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INTERSTELLAR $\text{H}_3^+$ LINE ABSORPTION TOWARD LkH$\alpha$ 101

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ABSTRACT

We present a detection of three lines of the $\text{H}_3^+$ ion in the near-infrared spectrum of the Herbig Be star LkH$\alpha$ 101. $\text{H}_3^+$ is the principal initiator of gas-phase chemistry in interstellar clouds and can be used to constrain the ionization rate or the path length through interstellar material along the line of sight. Essentially all of the observed $\text{H}_3^+$ column of $(2.2 \pm 0.3) \times 10^{14}$ cm$^{-2}$ toward LkH$\alpha$ 101 originates in the same dense, dark cloud; less than 1 mag of the $\sim$11 total magnitudes of visual extinction is attributable to diffuse material. Constraints on the density [$1 \times 10^6$ cm$^{-3}$ < n($\text{H}_2$) < $4 \times 10^4$ cm$^{-3}$], along with estimates of distances to the obscuring cloud, imply $\text{H}_2$ ionization rates of $6.7 \times 10^{-17}$ s$^{-1}$ < $\zeta$ < $2.7 \times 10^{-16}$ s$^{-1}$. The nondetection of fluorescent $\text{H}_2$ emission at the cloud surface implies that the obscuring dark cloud is located at least 20 pc from LkH$\alpha$ 101 and is therefore decoupled from its evolution. The confirmation of significant $\text{H}_3^+$ in dense material addresses earlier concerns that $\text{H}_3^+$ may originate in diffuse material surrounding dense clouds.

Subject headings: cosmic rays — infrared: ISM — ISM: clouds — ISM: molecules — stars: individual (LkH$\alpha$ 101)

1. INTRODUCTION

The molecular ion $\text{H}_3^+$ plays a special role in the chemistry of interstellar clouds. A by-product of the (cosmic ray) ionization of $\text{H}_2$, it initiates the diverse gas-phase reactions that form many of the 120+ known molecules in interstellar clouds. $\text{H}_3^+$ is formed by the ionization of $\text{H}_2$ into $\text{H}_2^+$, followed by the rapid reaction $\text{H}_2^+ + \text{H}_2 \rightarrow \text{H}_3^+ + \text{H}$. It is destroyed by recombination with free electrons and reaction with species that have a larger proton affinity than $\text{H}_2$. In diffuse clouds electron recombination dominates the destruction of $\text{H}_3^+$, whereas reaction with CO dominates its destruction in dense clouds. The relative simplicity of the formation and destruction mechanisms of $\text{H}_3^+$ makes it possible, in principle, to derive fundamental physical characteristics of diffuse and dense clouds from its abundance.

$\text{H}_3^+$ was first observed in laboratory spectra by Oka (1980), and nearly a decade later in the upper atmosphere of Jupiter (Drossart et al. 1989). With the advent of more sensitive echelle spectrometers operating at infrared wavelengths on large telescopes, $\text{H}_3^+$ has now been detected in a variety of interstellar environments (Geballe & Oka 1996; McCall et al. 1998, 1999, 2003; Geballe et al. 1999; Goto et al. 2002; Kulesa & Black 2003).

While the molecular physics of $\text{H}_3^+$ is simple, an understanding of the chemistry and abundance of $\text{H}_3^+$ in diffuse clouds is not well established. Interpretation of $\text{H}_3^+$ abundances in diffuse clouds is complicated by the uncertainty in the rate of $\text{H}_2$ ionization, in the abundances of species that destroy $\text{H}_3^+$, and especially in the electron recombination rate. McCall (2001) has found that the abundance of $\text{H}_3^+$ in some diffuse clouds is much larger than models predict, and later attributed this discrepancy to an enhanced cosmic-ray ionization rate (McCall et al. 2003).

In contrast, the theoretical picture of the chemistry of $\text{H}_3^+$ in dense clouds is clearer. Its formation depends entirely on the ionization rate of $\text{H}_2$. Unlike diffuse clouds, the ionization rate in dense clouds is constrained. The rate must be much greater than $10^{-18}$ s$^{-1}$ to initiate observed gas-phase chemistry, but it cannot exceed $\sim 10^{-16}$ s$^{-1}$ to prevent overproduction of atomic hydrogen (Solomon & Werner 1971). The destruction of $\text{H}_3^+$ in dense clouds is also better understood since measurement of the abundance of CO (relative to $\text{H}_2$), its most potent dissociative agent, is possible (Lacy et al. 1994) and the reaction rate of CO with $\text{H}_3^+$ is well established (Anicich & Huntress 1986). In principle, it is possible to determine the path length through a dense cloud or the cosmic-ray ionization rate by measuring the column densities of CO, $\text{H}_3^+$, and $\text{H}_2$.

There is, however, some controversy as to whether the $\text{H}_3^+$ observed along lines of sight toward dense clouds actually originates in the dense clouds themselves. Van der Tak & van Dishoeck (2000) point out that more distant dark clouds tend to have larger columns of $\text{H}_3^+$ than do nearby clouds. They conclude that $\text{H}_3^+$ largely resides in the diffuse interstellar medium between distant dense clouds and not necessarily in the dense clouds themselves. If this is correct, the lack of $\text{H}_3^+$ production in dense clouds could significantly alter our picture

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of the thermal and ionization balance in star-forming cloud cores. Resolution of this controversy requires a line of sight that is dominated by dense cloud material in which the extinction, density, and temperature of the cloud (inferred by rovibrational CO observations), H$_2$ abundance, and radiation field can be measured.

The direction toward the Herbig Be star LkH$\alpha$ 101 (HBC 40: Herbig & Bell 1988) is a good candidate for such a study. LkH$\alpha$ 101 is among the brightest ($m_L = 0.48$) Herbig Be stars and is the illuminating source of the NGC 1579 reflection nebula (Herbig 1971). It lies behind an obscuring cloud and is surrounded by an extended H $\pi$ region, S222 (Redman et al. 1986). Other clouds lie to the north, south, and southwest. The column density of CO in these clouds ranges from less than $10^{18}$ up to $5 \times 10^{18}$ cm$^{-2}$. Kelly, Rieke, & Campbell (1994) have determined the foreground extinction, $A_V = 11.2^{+0.3}_{-0.2}$ mag, based on a variety of infrared line ratios. Tuthill et al. (2002) have imaged LkH$\alpha$ 101 with an infrared interferometer and found a nearly face-on disk ($i < 35^\circ$). This orientation suggests that the observed extinction is likely due to interstellar rather than circumstellar material. In this work, we present our detection of the $Q(1, 0)$, $R(1, 0)$, and $R(1, 1)^a$ lines of H$_3^+$ along the line of sight toward LkH$\alpha$ 101, which serves as a test case that constrains the origin of H$_3^+$ in dark clouds.

## 2. OBSERVATIONS

Absorption spectra of the $P_2 \leftarrow 0$ fundamental lines $Q(1, 0)$, $R(1, 0)$, and $R(1, 1)^a$ of H$_3^+$ in the 4 $\mu$m $L'$-band atmospheric window were obtained at the W. M. Keck Observatory. We used the cross-dispersed NIRSPEC echelle spectrograph, which provides a spectral resolving power of 25,000 (McLean et al. 1998). The complete set of observations is summarized in Table 1. See Brittain et al. (2003) for a discussion of the data acquisition and reduction procedures.

After a correction for atmospheric absorption, the residual spectral extracts were found to have a fringe with an amplitude of $\approx 1\%$ (Figs. 1 and 2). We removed this fringe by examining the power spectrum and deleting the corresponding frequency spikes from the power spectrum. The defringed segments containing the H$_3^+$ lines are displayed in Figures 3 and 4.

## 3. ANALYSIS

We detected three absorption lines of H$_3^+$ along the line of sight toward LkH$\alpha$ 101. Table 2 presents the observed position, rest position, heliocentric radial velocity, equivalent width, and inferred column density for these lines.

LkH$\alpha$ 101 is a rich source of atomic emission lines (Herbig 1971), which may originate from the H $\pi$ region that surrounds the central star (Redman et al. 1986). Herbig (1971) notes a radial velocity of 8 km s$^{-1}$ for the optical and near-infrared lines of LkH$\alpha$ 101, but with a large scatter. Millimeter observations of CO by Redman et al. (1986) indicate the obscuring cloud in front of the star has a $v_{\text{rad}} = 4.5$–6.3 km s$^{-1}$, with the peak of the emission at $v_{\text{rad}} = 5.8$ km s$^{-1}$. A CO survey by Ungerechts & Thaddeus (1987) finds the cloud along the line of sight toward LkH$\alpha$ 101 (cloud 12e) is at $v_{\text{rad}} = 6.2$ km s$^{-1}$. In our NIRSPEC spectra of 2002 November and 2003 March, we measure a heliocentric radial velocity for H$_3^+$ of 6 ± 1 and 5 ± 1 km s$^{-1}$, respectively. The mean radial velocities of the CO emission at submillimeter wavelengths and the H$_3^+$ absorption features at infrared wavelengths are consistent, suggesting that they originate from within the same cloud. The uncertainty quoted here for H$_3^+$ on each date is the standard deviation of the Doppler shifts measured from the three absorption lines. The H$_3^+$ features have a FWHM = 16 ± 5 km s$^{-1}$ and thus are marginally resolved at the resolution of NIRSPEC (12 km s$^{-1}$). We used a

### Table 1: Journal of Observations

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<td>H$_3^+$ $R(1, 0)$, $R(1, 1)^a$</td>
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<td>200</td>
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Fig. 1.—Initial (atmospheric and H$_3^+$) spectrum and atmospheric model. The two emission features at 2742.8 and 2730.9 cm$^{-1}$, from H i and O i, result from the surrounding gas. The location of the H$_3^+$ lines is indicated. The telluric absorption features dominate the spectrum of LkH$\alpha$ 101. The transmittance function of the night sky was modeled (dashed line) using the Spectrum Synthesis Program (SSP; Kunde & Maguire 1974), which accesses the '92HITRAN molecular database (Rothman et al. 1992). The optimized model establishes the columns of absorbing atmospheric species, the spectral resolving power, and the wavelength calibration. The position of the $R(1, 1)^a$, R(1, 0) doublet of H$_3^+$ is indicated, but further analysis is needed to remove atmospheric and instrumental effects.
Gaussian line fit to the profiles to measure their equivalent widths, \( W_0 \), and present the results of the fits in Table 2.

From the observed equivalent widths (assumed to be on the linear part of the curve of growth), we computed the column density of gas in the lower molecular levels of each transition by means of the standard relation,

\[
W_0 = \left( \frac{8\pi^3 \nu}{3hc} \right) N_{\text{level}} |\mu|^2,
\]

where \( \mu \) is the transition dipole moment (McCall 2001). The level populations inferred for the lower states of the \( Q(1, 0) \), \( R(1, 0) \), and \( R(1, 1)^\nu \) transitions are listed in Table 2. The \( Q(1, 0) \) and \( R(1, 0) \) lines probe the same lower state, and the \( R(1, 1)^\nu \) line probes the only other state that can be populated at temperatures of less than a few hundred kelvins. Thus, the total column density of \( H_3^+ \) can be calculated from the sum of the \( J = 1, K = 0 \) state, probed by \( Q(1, 0) \) and \( R(1, 0) \), and the \( J = 1, K = 1 \) state, probed by \( R(1, 1)^\nu \). Averaging the level populations for the two nights of observations, we obtain \( N(H_3^+) = (2.2 \pm 0.3) \times 10^{18} \text{ cm}^{-2} \). McCall et al. (1999) included LkH\( \alpha \) 101 in their \( H_3^+ \) survey of dense clouds and derived a 3 \( \sigma \) upper limit for the column density of \( 7 \times 10^{13} \text{ cm}^{-2} \) for the \( J = 1, K = 1 \) level. It seems likely that systematic uncertainties in the continuum fit and incomplete removal of telluric features may have led to their underestimation of the abundance of \( H_3^+ \) toward LkH\( \alpha \) 101.

The ortho and para levels of \( H_3^+ \) are expected to be thermalized at the local gas temperature through collisional processes and proton exchange with \( H_2 \). The thermalization of these levels has been confirmed for multiple lines of sight through dense clouds for both \( H_2 \) (Kulesa & Black 2003) and \( H_3^+ \) (McCall et al. 1999). Thus, the ortho/para ratio provides a sensitive and reliable diagnostic of the kinetic temperature of the gas in which \( H_3^+ \) is found. The \( R(1, 0) \) and \( R(1, 1)^\nu \) doublet probes the ortho as well as para spin modifications of the \( H_3^+ \) molecule. The ratio of the strengths of these lines defines the excitation temperature of the gas, according to the Boltzmann formula

\[
\frac{N_{\text{ortho}}}{N_{\text{para}}} = \left( \frac{g_{\text{ortho}}}{g_{\text{para}}} \right) e^{-\Delta E/kT} = 2e^{-32.87/T}.
\]

The excitation temperature we derive from our observations of \( H_3^+ \) in 2002 November is \( 32 \pm 5 \) K, and that from the data taken in 2003 March is \( 23 \pm 8 \) K.

4. CHARACTERIZING THE GASEOUS LINE OF SIGHT TOWARD LkH\( \alpha \) 101

4.1. Evidence for a Single Dark Cloud

In order to interpret the presence of \( H_3^+ \) line absorption toward LkH\( \alpha \) 101, it is first necessary to characterize the nature of the intervening cloud(s), since the chemistry of \( H_3^+ \) differs from diffuse to dense clouds. The foreground extinction of LkH\( \alpha \) 101 is \( A_V = 11.2^{+0.3}_{-0.7} \) mag (Kelly et al. 1994). If the ratio of total to selective extinction is normal [i.e., \( R_V = A_V/(E(B-V)) = 3.1 \); Cardelli, Clayton, & Mathis 1989], then the column density of gas implied by the empirical relation of Bohlin, Savage, & Drake [1978; \( N_H/(E(B-V)) = 5.5 \times 10^{21} \text{ atoms cm}^{-2} \text{ mag}^{-1} \)] is \( N_H = 2.2 \times 10^{22} \text{ atoms cm}^{-2} \). If our line of sight passes through a dense cloud, hydrogen is mostly in molecular form, and \( N(H_2) = N_H/2 = 1.1 \times 10^{22} \text{ molecules cm}^{-2} \).
The amount of CO in the foreground gas can be used to determine whether it is consistent with a dense or diffuse cloud environment because the CO abundance varies strongly with environment. The CO/H$_2$ ratio varies from 1.5 $\times$ 10$^{-4}$ in dark clouds (Kulesa & Black 2003) to as little as 10$^{-7}$ in diffuse clouds exposed to a substantial radiation field (van Dishoeck & Black 1988). Mitchell et al. (1990) observed the 4.7 $\mu$m fundamental band of 12CO in absorption toward LkH$\alpha$ 101 and derived a CO column density, $N$(12CO) = 1.1 $\times$ 10$^{17}$ cm$^{-2}$, under the assumption that the lines are optically thin. However, recent work by Goto et al. (2003) provides more sensitive infrared spectroscopy toward LkH$\alpha$ 101, including observations of the 13CO fundamental band at 2.3 $\mu$m. Those authors note that the 12CO fundamental band lines are heavily saturated and find an order of magnitude larger CO abundance, $N$(CO) = (1.84 $\pm$ 0.11) $\times$ 10$^{18}$ cm$^{-2}$, using the 13CO bands and the 12CO overtone bands. Thus the CO/H$_2$ ratio is $\sim$10$^{-4}$, typical for a dense cloud. Also, the excitation temperature they find for the 13CO lines is 30 K, which is indicative of cold, dense cloud material and consistent with the temperature we derive for H$_3^+$. We have computed a suite of cloud models based on work by van Dishoeck & Black (1986, 1988), which calculate the abundances of important species such as H, H$_2$, C$^+$, C, and CO as a function of depth into a cloud. Figure 5 demonstrates the depth dependence of the hydrogen- and carbon-bearing species for one interstellar cloud model appropriate to LkH$\alpha$ 101, a dense cloud with $n_H$ = 10$^4$ cm$^{-3}$ in a uniform 2.2 $\times$ Habing ($A_V$ = 1) radiation field.$^2$ The integrated column densities from this model provide $A_V$ = 11–13 mag and account for all of the observed CO. The 3 $\sigma$ upperlimit for the extinction toward LkH$\alpha$ 101 is $A_V$ $\sim$ 12 (Kelly et al. 1994); thus we find that at most 1 mag of diffuse material is warranted for this line of sight. Therefore, $N_H$ $<$ 2 $\times$ 10$^{21}$ cm$^{-2}$ for a typical diffuse cloud gas-to-dust ratio (Bohlin et al. 1978).

Can a diffuse cloud that provides $\sim$1 mag of visual extinction contain the observed H$_3^+$? For a typical diffuse cloud, $N$(H$_3^+$) = [C$(L(N(H_2))/[k_e N(e^{-})]$) (McCall et al. 2003), so that $\zeta L = [k_e N(e^{-}) N(H_3^+)]/N(H_2)$, where $\zeta$ is the ionization rate of H$_2$, $L$ is the path length through the cloud, and $k_e$ is the electron recombination rate, 2 $\times$ 10$^{-7}$ cm$^{-3}$ s$^{-1}$ (McCall et al. 2003). We adopt $N(e^{-})$ $\sim$ 5 $\times$ 10$^{17}$ cm$^{-2}$ if all elemental carbon (C/H $\sim$ 2.4 $\times$ 10$^{-4}$; Cardelli et al. 1996) is singly ionized, assuming that $L$ is not larger than a few parsecs. The resulting ionization rate, $\zeta$ $>$ 10$^{-18}$ s$^{-1}$, has profound consequences for the dense cloud. The ionization would increase the atomic hydrogen fraction to nearly 10$^{-1}$, but observations by Dewdney & Roger (1982) show that cold atomic hydrogen in 21 cm absorption toward LkH$\alpha$ 101 contributes only 10$^{-2}$ of the total hydrogen.
If we consider the limiting case in which all production of atomic hydrogen is governed by cosmic-ray ionization and balanced by the formation of molecular hydrogen at the Jura (1974) rate, then $\zeta < 10^{-15}$ s$^{-1}$. This is a strong upper limit because efficient dissociation of $H_2$ by UV radiation has been entirely neglected. Even if the cosmic-ray power spectrum is dominated by low-energy particles incapable of penetrating dark clouds, the high ionization rate measured by McCall et al. (2003) toward the diffuse cloud around $\zeta$ Per only manages to produce a small fraction ($\sim 10\%$) of the observed $H_3^+$ toward LkH$\alpha$ 101. It is also important to note that the temperature of $H_3^+$ that we observe, $\sim 30$ K, is identical to the rotational temperature of the dark cloud CO observed in absorption (Goto et al. 2003) and significantly lower than the $70$–$1200$ K spin temperature of the diffuse H I emission observed by Dewdney & Roger (1982). We conclude that most of the observed $H_3^+$ originates in the dense material, although a small fraction of the $H_3^+$ may reside in warmer diffuse material along the line of sight.

4.2. Location of the Cloud along the Line of Sight

The distance to LkH$\alpha$ 101 is uncertain. It has been estimated to be 160 pc by Stone & O’Neil (1998), 350 pc by Ungerechts & Thaddeus (1987), and at least 800 pc by Herbig (1971). Redman et al. (1986) suggest that the obscuring cloud is not intimately associated with LkH$\alpha$ 101, but this does not tightly constrain the cloud’s location. A tighter constraint on the proximity of the cloud is provided by the upper limit on the $H_2$ features in our 2 $\mu$m spectroscopy. If the cloud is close to the star, a significant nonionizing UV continuum and Ly$\alpha$ flux from LkH$\alpha$ 101 should lead to measurable $H_2$ fluorescence from the surface of the cloud. We measure an upper limit of the $H_2$ (1–0) S(1) line emission at 4712.9 cm$^{-1}$ (2.1218 $\mu$m) of $10^{-7}$ ergs s$^{-1}$ cm$^{-2}$ sr$^{-1}$, which limits exposure of $H_2$ within the intervening cloud to a radiation field of $k_{UV} \ll 1$.

We interpolate the ATLAS 9 (Kurucz 1993) and CoStar models (Schaefer et al. 1996) to estimate the specific luminosity of $H_2$-fluorescing photons from a 24,000 K star: $2.7 \times 10^{32}$ photons s$^{-1}$. The distance from LkH$\alpha$ 101 at which this ultraviolet radiation field would be quenched to $k_{UV} \ll 1$ is at least 20 pc.

4.3. $H_3^+$ Abundance and Ionization Rate in Dense Molecular Environments

Our characterization of the gaseous environment toward LkH$\alpha$ 101 constrains our physical interpretation of $H_3^+$ line absorption. $H_3^+$ is a unique molecule in that, to first order, its number density is independent of the total number density of the dense cloud (McCall et al. 1998). The formation rate of $H_3^+$ is determined by the ionization rate of $H_2$, $\zeta$, which is dominated by cosmic rays. The rate can be enhanced by a local X-ray radiation field such as that produced by a young star or group of stars that form in such environments (Black 2000). In a dense cloud, the destruction of $H_3^+$ is dominated by reaction with CO, whose reaction rate is $k_{CO} = 2 \times 10^{-7}$ cm$^3$ s$^{-1}$. Disregarding any other species that can react with $H_3^+$ places a lower limit on the cosmic-ray ionization rate of $H_2$ that is needed to maintain a steady state solution, $\zeta n(H_2) = k_{CO} n(CO) n(H_2)$, so that $n(H_3^+) = [\zeta n(H_2)] / [k_{CO} n(CO)]$. This can be rewritten as

$$\zeta L = k_{CO} N(CO) n(H_2^+)/N(H_2).$$

Adapting $N(H_3^+) = 2.2 \times 10^{14}$ cm$^{-2}$ from § 3, $N(H_2) = 1.1 \times 10^{22}$ cm$^{-2}$ and $N(CO) = 2 \times 10^{18}$ cm$^{-2}$ from § 4.1, we find $\zeta L \approx 80$ cm s$^{-1}$.

The angular extent of the obscuring cloud in the plane of the sky is $2'$ (Redman et al. 1986). The physical dimension of the cloud depends on its distance, and our only constraint is that it be at least 20 pc from LkH$\alpha$ 101. At the distances mentioned earlier, $d = 160, 350$, and 800 pc, the path length through the cloud is 0.09, 0.2, and 0.4 pc, respectively, assuming that it is spherical. The implied gas densities, $n(H_3^+)/N(H_2)/L_\alpha$ are $4 \times 10^4, 2 \times 10^4$, and $1 \times 10^4$ cm$^{-3}$. These are consistent with the firm upper limit of $2 \times 10^6$ cm$^{-3}$ that we find from a detailed analysis of the infrared CO absorption lines (C. A. Kulesa et al. 2004, in preparation). The resulting ionization rate indicated for each distance is $3 \times 10^{-16}$, $1.3 \times 10^{-16}$, and $6.7 \times 10^{-17}$ s$^{-1}$.

These derived ionization rates are lower limits, since we neglect other destructive species. In particular, O/CO ranges from $\sim 0.5$ to 1, and $k_{O}/k_{CO} \sim 0.5$. Thus the ionization rate can be enhanced by as much as 50%. If the dark cloud is at 800 pc preferred by Herbig (1971), then the observed ionization rate of the $H_3^+$ is consistent with the constraints determined by Solomon & Werner (1971). No sources of local ionization can explain the larger derived ionization rates at the nearer cloud distances. The only possible local source of ionization is a cluster of T Tauri stars located 0–5'–2' from the line of sight toward LkH$\alpha$ 101, at a distance of 160 pc. Following the treatment of Maloney, Hollenbach, & Tielens (1996), we derive a maximal local ionization enhancement of only $1.2 \times 10^{-17}$ s$^{-1}$ for an X-ray luminosity of $10^{32}$ ergs s$^{-1}$ and the minimum projected star-cloud distance of 0.1 pc. The derived ionization rate is therefore dominated by cosmic rays and not by a local enhancement of the radiation field. The cosmic-ray ionization rate will be better constrained once the gas density or the relationship of the obscuring cloud and LkH$\alpha$ 101 can be better established.

5. CONCLUSION

We have presented observations of $H_3^+$ absorption toward LkH$\alpha$ 101. The study of this relatively simple line of sight allows the interstellar material to be studied unambiguously. Our upper limit on the column of diffuse material is insufficient to account for the quantity of observed $H_3^+$; thus most of the $H_3^+$ must originate in a dense cloud. Furthermore, the spin temperature of the $H_3^+$ ($\sim 30$ K) is consistent with the same cold dense gas probed by CO. The identification of $H_3^+$ in the obscuring cloud toward LkH$\alpha$ 101 supports the previous attribution of significant $H_3^+$ absorption to dense cloud material (McCall 2001).

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