  ratio. Observations of  $\text{HCO}^+$ ,  $\text{DCO}^+$ , and  $\text{H}^{13}\text{CO}^+$  toward NGC 2264 IRS indicate an enhancement of deuterium no larger than normal in this ion (Guélin, Langer, and Wilson 1982), although its exact value is difficult to determine owing to effects of line saturation and to confusion among cloud components at different temperatures. If  $\text{H}_2\text{D}^+$  is not enhanced, the emitting gas sampled by the  $\text{H}_2\text{D}^+$  radio observations must lie outside the direct column to the infrared source, either behind the infrared source or displaced to the side.

#### b) AFGL 2591

As discussed above (§ IIIb), the upper limit on the total column density in cold molecular gas toward AFGL 2591 is  $N(\text{H}_3^+) < 5.1 \times 10^{14} \text{ cm}^{-2}$ . The absorption-line measurements of Mitchell *et al.* (1989) reveal several distinct velocity components in  $^{12}\text{CO}$  and  $^{13}\text{CO}$  with a range of excitation temperatures. The  $^{12}\text{CO}$   $v = 1 \leftarrow 0$  lines of the cold, quiescent component are too highly saturated to provide direct determinations of the abundance and excitation of that species. The cold component, at  $T_{\text{rot}} = 38$  K, of  $^{13}\text{CO}$ , however, has a well-determined column density  $N(^{13}\text{CO}) = 1.2 \times 10^{17} \text{ cm}^{-2}$ . For simplicity, we will assume the same abundance ratio as Mitchell *et al.* (1989),  $N(^{12}\text{CO})/N(^{13}\text{CO}) = 60$ , and we will assign their adopted  $^{12}\text{CO}$  column density  $N(^{12}\text{CO}) = 7.2 \times 10^{18} \text{ cm}^{-2}$  to the cold molecular component. Unfortunately, we have no direct limit on the column density of  $\text{H}_2$  toward AFGL 2591. The excitation of CO in this direction is very complicated and may have a significant contribution from infrared radiative pumping close to the infrared source. Although Mitchell *et al.* (1989) interpret the “hot” molecules as evidence of hot gas with kinetic temperature  $T \approx 1000$  K and densities exceeding  $10^7 \text{ cm}^{-3}$ , alternative explanations that include infrared radiative excitation are plausible (Katriss *et al.* 1990). The excitation of low-lying levels of  $^{13}\text{CO}$  in the cold component can be explained with densities  $n(\text{H}_2) \approx 10^5\text{--}10^6 \text{ cm}^{-3}$ . Following the discussion in § IVa, we find that the observed limit on  $\text{H}_3^+$  in the cold molecular component toward AFGL 2591 is consistent with a cosmic-ray ionization rate  $\zeta_0 < 3 \times 10^{-17} \text{ s}^{-1}$  if  $N(\text{H}_2)/N(\text{CO}) < 2 \times 10^4$  and  $n(\text{H}_2) \approx 10^5 \text{ cm}^{-3}$ .

#### c) Other Sources

We noted in § II that the oscillator strengths adopted here for the CO  $v = 2 \leftarrow 0$  lines are approximately 17% larger than

those used by Black and Willner (1984) in analyzing infrared absorption-line data on NGC 2024 IRS 2. This means that the column density of and abundance limit on CO in that direction should be adjusted to  $N(\text{CO}) = 7 \times 10^{18} \text{ cm}^{-2}$  and  $\text{CO}/\text{H}_2 > 7.8 \times 10^{-5}$ , values which are not significantly different from the original results in view of the uncertainties. The upper limit on  $\text{H}_3^+$  toward NGC 2024 of Geballe and Oka (1989) is  $H(\text{H}_3^+) < 3.5 \times 10^{14} \text{ cm}^{-2}$  for a thermal population distribution at the observed temperature of the CO molecules (§ IIIc). The analysis discussed for NGC 2264 IRS above, if applied here, suggests that the limit on the  $\text{H}_3^+$  abundance is consistent with a cosmic-ray ionization rate  $\zeta_0 < 6 \times 10^{16} \text{ s}^{-1}$ . This presumes that the thickness of the CO absorbing region  $L < N(\text{H}_2)/n(\text{H}_2) \approx 8.8 \times 10^{16} \text{ cm}$ , based upon an estimated density  $n(\text{H}_2) = 10^6 \text{ cm}^{-3}$  from the multitransition analyses of CS and  $\text{H}_2\text{CO}$  emission lines in the same direction (Mundy *et al.* 1986, 1987). The constraint on  $\zeta_0$  would be more restrictive if the density of the CO absorbing column were lower.

Microwave absorption lines of OH toward NGC 2024 show some of the highest optical depths observed anywhere outside the Galactic center and imply  $N(\text{OH}) = 1.8 \times 10^{15} \text{ cm}^{-2}$  (Goss *et al.* 1976). In this case, the upper limit on  $\text{H}_3^+$  and the chemical analysis of Lepp, Dalgarno, and Sternberg suggest that

$$\left[ 10^{-4} \frac{n(\text{H}_2)}{n(\text{O})} \right] \left( \frac{\zeta_0}{10^{-17} \text{ s}^{-1}} \right) \left( \frac{L}{8.8 \times 10^{16} \text{ cm}} \right) < 390. \quad (15)$$

#### V. CONCLUSIONS

Interstellar absorption-line spectroscopy has been applied to three sources. In principle, these observations permit the determination of the temperature,  $T$ , the abundance ratio,  $N(\text{CO})/N(\text{H}_2)$ , and the column density of  $\text{H}_3^+$ . The basic chemistry of  $\text{H}_3^+$  is thought to be sufficiently straightforward that such data can be used to determine the cosmic-ray ionization rate. In NGC 2264 IRS, the CO molecule has a column density  $5 \times 10^{18} \text{ cm}^{-2}$  and a rotational excitation temperature of 28 K. A direct upper limit on the  $\text{H}_2$  column density implies that at least 6% of a solar carbon abundance is in the form of CO. The upper limit on the  $\text{H}_3^+$  abundance implies that the cosmic-ray ionization rate is of the order of  $10^{-16} \text{ s}^{-1}$  or less. The  $\text{H}_3^+$  upper limit, together with a previous radio detection of  $\text{H}_2\text{D}^+$  emission, implies either an enormous overabundance of the deuterated molecule or else that most of the radio emission comes from clouds not located directly between us and the infrared source.

In the sources AFGL 2591 and NGC 2024 IRS 2, the upper limits on  $\text{H}_3^+$  imply cosmic-ray ionization rates less than 3 and  $60 \times 10^{-17} \text{ s}^{-1}$ , respectively.

In the future, a cooled spectrometer and sensitive array detector, operating at a resolving power of  $\lambda/\Delta\lambda \approx 10^5$  (3 km  $\text{s}^{-1}$  resolution in Doppler velocity), might improve the signal-to-noise ratio achievable in interstellar spectra by a factor of 10 or more in comparison with the data discussed here. This would make it possible to measure directly the abundances of cold, quiescent  $\text{H}_2$  and  $\text{H}_3^+$ . It would allow observations of CO  $v = 2 \leftarrow 0$  lines to be used to estimate mean densities from accurately determined rotational population distributions. The determination of ionization rates would be possible. In combination with observations of other ions, the  $\text{H}_3^+$  measurements could be used as a stringent test of a cornerstone of theories of ion-molecule chemistry.



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