DETECTION OF THE 2165 INVERSE CENTIMETER (4.619 MICRON) XCN BAND IN THE SPECTRUM OF L1551 IRS 5

STEPHEN C. TEGLER, 1, 2 DAVID A. WEINTRAUB, 2, 3 LOUIS J. ALLAMANDOLA, 4 SCOTT A. SANDFORD, 4
TERENCE W. RETTIG, 1, 2 AND HUMBERTO CAMPINS 5

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ABSTRACT

We report the detection of a broad absorption band at 2165 cm⁻¹ (4.619 μm) in the spectrum of L1551 IRS 5. New laboratory results over the 2200–2100 cm⁻¹ wavenumber interval (4.55–4.76 μm), performed with realistic interstellar ice analogs, suggest that this feature is due to a CN-containing compound. We will refer to this compound as XCN. We also confirm the presence of frozen CO (both in nonpolar and polar matrices) through absorption bands at 2140 cm⁻¹ (4.67 μm) and 2135 cm⁻¹ (4.68 μm). The relative abundance of solid-state CO to frozen H₂O is ~0.13 while the abundance of XCN seems comparable to that of frozen CO.

Subject headings: infrared: interstellar: lines — ISM: individual (L1551 IRS 5) — ISM: molecules — line: identification

1. INTRODUCTION

Mid-infrared spectroscopic studies of protostars embedded in dense molecular clouds show the presence of interstellar ices and dust (Willner et al. 1982; Tielens 1989). The ices are known to contain H₂O, CH₃OH, CO, and CH₄ (Lacy et al. 1984; Allamandola & Sandford 1988; Lacy et al. 1991; Tielens et al. 1991; Allamandola et al. 1992), and probably CO₂ (d’Hendecourt & Jourdain de Muizon 1989), NH₃, and H₂CO. Additional components of the ices in these clouds are an unidentified CN-containing material (Lacy et al. 1984), as well as carbonyl containing species such as esters, ketones, and aldehydes (Tielens & Allamandola 1987). Observations of comets also show the presence of H₂O (Weaver, Mumma, & Larson 1987), CH₃OH (Bockelee-Morvan et al. 1991), CO (Balsiger et al. 1986), CH₄ (Larson et al. 1989), CO₂ (Moroz et al. 1987), and a C=NT containing material (Cruikshank et al. 1991). Although the relative abundance of ice components in protostellar and cometary environments has been under study for several years, few such measurements have been made for material surrounding pre-main-sequence stars. Ices in these environments are intermediate in an evolutionary sense between interstellar ices around protostars and ices in comets; hence, such measurements may provide evidence for determining whether cometary ices formed in situ or whether they survived in abundant enough quantities from interstellar ice reservoirs to permit comet formation without any additional ice evolution. The only relative abundance measurement that exists for frozen material of any type in these pre-main-sequence star environments is for the abundance of CO (Tielens et al. 1991) relative to H₂O (Sato et al. 1990) around L1551 IRS 5.

IRS 5, which is the exciting and driving source for the extremely well separated, prototypical bipolar outflow in the dark cloud L1551, shows a K2 III or later spectral type (Carr, Harvey, & Lester 1987; Stocke et al. 1988), emits a modest bolometric luminosity of ~40 L_⊙ (Stocke et al.), likely has a mass of less than ~2.5 M_⊙ (Strom et al. 1985) and is shrouded by ≥19 mag of optical extinction (Snell et al. 1985; Cohen 1975; Davidson & Jaffe 1984) along our line of sight. The outflow lobes are well collimated from within 0′.5 out to ≥10′ (≥0.5 pc at a distance of 160 pc) from the central source (e.g., Bieging & Cohen 1985). These results suggest that L1551 IRS 5 is more evolved than typical protostars and is surrounded by a thick circumstellar disk, viewed nearly edge-on to the plane of the sky (Stocke et al. 1988). In fact, Mundt et al. (1985), Carr et al. (1987), and Stocke et al. (1988) have shown that L1551 IRS 5 is probably an FU Orionis star. Keene & Masson (1990) have found that L1551 IRS 5 has a greater than 2000 AU radius envelope surrounding a compact core. They suggest the core, which has a radius of 45 ± 20 AU and a column density of ~10⁰⁰ g cm⁻², is the preplanetary disk inferred to exist around this star.

FU Orionis stars are a subclass of low-mass pre-main-sequence stars known as T Tauri stars. They are characterized by active growth of the star due to rapid accretion from a massive circumstellar disk (Hartmann et al. 1991). T Tauri stars are observed to have strong stellar winds and outbursts of ultraviolet radiation, especially during the FU Orionis star evolutionary stage. Consequently, icy grains in disks around T Tauri stars may be exposed to high levels of ion bombardment and ultraviolet irradiation. Laboratory experiments have demonstrated that certain ices undergo chemical changes—some new ice components form and others are destroyed—when exposed to ion bombardment and ultraviolet irradiation. In particular, Moore et al. (1983) and Lacy et al. (1984) report the growth of a broad absorption band centered at 2165 cm⁻¹ (4.619 μm) in the spectra of some laboratory ice mixtures, after exposing the ices to ion bombardment and ultraviolet irradiation, respectively. The laboratory results reported by Lacy et al. showed that the 2165 cm⁻¹ band is produced by irradiating laboratory ice mixtures containing carbon and nitrogen atoms. A carbon atom triply bonded to nitrogen atom has a range of stretching vibrations...
that depend on the group to which it is attached. Because the laboratory 2165 cm⁻¹ band falls in this range Lacy et al. concluded the measured absorption band is due to an unidentified molecule containing a nitrile or iso-nitrile group (\(\text{C}==\text{N}\) or \(\text{C}==\text{N}\), respectively) in a compound they designated as X(C==N). Alternative identifications for this band have been suggested, namely the CN stretch in the ion OCN⁻ (Grím & Greenberg 1987) and the SiH stretching vibration (Nuth & Moore 1988; Moore, Tanabe, & Nuth 1991). Because (i) the SiH feature seen in published laboratory spectra are too broad (50–200 cm⁻¹, as compared to a value of ~25 cm⁻¹ for the interstellar feature) and the narrowest bands do not match in position (2270 cm⁻¹ for the laboratory spectra vs. 2165 cm⁻¹ for the interstellar feature) and (ii) the laboratory feature produced by UV irradiation of mixed C- and N-containing ices fits the interstellar feature in both position and width (Lacy et al. 1984; this paper), we prefer an assignment to a CN-containing material and will refer here to the carrier as XCN and the feature as the XCN band.

Very few studies have been done on XCN in astronomical sources. XCN has been positively detected through the 2165 cm⁻¹ band only toward two protostars, W33 A, where it is particularly strong, and NGC 7538 IRS 9 (Lacy et al. 1984). Cruikshank et al. (1991) have identified a similar or identical CN-containing material through the 4550 cm⁻¹ (2.2 μm) overtone on the surfaces of certain asteroids, in the dust around some comets, on the surface of Iapetus, and in the rings of Uranus.

Previously, several groups (see discussion in Cruikshank et al. 1991) showed that absorption bands exist between 2270 and 2040 cm⁻¹ (4.4–4.9 μm) and 4550–4530 cm⁻¹ (2.2–2.3 μm) in laboratory reflectance spectra of nitrogen-bearing organic solids. In these studies, the bands were definitely identified with the fundamental and overtone of a C==N stretch. The good match between the astronomical spectra (Lacy et al. 1984), laboratory reflectance spectra (Cruikshank et al. 1991), and irradiated interstellar ice analogs (Lacy et al.; Moore et al. 1983) has been taken as evidence that energetic processing of interstellar ices occurs and plays an important interstellar chemical role. Even though there is limited astrophysical data, XCN has been extensively studied in the laboratory (d'Hendecourt & Allamandola 1986; Grim & Greenberg 1987; Allamandola, Sandford, & Valero 1988).

An understanding of the source and behavior of the 2165 cm⁻¹ (4.619 μm) feature is potentially very important and may help us address questions concerning the formation of stars and planetary systems. For example, is the carrier associated with the general dense cloud medium or is it specifically associated with circumstellar disks known to surround pre-main-sequence stars and embedded protostellar objects? Is it part of the icy or the refractory grain component? Cruikshank et al. (1991) propose that the CN-bearing materials found on solar system bodies may have formed in situ in the solar nebula and are thus part of a refractory material. Observations of XCN in many preplanetary disks could establish whether such materials formed on the surfaces of small bodies in the outer solar system or whether the CN-rich grains formed during an earlier epoch, before accretion produced planetsimals.

No XCN studies have been carried out yet for T Tauri stars. The strong ultraviolet excess associated with FU Orionis stars and the favorable, edge-on morphology of a disk around L1551 IRS 5 suggests the XCN column density along the line of sight to this source could be large enough to be measured.

L1551 IRS 5 therefore offers an excellent opportunity to determine whether icy grains in disks are chemically processed before they accrete to form planetsimals.

In this paper, we report the results of our spectroscopic study of L1551 IRS 5 and present new laboratory results for ice analogs over the 2200–2100 cm⁻¹ (4.55–4.76 μm) interval. In our spectrum of L1551 IRS 5, we find strong evidence for a broad absorption band centered near 2165 cm⁻¹. Our comparison of this spectrum with the spectra of laboratory ice analogs suggests the band is produced by XCN in the disk around this source. We address some of the questions raised by Lacy et al. (1984) about the nature of the carrier. In particular, the new laboratory results relax some of the restrictions on the XCN band carrier presented earlier by Lacy et al. We also confirm the existence of a narrow absorption band at 2140 cm⁻¹ (4.67 μm) produced by frozen CO trapped in a nonpolar matrix and a broader absorption band at 2135 cm⁻¹ (4.68 μm) produced by frozen CO in a polar matrix.

2. OBSERVATIONS

We obtained spectra of L1551 IRS 5 using the cooled grating array spectrometer (CGAS) (Tokunaga, Smith, & Irwin 1987) and the Infrared Telescope Facility (IRTF) on Mauna Kea, Hawaii, on 1991 October 22–24 UT. CGAS is a grating spectrometer with a linear array of 29 consecutive working InSb detectors. The observations were obtained with a 2′7 circular aperture and a 25′ north–south chop. The spectrometer, used in second order with grating B, provided a resolving power λ/Δλ of ~1300. Absolute wavelength calibration was obtained with a krypton lamp inside CGAS. Observations of L1551 IRS 5 were obtained at two grating positions resulting in spectra centered at 2132 cm⁻¹ (4.690 μm) and 2170 cm⁻¹ (4.608 μm) with a seven detector overlap. We obtained eight, 32 s spectra of L1551 IRS 5, four at each grating position. We also obtained six, 16 s spectra of the calibrator BS 1412, three at each grating position. By restricting the air-mass difference between L1551 IRS 5 and BS 1412 to less than 0.10, we ensured that telluric absorption features were accurately removed. To achieve a relative flux calibration, the spectrum of L1551 IRS 5 was multiplied by a T = 8190 K blackbody function appropriate for BS 1412.

In Figure 1, we present the calibrated 2200 to 2100 cm⁻¹ spectrum of L1551 IRS 5. The narrow and broad frozen CO features centered at 2140 cm⁻¹ and 2135 cm⁻¹, respectively, and the broad XCN feature centered at 2165 cm⁻¹ clearly are present in the data.

3. RESULTS

3.1. Astronomical Observations of L1551 IRS 5

The original spectrum of L1551 IRS 5 was converted to the absorbance spectrum shown in Figure 2a using the straight baseline (dashed line) drawn in Figure 1. The three high points between 2193 and 2185 cm⁻¹ are due to absorption in the bright star spectrum and were not used to define the baseline. Similar absorbance spectra from NGC 7538 IRS 9 (Fig. 2b) and W33A (Fig. 2c) are given for comparison. As laboratory spectra show that the XCN band extends into the tellurically obscured region, the baseline drawn produces a slightly conservative underestimate of the optical depth of both the CO and XCN bands and the width of the XCN band.

Figure 2a shows that the optical depth of the 2140 cm⁻¹ frozen CO feature in the spectrum of L1551 IRS 5 is ~4 times
that of the XCN band. This component, assigned to CO frozen in a nonpolar ice, is ≈ 2 times as deep as the 2135 cm⁻¹ shoulder which is due to CO in a polar-dominated interstellar ice (Sandford et al. 1988). The CO bands toward L1551 IRS 5 are discussed in detail by Tielens et al. (1991) and will not be treated further here.

Comparison of the 2200 to 2100 cm⁻¹ absorbance spectra of L1551 IRS 5, NGC 7538 IRS 9, and W33 A shows no obvious correlation between the absorbance in the XCN and frozen CO bands. The optical depths of various grain components toward these three objects with the XCN band are summarized in Table 1. Inspection of Table 1 suggests at best only a weak correlation between the XCN band and other ice features. This suggests that the XCN carrier is an independent grain component which is only loosely connected with other known solid constituents.

3.2. Laboratory Ice Analogs

Figure 3 shows the spectral evolution in the 2200–2100 cm⁻¹ (4.55–4.76 μm) region of an interstellar ice analog that was irradiated by ultraviolet light and subsequently warmed under vacuum. The composition of the starting ice was H₂O : CH₃OH : CO : NH₃ = 100 : 50 : 10 : 10, a composition chosen because its mid-infrared spectrum reproduces the main ice absorption features in the spectra of embedded objects such as W33 A and NGC 7538 IRS 9. The CO and NH₃ concentrations are enhanced by a factor of 2–5 relative to the normal interstellar ice abundance to increase the XCN yield and thereby facilitate its study. It is important to study the band carrier in a realistic ice as matrix effects can produce significant spectral variations. A full description of the experimental procedure and equipment used to obtain this laboratory data can be found elsewhere (Allamandola et al. 1988).

TABLE 1

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Band Center (cm⁻¹)</th>
<th>L1551 IRS 5</th>
<th>NGC 7538 IRS 9</th>
</tr>
</thead>
<tbody>
<tr>
<td>XCN</td>
<td>2165</td>
<td>0.16ᵇ</td>
<td>1.30ᵇ</td>
</tr>
<tr>
<td>CO</td>
<td>2140</td>
<td>0.80ᵇ</td>
<td>1.20ᵇ</td>
</tr>
<tr>
<td>CO</td>
<td>2135</td>
<td>0.16ᵇ</td>
<td>0.43ᵇ</td>
</tr>
<tr>
<td>H₂O</td>
<td>3275</td>
<td>2.10ᵇ</td>
<td>&gt; 5.40ᵇ</td>
</tr>
<tr>
<td>H₂O</td>
<td>1670</td>
<td>1.75ᵇ</td>
<td>0.45ᵇ</td>
</tr>
<tr>
<td>CH₃OH</td>
<td>1450</td>
<td>1.49ᵇ</td>
<td>0.36ᵇ</td>
</tr>
<tr>
<td>SiO</td>
<td>1030</td>
<td>1.4ᵇ</td>
<td>7.8⁴ᵇ</td>
</tr>
</tbody>
</table>

Notes—(a) this paper; (b) Lacy et al. 1984; (c) Tielens et al. 1991; (d) Sato et al. 1990; (e) Willner et al. 1982; (f) Cohen & Schwartz 1983.
The XCN Feature

In Figure 4, we compare the XCN band in the spectra of W33A, NGC 7538 IRS 9, L1551 IRS 5, and the 10 K irradiated laboratory sample warmed to 60, 125, and 175 K. All the spectra in this figure have been scaled to have the same optical depth in the center of the XCN band. This figure demonstrates that the profile and position of the interstellar XCN band are essentially the same in all three astronomical objects, and that the feature is well reproduced by the laboratory spectra. Temperature cycling is not necessary to shift the laboratory band to match the interstellar band as was the case in the earlier study reported by Lacy et al. (1984) on the simpler CO : NH₃ ice. Thus, there is no need for the scenarios that invoke warming by local infrared sources or long time scales in cooler regions considered by Lacy et al.; however, the questions of production efficiencies and production sites discussed by Lacy et al. remain valid.

4. DISCUSSION

The column density of an absorbing species \( N_x \) is given by the formula

\[
N_x \approx \frac{\Delta V_x \tau_x}{A_x},
\]  

(1)
we use the higher signal-to-noise ratio than our frozen CO observations, the frozen CO observations obtained by Tielens et al. have a value of 0.16. Our values for CO are in agreement with those reported by Tielens et al. 1991 (see Table 1). Since the ratio of frozen CO to frozen H$_2$O is $N_{CO}(total)/N_{H_2O} \approx 0.09$, although the ratio of frozen CO to frozen H$_2$O in the polar matrix, where the CO is less abundant, is $N_{CO}(polar)/N_{H_2O} \approx 0.02$. The relative abundance of XCN to frozen H$_2$O is $0.02 \leq N_{XCN}/N_{H_2O} \leq 0.05$. These ice abundance ratios, derived from the astronomical data alone, are consistent with the composition of the starting ice used in the laboratory experiments.

With the 2.7' aperture of CGAS, we do not have sufficient angular resolution to uniquely constrain the location of the absorbing ices. The results of other studies (Stocke et al. 1988), however, suggest that the visual optical depth through material in the immediate circumstellar environment of L1551 IRS 5, and along the direct line of sight to L1551 IRS 5 ($A_v \geq 19$ mag), is much greater than the visual optical depth through material in the immediate circumstellar environment of L1551 IRS 5, but not along the line of sight to the central source ($A_v \approx 0$). Thus it appears this ice-rich column is not representative of a grain population distributed in a spherically symmetric cloud around the central core. We conclude that most of these ices may lie in the circumstellar disk oriented nearly edge-on to our line of sight.

The laboratory ice experiments show that neither the CO nor the H$_2$O ices remain stable above ~150 K while the more refractory XCN remains solid only below ~250 K. These ices therefore could not exist in the inner region of the disk, closer than ~5-10 AU from the protostellar photosphere of L1551 IRS 5. They could exist in regions of this disk that are comparable in temperature to the outer planet region of our solar system, where comets in the Sun’s Oort cloud are thought to have formed.

5. CONCLUSIONS

We have measured a broad and shallow absorption band at 2165 cm$^{-1}$ in the spectrum of L1551 IRS 5 that we interpret as produced by XCN in a circumstellar disk around this source. Thus, there are now three extra-solar system sources, two embedded sources and an FU Orionis object, for which this feature has been detected. This XCN feature is similar in all three of these objects and can be well fitted with spectra obtained by photolyzing an ice of reasonable interstellar com-

**TABLE 2**

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Band Width$^a$ ($\Delta v$ cm$^{-1}$)</th>
<th>Absorbance $^b$ ($A_{cm molecule}^{-1}$)</th>
<th>Column Density $N$ (molecules cm$^{-2}$)</th>
<th>Column Mass $m$ (g cm$^{-2}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>XCN</td>
<td>20</td>
<td>2.4 x $10^{-17}$</td>
<td>0.8-1.6 x $10^{-17}$</td>
<td>&gt;3.5 x $10^{-6}$</td>
</tr>
<tr>
<td>CO(2140 cm$^{-1}$)</td>
<td>6</td>
<td>2.0 x $10^{-17}$</td>
<td>2.4 x $10^{-17}$</td>
<td>1.1 x $10^{-4}$</td>
</tr>
<tr>
<td>CO(2135 cm$^{-1}$)</td>
<td>10</td>
<td>2.0 x $10^{-17}$</td>
<td>0.8 x $10^{-17}$</td>
<td>3.7 x $10^{-10}$</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>335</td>
<td>2.0 x $10^{-16}$</td>
<td>3.5 x $10^{10}$</td>
<td>1.1 x $10^{-4}$</td>
</tr>
</tbody>
</table>

$^a$ Band width ($\Delta v$) and absorbance ($A$) values for XCN from d'Hendecourt & Allamandola (1986); for CO from Sandford et al. (1988); for H$_2$O from d'Hendecourt & Allamandola (1988).
position. The fit is temperature insensitive up to ~250 K, so the XCN-containing material could exist in the ice phase or reside in warmer organic residues. With spectra from only three objects, we are unable to determine whether the XCN around L1551 IRS 5 has been preserved in a dense disk from the protostellar cloud or whether intense particle and high-energy photon flux from the FU Orionis star has stimulated production of these ices in the disk.

We confirm the existence of a narrow absorption band at 2140 cm\(^{-1}\) (4.67 \(\mu\)m) produced by frozen CO trapped in a nonpolar matrix and a broader, weaker absorption band at 2135 cm\(^{-1}\) (4.68 \(\mu\)m) produced by CO frozen in a polar matrix (probably H\(_2\)O). Frozen H\(_2\)O is approximately 10 times more abundant than frozen CO and 20 times more abundant than XCN.

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