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MORE METAL CYANIDE SPECIES: DETECTION OF AlNC ($X\ ^1\Sigma^+$) TOWARD IRC +10216

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ABSTRACT

A new metal-containing species, AlNC, has been detected toward the circumstellar envelope of the late-type carbon star IRC +10216, using the IRAM 30 m telescope. The $J = 11 \rightarrow 10$, $12 \rightarrow 11$, and $13 \rightarrow 12$ rotational transitions at 2 mm and the $J = 18 \rightarrow 17$ and $J = 21 \rightarrow 20$ transitions at 1.2 mm of this linear, closed-shell molecule were observed in this object. The line profiles appear U-shaped, indicating a source $\gtrsim 20''$, and the horn-to-center ratios suggest a shell-like distribution. In contrast, the other two Al-bearing molecules previously detected, AlF and AlCl, exist exclusively near the stellar photosphere. Modeling of the detected transitions, assuming a spherical-shell distribution, indicates a column density of $N_{\rm tot} \sim 9 \times 10^{11}$ cm^{-2} and a fractional abundance relative to H_2 of $\sim 3 \times 10^{-10}$ for AlNC. A rotational temperature of $T_{\rm rot} \sim 60$ K was also derived for this molecule, suggesting that shock waves may be synthesizing AlNC in the outer envelope. This species is the fourth metal cyanide/isocyanide compound discovered in this object, along with MgNC, MgCN, and NaCN. These data suggest that cyanide/isocyanide species are the major molecular carriers of metals in circumstellar gas.

Subject headings: circumstellar matter — ISM: molecules — line: identification — radio lines: stars — stars: individual (IRC +10216)

1. INTRODUCTION

Refractory molecules are known to be heavily depleted in the gas phase in molecular clouds. In fact, the only refractory species observed in such objects to date are SiO and SiS (e.g., Ziurys 1991). Such compounds, on the other hand, are significantly more abundant toward the circumstellar shells of late-type stars. For example, eight silicon-bearing molecules thus far have been detected toward the expanding envelope of the evolved carbon star IRC +10216, including such unusual species as SiC_3 (Apponi et al. 1999) and SiCN (Guélin et al. 2000). Furthermore, several molecules containing the metals aluminum, magnesium, sodium, and potassium have been discovered toward IRC +10216 (e.g., Cernicharo & Guélin 1987) and toward other evolved stars as well (Highberger et al. 2001). Although grain formation is thought to occur on a large scale in the envelopes of such objects (e.g., Glassgold 1996), the physical conditions there must nevertheless support a rich and varied gas-phase chemistry for refractory elements.

The most prevalent molecular form of silicon in circumstellar shells is in carbon-chain and ring-type compounds, as might be expected given the C-rich environment of these objects. In contrast, the metal-bearing molecules either are halide species (AlCl, AlF, NaCl, and KCl: Cernicharo & Guélin 1987) or contain the CN moiety (MgNC, NaCN, and MgCN: Kawaguchi et al. 1993; Turner, Steimle, & Meerts 1994; Ziurys et al. 1995). Searches for monoacetylides (MCCH) and monocarbides (MC) have been curiously unsuccessful. While the metal halide compounds are predicted to be abundant in stellar envelopes by thermochemical equilibrium models (Tsuji 1973), the appearance of cyanide/isocyanide species has been totally unexpected. Their chemical synthesis in IRC +10216 and other objects such as CRL 2688 and CRL 618 (Highberger et al. 2001) has yet to be adequately explained (Glassgold 1996; Petrie 1996a).

In this Letter we report the detection of a new metal-isocyanide compound, AlNC, which has been observed toward IRC +10216 using the IRAM 30 m telescope. These measurements were made possible because of the laboratory work of Robinson, Apponi, & Ziurys (1997) and the theoretical calculations of Ma, Yamaguchi, & Schaefer (1995). Five unblended rotational transitions were observed for AlNC, which is a linear, closed-shell species. Here we describe our results and discuss their implications for circumstellar chemistry.

2. OBSERVATIONS

The measurements were carried out in a series of observing runs from 1997 May through 2001 September, using the IRAM 30 m telescope at Pico Veleta, Spain. The receivers used were cooled SIS mixers at 2 and 1.2 mm in wavelength, operated in single-sideband mode with approximately 15 dB rejection. The initial observations were carried out with single-channel receivers, while measurements in 2000 October and thereafter were conducted with dual-polarization mixers. The backend used was a 1024 channel, 1 MHz filter bank split into several configurations (4 × 256 and 2 × 512, etc.), depending on the number of receiver channels. The temperature scale used was T_A^*, the chopper wheel-corrected antenna temperature, and therefore conversion to radiation temperature is $T_R = T_A^*/\eta_B$, where η_B is the main-beam efficiency. Observations were conducted by wobble-switching, with a throw of typically $\pm 1\rlap{.}'5$. The data were taken toward the IRC +10216 position $\alpha = 9^{\rm h}45^{\rm m}14\rlap{.}^{\rm s}8$, $\delta = 13°30'40\rlap{.}''0$ (B1950.0). Pointing was established by observations of the planets and OJ 287. Local

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TABLE 1

OBSERVATIONS OF AlNC TOWARD IRC +10216

Transition	Frequency (MHz)	θ_b (arcsec)	η_B	T_A^* (mK)	V_{LSR} (km s^{-1})	$\Delta V_{1/2}$ (km s^{-1})	$\int T_A^* dV$ (K km s^{-1})
$J = 11 \rightarrow 10$	131642.2	19	0.72	5 ± 2	−27.0 ± 2.3	29.6 ± 2.3	0.084 ± 0.023
$J = 12 \rightarrow 11$	143605.4	17	0.69	6 ± 3	−27.5 ± 2.1	33.4 ± 2.1	0.153 ± 0.026
$J = 13 \rightarrow 12$	155567.4	16	0.67	5 ± 2	−27.5 ± 1.9	28.9 ± 1.9	0.102 ± 0.027
$J = 18 \rightarrow 17$	215357.9	12	0.56	6 ± 3	−26.5 ± 1.4	29.2 ± 1.4	0.100 ± 0.026
$J = 21 \rightarrow 20$	251213.0	10	0.48	5 ± 2	−26.5 ± 1.1	28.5 ± 1.1	0.099 ± 0.030

NOTE.—Errors are 3 σ; observed toward $\alpha = 09^{\mathrm{h}}45^{\mathrm{m}}14\overset{\mathrm{s}}{.}8$, $\delta = 13°30'40\overset{''}{.}0$ (B1950.0).

oscillator shifts were conducted for every line to confirm sideband identity.

3. RESULTS

A summary of the AlNC observations toward IRC +10216 is given in Table 1, including rest frequencies, beam sizes, and beam efficiencies η_B, as well as line parameters. As is shown in the table, the detected lines of aluminum isocyanide have intensities typically less than 10 mK (T_A^*), but with the usual LSR velocity ($V_{\mathrm{LSR}} \sim -26.5$ km s^{-1}) and line width ($\Delta V_{1/2} \sim 30$ km s^{-1}) for molecules present in the outer envelope (Cernicharo, Guélin, & Kahane 2000). The line parameters are also consistent among the five features, additional proof that they arise from the same molecule, and the lines appear exactly at the frequencies measured in the laboratory for AlNC within 0.5 MHz (Robinson et al. 1997). Moreover, there are no known identifications of these spectral features other than aluminum isocyanide.

Spectra of four transitions of AlNC are presented in Figure 1, which includes the three lines observed at 2 mm ($J = 11 \rightarrow 10$, $J = 12 \rightarrow 11$, and $J = 13 \rightarrow 12$) and a 1.2 mm feature ($J = 18 \rightarrow 17$). The four transitions appear to exhibit U-shaped profiles. This line shape indicates that the source of AlNC emission in this circumstellar shell must be extended with respect to the largest 2 mm beam ($\theta_b \sim 19''$ or $r \gtrsim 10''$; see Table 1). Therefore, AlNC must be present toward the outer regions of the envelope.

The spectra shown in Figure 1 also contain features from other molecules; the stronger lines have been already reported in Cernicharo et al. (2000). A summary of the features appearing in the AlNC bandpasses is given in Table 2. Several weak unidentified lines were observed, as well as transitions arising from carbon chains or rings, including those containing a sulfur or a silicon heteroatom.

4. DISCUSSION

4.1. AlNC*: The Third Interstellar Aluminum-bearing Compound*

The unambiguous detection of five transitions of AlNC, a linear species with a $^1\Sigma^+$ ground electronic state, confirms the presence of this new molecule in the circumstellar envelope of IRC +10216. This compound is the third molecule identified in interstellar/circumstellar gas that contains the element aluminum. Previously, only AlCl and AlF had been observed (Cernicharo & Guélin 1987; Ziurys, Apponi, & Phillips 1994). However, in contrast to AlNC, the aluminum halide species are confined to the *inner* envelope of IRC +10216, as suggested by their flat-topped line profiles (Cernicharo & Guélin 1987) and Plateau de Bure interferometer maps (Guélin, Lucas, & Neri 1997). Their total spatial extent is on the order of 5″. They are thus likely formed at chemical equilibrium close to the stellar photosphere where temperatures are approximately 2000 K, as predicted by Tsuji (1973).

The cusped appearance of the AlNC profiles suggests a concentration near the outer envelope of IRC +10216, at least up to a radius of 10″ from the star. However, detection of the $J = 18 \rightarrow 17$ and $J = 21 \rightarrow 20$ transitions, which lie over 100 K above the ground rotational level, indicates that AlNC emission originates in warm material. Species solely confined to the outer envelope, such as the free radicals C_4H or MgNC, often have low rotational temperatures ($T_{\mathrm{rot}} \sim 15$–35 K: Guélin, Lucas, & Cernicharo 1993). On the other hand, the presence of vibrationally excited C_4H and rotational temperatures derived from C_5H and C_6H (e.g., Guélin et al. 1997) indicate $T_{\mathrm{rot}} \sim 50$–60 K in the outer shell. Moreover, cross K-ladder transitions of SiC_2, which also has U-shaped line profiles, suggest an origin in gas with $T_K \sim 140$ K (Thaddeus, Cummins, & Linke 1984). Hence, observation of higher energy lines of AlNC is still consistent with an outer shell source. Consequently, the distribution of AlNC is very different from its halide counterparts AlCl and AlF.

4.2. AlNC *and Other Cyanide Abundances in IRC +10216*

The column density and fractional abundance of AlNC was estimated using a model of a spherically- symmetric, expanding envelope (see Guélin et al. 1997). The input parameters are source distribution and rotational temperature, which are adjusted to reproduce the observed line profiles and hence derive column densities and abundances. A mass-loss rate of 3×10^{-5} $M_\odot$ yr^{-1} and a distance to IRC +10216 of 200 pc were assumed (Crosas & Menten 1997), and a dipole moment for AlNC of 3.14 D was used (Ma et al. 1995). The best fit to the line profiles was achieved for a hollow-shell source with an inner radius of 5″ and an outer radius of 15″ for a rotational temperature of $T_{\mathrm{rot}} = 60$ K. The subsequent column density for AlNC through the shell was found to be $N_{\mathrm{tot}} \sim 9 \times 10^{11}$ cm^{-2}, with $f(\mathrm{AlNC/H_2}) \sim 3 \times 10^{-10}$.

In comparison, the fractional abundance of MgCN in IRC +10216 of $f \sim 7 \times 10^{-10}$ is similar to that of AlNC (Ziurys et al. 1995), while MgNC is more abundant, with $f \sim 5 \times 10^{-8}$ (Kawaguchi et al. 1993; Highberger et al. 2001). The magnesium compounds are present in the outer shell, both being free radicals. The other metal cyanide species detected, NaCN, is confined to the inner shell ($\theta_s \sim 5''$) with a far greater abundance than any of its counterparts: $f(\mathrm{NaCN/H_2}) \sim 10^{-7}$ (Guélin et al. 1997; Highberger et al. 2001).

In the inner envelope of IRC +10216, AlF and AlCl have fractional abundances of $f(\mathrm{AlF/H_2}) \sim 1.5 \times 10^{-7}$ and $f(\mathrm{AlCl/H_2}) \sim 2.2 \times 10^{-7}$, respectively, if a 5″ source size is assumed (Highberger et al. 2001). Thus, they are by far the dominant molecular carriers of aluminum, at least in this region. If the abundance of aluminum in IRC +10216 is roughly cosmic (i.e., $\mathrm{Al/H} \sim 3 \times 10^{-6}$: Savage & Sembach 1996), then

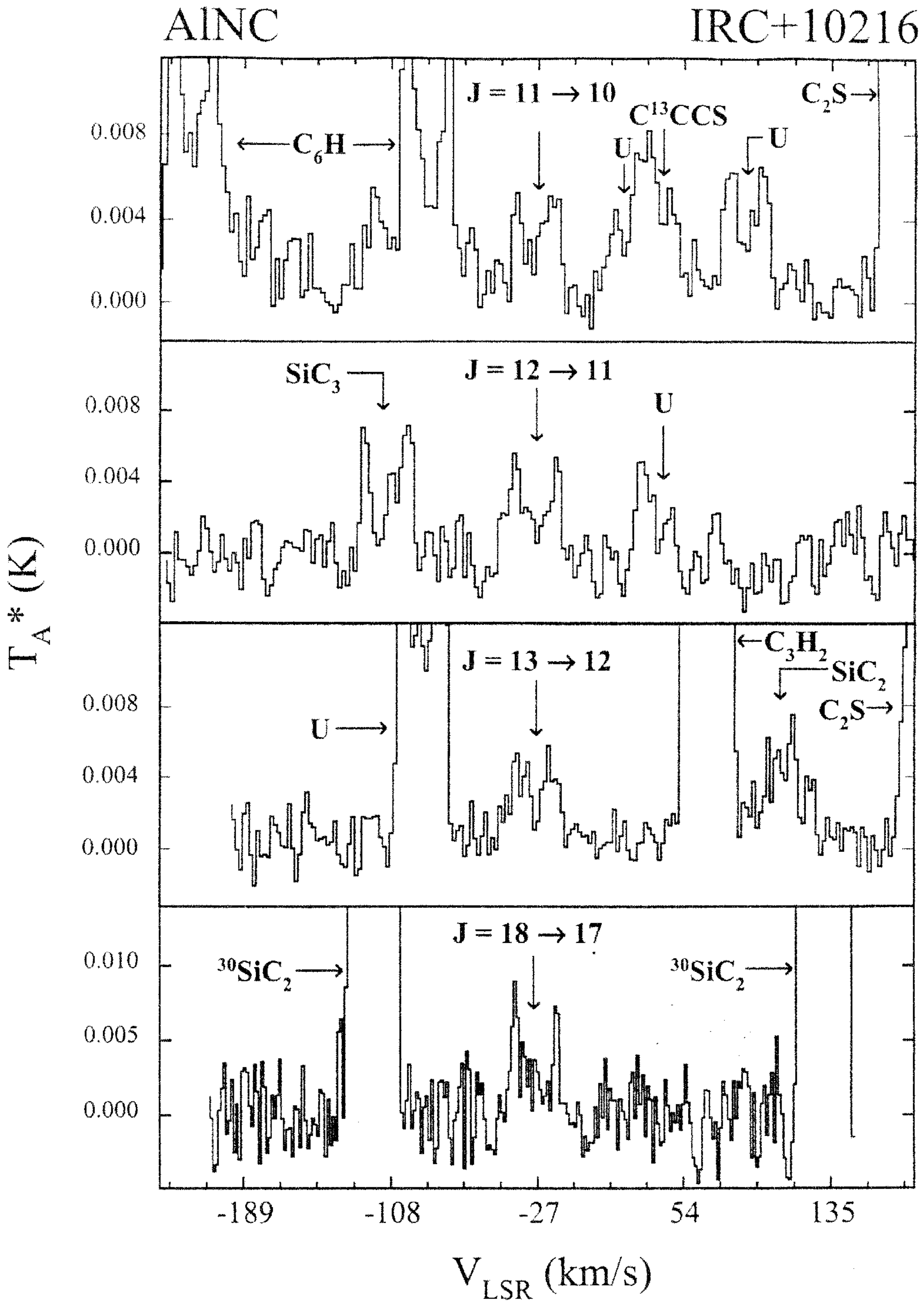

FIG. 1.—Spectra of the $J = 11 \rightarrow 10$, $12 \rightarrow 11$, $13 \rightarrow 12$, and $18 \rightarrow 17$ rotational transitions of AlNC($X^1\Sigma^+$) at 131, 143, 155, and 215 GHz, respectively, observed toward IRC +10216 using the IRAM 30 m telescope. The line profiles are U-shaped, indicating that AlNC emission is likely to be extended into the outer circumstellar shell. The spectral resolution is 1 MHz.

about 5% of this element is in the form of these two compounds. It is not clear, however, that cosmic abundances apply to envelopes of asymptotic giant branch stars (Forestini & Charbonnel 1997). Nevertheless, AlNC is still a very minor sink for aluminum and a very large fraction of Al must be incorporated into grains quite close to the star.

4.3. *Metal Cyanide Chemistry in IRC +10216*

AlNC is the fourth metal cyanide/isocyanide molecule observed in IRC +10216, along with MgNC, MgCN, and NaCN. Therefore, the cyanides appear to be an important carrier of refractory elements. It was initially proposed that the magnesium species were produced via the radiative association reaction (Kawaguchi et al. 1993),

$$Mg^+ + HCN \rightarrow MgNCH^+ + h\nu, \quad (1)$$

followed by dissociative recombination. However, calculations have shown that this process is too slow to be viable for Mg, Al, or Na (Petrie 1996a). Petrie has suggested that the same

TABLE 2

ADDITIONAL MOLECULES OBSERVED IN THE BANDPASS

Molecule	Transition	Frequency (MHz)	T_A^* (K)	V_{LSR} (km s^{-1})	$\Delta V_{1/2}$ (km s^{-1})
C_2S	$N_J = 10_{11} \rightarrow 9_{10}$	131552.0	0.134 ± 0.003	−26.2 ± 2.3	29.6 ± 2.3
$C^{13}CCS$[a]	$J = 23 \rightarrow 22$	131612.1	0.004 ± 0.002	∼−27	∼28
$C_6H(^2\Pi_{3/2})$	$J = 47.5 \rightarrow 46.5e$	131668.5	0.019 ± 0.003	−26.1 ± 2.3	29.7 ± 2.3
	$J = 47.5 \rightarrow 46.5f$	131725.5	0.016 ± 0.003	−25.6 ± 2.3	29.7 ± 2.3
SiC_3	$J(K_a, K_c) = 12(2, 10) \rightarrow 11(2, 9)$	143645.4	0.008 ± 0.002	−26.2 ± 2.6	26.5 ± 2.6
C_2S	$N_J = 12_{12} \rightarrow 11_{11}$	155454.5	0.038 ± 0.003	−26.6 ± 1.9	28.9 ± 1.9
C_3H_2	$J(K_a, K_c) = 3(2, 2) \rightarrow 2(1, 1)$	155518.3	0.101 ± 0.003	−26.3 ± 1.9	28.9 ± 1.9
SiC_2[b]	$J(K_a, K_c) = 7(2, 6) \rightarrow 6(2, 5)$	164069.1	0.005 ± 0.002	−26.7 ± 2.1	29.2 ± 2.1
$^{30}SiC_2$	$J(K_a, K_c) = 9(2, 7) \rightarrow 8(2, 6)$	215247.7	0.069 ± 0.003	−27.8 ± 1.4	29.2 ± 1.4
$^{30}SiC_2$	$J(K_a, K_c) = 10(0, 10) \rightarrow 9(0, 9)$	215424.5	0.068 ± 0.003	−27.9 ± 1.4	30.6 ± 1.4
Unidentified[a]	…	131620	0.003 ± 0.002	∼−27	∼28
Unidentified	…	131590	0.005 ± 0.002	−27	27.3 ± 2.3
Unidentified	…	143574	0.006 ± 0.003	−27	25.0 ± 2.6
Unidentified	…	155601	0.014 ± 0.002	−27	28.9 ± 1.9

NOTE.—Errors are 3 σ; beam sizes and efficiencies given in Table 1.

[a] Blended line; see text.

[b] Image sideband.

type of reaction with longer carbon-chain molecules such as HC_5N might be more feasible, because the rate is increased through vibrational stabilization of the intermediate ion, such as $MgNC_5H^+$. This mechanism might be possible for MgNC, MgCN, and AlNC, which exist predominantly in the outer envelope—the only region where there is significant photoionization. The inner-shell distribution of NaCN on the other hand requires an alternative production scheme.

On the basis of calculations of heats of formation (Petrie 1996b), NaCN appears to be a relatively stable compound; it is also closed shell. Hence, it is likely formed at LTE in the inner envelope. (Curiously, the radiative association reaction of $Na^+ + HC_5N$ is not very efficient.) Considering theoretical predictions of Gibbs free energies (Politzer, Lane, & Grice 2001), AlNC should be relatively stable as well, but not quite as robust as AlCl and AlF. LTE chemistry in the inner envelope must clearly favor the halide compounds. Why AlF and AlCl do not survive into the outer envelope is a puzzling question.

Another possible pathway for AlNC formation in the outer shell may be shock waves. Several theoretical studies have suggested shock chemistry for molecule production near the stellar photosphere (Duari, Cherchneff, & Willacy 1999). Furthermore, observations of HCN toward a large sample of AGB circumstellar shells by Bieging, Shaked, & Gensheimer (2000) indicate that the higher energy rotational lines of this species are unusually bright. These data suggest that HCN is produced by nonequilibrium chemical processes—likely shock waves. Such shocks could also be creating AlNC. Such formation would additionally explain the relatively high rotational temperature observed in this species. Shock waves could be destroying AlF and AlCl at the same time, causing their abundances to drop sharply a short distance from the star, and perhaps releasing aluminum for later AlNC creation. Certainly additional observations and chemical modeling are needed to explain these current findings.

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