The Astrophysical Journal, 582:L101–L104, 2003 January 10

FIRST DETECTION OF VIBRATIONALLY EXCITED HNC IN SPACE

Peter Schilke and Claudia Comito
Max-Planck-Institut für Radioastronomie, Auf dem Hügel 69, 53121 Bonn, Germany; schilke@mpifr-bonn.mpg.de, ccomito@mpifr-bonn.mpg.de
and
Sven Thorwirth
I. Physikalisches Institut, Universität zu Köln, Zülpicher Strasse 77, 50937 Cologne, Germany; sven@ph1.uni-koeln.de
Received 2002 August 14; accepted 2002 November 27; published 2003 December 11

ABSTRACT

We report the first detection of vibrationally excited HNC in space, found toward the proto–planetary nebula CRL 618. Three lines of HNC in the $v_2 = 1$ vibrationally excited state have been found, making the detection unambiguous. The lines are emitted in a hot region close to the inner radius of the molecular envelope of CRL 618, but quantitative estimates of the column density are not possible, since the lines are most likely optically thick. In other astrophysical environments, HNC is found only in cold gas, and the presence of HNC in the hot layer toward CRL 618 is most likely due to time-dependent photochemistry in the boundary between the inner H II region and the molecular envelope.

Subject headings: astrochemistry — circumstellar matter — line: identification — radio lines: stars — stars: AGB and post-AGB — stars: individual (CRL 618)

1. INTRODUCTION

The observation of rotational transitions of vibrationally excited molecules is a unique probe of very hot gas around stars and young stellar objects (see, e.g., Schilke et al. 1992b, 2000; Schilke & Menten 2003 or Wyrowski, Schilke, & Walmsley 1999 and references therein). This is because vibrational transitions are generally pumped by IR radiation, and thus the excitation analysis offers a probe of the IR radiation field close to the exciting object, often at wavelengths at which direct observations in the IR are not possible, because the dust in the object is optically thick there. In the millimeter/submillimeter range at which the rotational lines are usually observed, the dust optical depth is usually negligible. Particularly in the carbon star IRC +10216, rotational lines of vibrationally excited HCN have been observed in a variety of vibrational states, up to 4000 K above the ground level (Schilke et al. 2000), and a careful study of these transitions can reveal the structure of the inner envelope in the dust formation zone.

In this Letter, we report the first detection of vibrationally excited HNC in interstellar space, toward the proto–planetary nebula CRL 618. HNC is a structural isomer of the more familiar hydrogen cyanide HCN. In interstellar molecular clouds, HNC has similar abundances to HCN in cold gas, while in hot gas it is much less abundant or even absent (Goldsmith et al. 1986; Schilke et al. 1992b). In the carbon star IRC +10216, HNC does not exist close to the star but is found only in an outer ring (Guélin, Lucas, & Neri 1996) and is supposed to be produced from the parent molecule HCN in the region where the expanding molecular envelope starts to be photodissociated by the interstellar UV radiation field.

In the proto–planetary nebula CRL 618, HCN and HNC are found to be of similar abundances by Bujarrabal et al. (1988), but at the time it was unknown where in the envelope HNC existed. Before we present and discuss our results, an introduction to this unusual object is in order.

Proto–planetary nebulae represent a short stage in the transition phase between asymptotic giant branch stars and planetary nebulae. These stars have gone through a phase of intense mass loss, and the central stellar remnant has heated up enough to start ionizing the inner envelope. CRL 618 is one of the few prominent representatives of this class. Its expanding envelope emits in a multitude of molecular lines (Bujarrabal et al. 1988), it shows a prominent high-velocity molecular outflow (Cernicharo et al. 1989; Neri et al. 1992; Hajian, Phillips, & Terzian 1996), and an H II region is just emerging around the central star (Martín-Pintado et al. 1993). Spectacular *Hubble Space Telescope* pictures of the outflow have been obtained by Trammell (2000). Very recently, *Infrared Space Observatory* (*ISO*) and single-dish observations have resulted in the detection of several organic molecular species, including benzene (Cernicharo et al. 2001a, 2001b). HCN and HNC have been observed with *ISO* (Herpin & Cernicharo 2000). Studies of vibrationally excited cyanoacetylene (HC_3N) and direct *l*-type transitions of vibrationally excited HCN (Wyrowski et al. 2003; Thorwirth et al. 2003) have established a good knowledge of the thermal profile of the inner envelope.

2. OBSERVATIONS

The observations were conducted 2001 March 11 and 12 and 2002 February 25 at the Caltech Submillimeter Observatory (CSO)[1] on Mauna Kea, Hawaii, using the facility receivers and back ends. The frequencies of vibrationally excited HNC were calculated on the basis of the results of Thorwirth et al. (2000) and are available in the Cologne Database for Molecular Spectroscopy (Müller et al. 2001).[2] We pointed on CRL 618 itself, using the HCN and HNC ground-state lines; hence, we estimate the pointing accuracy to be around 2″. Beam sizes and beam efficiencies were taken from the CSO Web page,[3] to be 30″ and 24″ and 76% and 77% at 270 and 360 GHz, respectively. Although in 2001 the weather was excellent (the 225 GHz atmospheric opacity $\tau_{225} \approx 0.04$), corresponding to roughly 0.8 mm of precipitable water vapor, typical single-sideband system temperatures were around 500 and 1400 K for 270 and 360 GHz, respectively, because the source was observed at low elevations. In 2002, τ_{225} was slightly worse, between 0.08 and 0.14, the

[1] The CSO is operated by the California Institute of Technology under funding from the National Science Foundation, grant AST 99-80846.
[2] See http://www.cdms.de.
[3] See http://www.submm.caltech.edu/cso/receivers/beam.html.

TABLE 1
LINE PARAMETERS FOR HCN AND HNC IN CRL 618

Line	$\int T_R^* \, dv$ (K km s^{-1})	T_R^* (K)	$v_{\rm LSR}$ (km s^{-1})	Δv (km s^{-1})
CRL 618				
HCN:				
$v_2 = 0$; $J = 3$–2	16.2 (0.5)	0.92 (0.05)	−21.2 (0.2)	16.5 (0.4)
	44.3 (0.8)	0.42 (0.05)	−17.8 (0.8)	97.7 (2.5)
$v_2 = 1f$; $J = 4$–3	3.6 (0.3)	0.10 (0.02)	−21.7 (1.4)	33.9 (3.3)
HNC:				
$v_2 = 0$; $J = 3$–2	9.5 (0.1)	0.40 (0.01)	−20.8 (0.1)	22.2 (0.2)
$v_2 = 1e$; $J = 3$–2	1.4 (0.1)	0.04 (0.01)	−24.4 (0.7)	30.7 (3.7)
$v_2 = 1f$; $J = 3$–2	0.4 (0.1)	0.02 (0.01)	−25.1 (1.9)	16.0 (3.3)
$v_2 = 0$; $J = 4$–3	19.8 (0.3)	0.78 (0.05)	−20.7 (0.2)	23.7 (0.5)
$v_2 = 1e$; $J = 4$–3	3.0 (0.2)	0.12 (0.05)	−24.4 (0.7)	23.4 (3.8)
IRC +10216				
HNC:				
$v_2 = 1f$; $J = 4$–3	...	<0.015	...	...

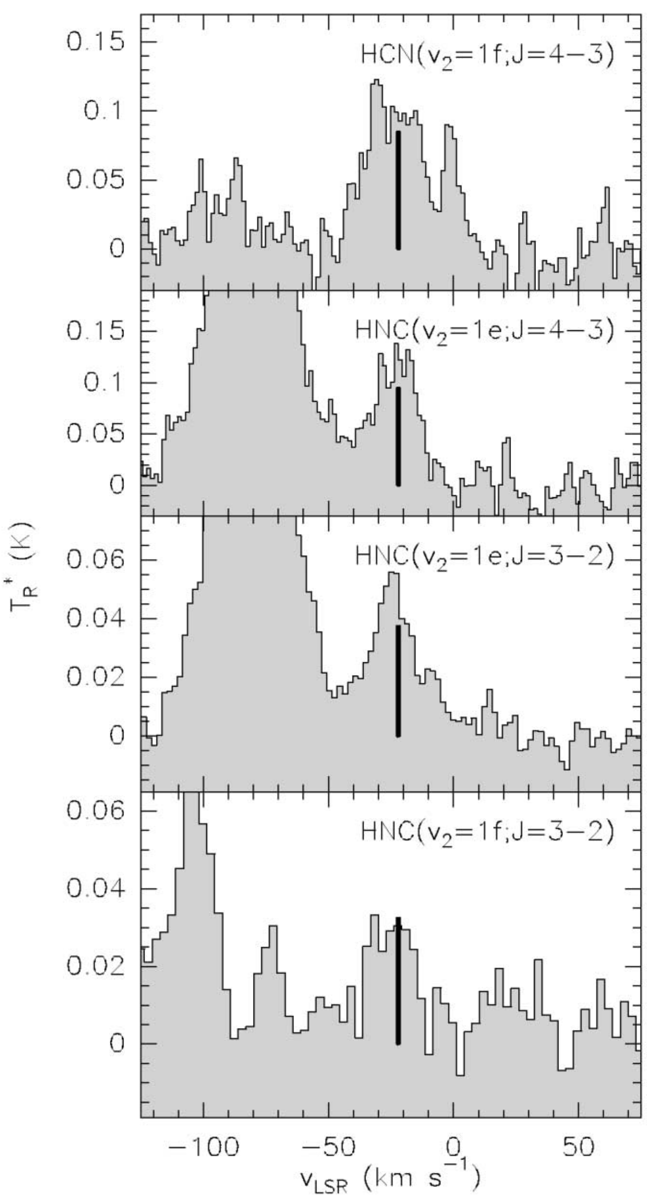

FIG. 1.—Spectra of vibrationally excited HCN and HNC toward CRL 618

observations were performed at higher elevations, and we had system temperatures comparable to 2001. In total, we estimate our calibration to be accurate to 30%.

3. RESULTS AND DISCUSSION

Three transitions of vibrationally excited HNC have been searched for in CRL 618, and all three have been found (Table 1, Fig. 1). A search toward IRC +10216 was conducted in the $v_2 = 1e$; $J = 4$–3 and $v_2 = 1f$; $J = 4$–3 vibrational satellites. While the $v_2 = 1e$; $J = 4$–3 line was blended with AlF (11–10), an upper limit of 45 mK (3 σ) could be obtained in the $v_2 = 1f$; $J = 4$–3 line.

Toward CRL 618, the $J = 4$–3 and $J = 3$–2 lines in the $v_2 = 1$ state have center velocities and line widths comparable with vibrationally excited HCN lines (cf. Table 1). Therefore, we consider the identification of all three lines with vibrationally excited HNC as secure, in particular since the line strengths of all three lines, taking the beam size and statistical weights into consideration, are comparable. The line density in CRL 618 at the frequencies in question, although high, is not high enough to allow for chance coincidences at all three frequencies with the correct intensities.

In addition to the HNC lines, we also observed the $J =$ 3–2 line of HCN. This line has also been observed by Cernicharo et al. (1989), who found a source size of ≈10″ for the spike component. Using this source size, the intensity we find is consistent with the results from Cernicharo et al. (1989) for the same transition, which were obtained with a much smaller beam of 11″. The HCN $v_2 = 1f$; $J = 3$–2 line is not detected, since it is buried by the line wings of the ground-state transition, but the ground-state line can be compared with the corresponding ground-state transition of HNC (Fig. 2). We note that HNC shows very weak line wings; thus, it has a low abundance in the outflowing gas. The ratio of integrated areas of the HCN (3–2) and HNC (3–2) spike component is 1.7, which has to be compared with the equal line strengths of the (1–0) transitions found by Bujarrabal et al. (1988), observed with a beam of similar size. These two results together, taken at face value, would hint at HNC being more abundant in the lower excitation gas [which is traced by the (1–0) transitions] than in the high-excitation gas [as traced by the (3–2) transitions], although a quantitative statement is difficult to make because of the un-

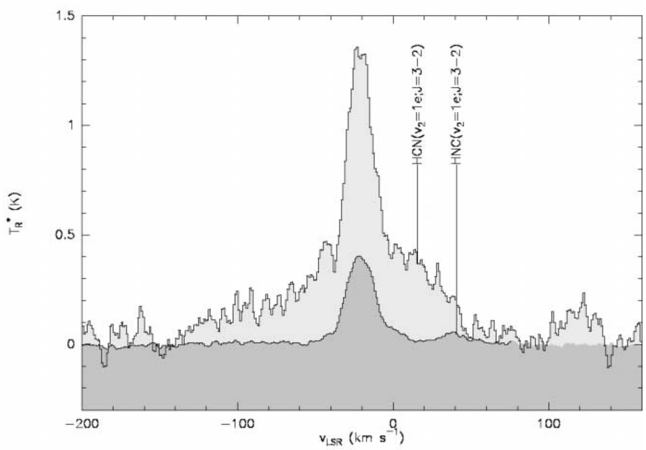

FIG. 2.—Spectra of ground-state HCN (3–2) and HNC (3–2). The $v_2 = 1e$; $J = 3$–2 component is visible for HNC but buried in the ground-state emission from the outflowing gas for HCN.

known optical depths of the lines. Moreover, the integrated area of the HCN (1–0) spectrum of Bujarrabal et al. (1988) is lower by a factor of about 2 than the integrated area of the same line reported by Cernicharo et al. (1989), observed with the same instrument, so that questions concerning the calibration accuracy of the HCN (1–0) and HNC (1–0) data and correspondingly the derived abundance ratios from Bujarrabal et al. (1988) arise. Using *ISO* observations, Herpin & Cernicharo (2000) find HCN and HNC to be equally abundant in their hot gas layer.

Our observations of vibrationally excited lines confirm the existence of HNC in the hot gas. Common wisdom is that vibrationally excited lines are pumped by IR radiation, since the critical densities are usually far higher than any densities encountered in the medium (e.g., Schilke et al. 1992a). The $v_2 = 1$ bending vibration state of HNC is much lower in energy than the corresponding state of HCN, ≈700 K versus ≈1050 K; i.e., HNC can be pumped by 21 μm radiation (which is close to the IR emission peak of CRL 618 at ≈22 μm; Knapp, Sandell, & Robson 1993), while HCN requires 14 μm. On the basis of this argument, one might expect that the region where HNC is excited is larger than the HCN excitation region. For the relatively low-lying HNC bending vibration, it also cannot be entirely excluded that the hot and dense gas [$T_{kin} \approx 200$ K, $n(H_2) \approx 10^7$ cm^{-3}; Cernicharo et al. 2001a, 2001b] can, after all, pump by collisions, which is unlikely to be the case for HCN.

For average source sizes of 0ʺ.5, guided by the results of Wyrowski et al. (2003) and Thorwirth et al. (2003), the intensities of the vibrationally excited lines of both HCN and HNC are consistent with optically thick emission at 200–300 K, in agreement with the temperatures expected at these radii. The fact that the HNC lines are of comparable strength to the HCN lines can mean either that the HNC lines come from a similar radius, because for optically thick lines

$$\begin{aligned} T_{MB} &= T_{kin}\eta_{MB} \\ &= T_0 \left(\frac{r}{r_0}\right)^{-\alpha} \left(\frac{r/D}{\Theta_{beam}}\right)^2 \\ &= \text{const}\,(r^{2-\alpha}), \qquad (1) \end{aligned}$$

which, with $\alpha = 0.8$ (Wyrowski et al. 2003), means that for optically thick lines, the rise of the filling factor overcompensates the drop of the temperature of the $\tau = 1$ "photosphere," or that the HNC lines come from a larger region as HCN but are not optically thick. A decision between these two alternatives could come only from spatially resolved observations, which is beyond the capabilities of present-day interferometers.

In § 1 it was mentioned that in the warm interstellar matter, HNC is virtually absent; also, in contrast to HCN, no HNC is found in the warm inner regions of carbon stars. The question arises of how HNC comes to exist in very warm gas in the very young proto–planetary nebula CRL 618, while it most likely did not exist in the envelope of its progenitor star, which probably resembled IRC +10216. Indeed, we failed to detect vibrationally excited HNC in the latter object, which is consistent with HNC in the vibrational ground state existing only in the outermost layer of the envelope (Guélin et al. 1996). The answer was probably given already by Bujarrabal et al. (1988), who claimed that the reason for the low HCN/HNC ratio and also for the high abundance of the ion HCO^+, which is virtually absent in IRC +10216, is the photodissociaton by UV photons from the star. Qualitatively, this can be seen in the models of IRC +10216 by Lafont, Lucas, & Omont (1982) or Nejad & Millar (1987), who consider photochemistry triggered by the interstellar radiation field on the *outside* of the envelope and indeed produce CN and HNC out of HCN, in agreement with the observations (Guélin et al. 1996). For CRL 618, the source of the UV photons is *inside* the envelope. First results of calculations aimed specifically at CRL 618 show that indeed HNC is produced as the result of chemical processes triggered by the intense UV field of the central star (P. A. Woods, T. J. Millar, & E. Herbst 2002, private communication).

We thank Tom Phillips for granting CSO observing time, Karl Menten for a critical reading of the manuscript, Friedrich Wyrowski for the vibrationally excited HCN data, and Eric Herbst and Tom Millar for discussions on the chemistry of CRL 618. An anonymous referee provided helpful hints concerning the excitation of the vibrationally excited lines. The CSO is supported by NSF grant AST 99-80846.

REFERENCES

Bujarrabal, V., Gómez-Gonzales, J., Bachiller, R., & Martín-Pintado, J. 1988, A&A, 204, 242
Cernicharo, J., Guélin, M., Martín-Pintado, J., Peñalver, J., & Mauersberger, R. 1989, A&A, 222, L1
Cernicharo, J., et al. 2001a, ApJ, 546, L123
———. 2001b, ApJ, 546, L127
Goldsmith, P. F., Irvine, W. M., Hjalmarson, A., & Ellder, J. 1986, ApJ, 310, 383
Guélin, M., Lucas, R., & Neri, R. 1996, in Science with Large Millimetre Arrays, ed. P. Shaver (Berlin: Springer), 276
Hajian, A. R., Phillips, J. A., & Terzian, Y. 1996, ApJ, 467, 341
Herpin, F., & Cernicharo, J. 2000, ApJ, 530, L129
Knapp, G. R., Sandell, G., & Robson, E. I. 1993, ApJS, 88, 173
Lafont, S., Lucas, R., & Omont, A. 1982, A&A, 106, 201
Martín-Pintado, J., Gaume, R., Bachiller, R., & Johnston, K. 1993, ApJ, 419, 725
Müller, H. S. P., Thorwirth, S., Roth, D. A., & Winnewisser, G. 2001, A&A, 370, L49
Nejad, L. A. M., & Millar, T. J. 1987, A&A, 183, 279
Neri, R., Garcia-Burillo, S., Guélin, M., Cernicharo, J., Guilloteau, S., & Lucas, R. 1992, A&A, 262, 544
Schilke, P., Güsten, R., Schulz, A., Serabyn, E., & Walmsley, C. M. 1992a, A&A, 261, L5
Schilke, P., Mehringer, D. M., & Menten, K. M. 2000, ApJ, 528, L37

Schilke, P., & Menten, K. M. 2003, ApJ, in press
Schilke, P., Walmsley, C. M., Pineau des Forêts, G., Roueff, E., Flower, D. R., & Guilloteau, S. 1992b, A&A, 256, 595
Thorwirth, S., Müller, H. S. P., Lewen, F., Gendriesch, R., & Winnewisser, G. 2000, A&A, 363, L37
Thorwirth, S., Wyrowski, F., Schilke, P., Menten, K. M., Müller, H. S. P., & Winnewisser, G. 2003, ApJ, in press
Trammell, S. R. 2000, in ASP Conf. Ser. 199, Asymmetrical Planetary Nebulae II: From Origins to Microstructures, ed. J. H. Kastner, N. Soker, & S. Rappaport (San Francisco: ASP), 147
Wyrowski, F., Schilke, P., Thorwirth, S., Menten, K. M., & Winnewisser, G. 2003, ApJ, in press
Wyrowski, F., Schilke, P., & Walmsley, C. M. 1999, A&A, 341, 882