THE ASTROPHYSICAL JOURNAL, 426:L97–L100, 1994 May 10

# DETECTION OF SODIUM CYANIDE (NaCN) IN IRC 10216

B. E. TURNER
National Radio Astronomy Observatory,[1] 520 Edgemont Road, Charlottesville, VA 22903-2475
T. C. STEIMLE
Arizona State University, Department of Chemistry, Tempe, AZ 85287
AND
LEO MEERTS
Katholieke University, Sterrenkundig Instituut, Toernooiveld, NL-6525 ED Nijmegen, The Netherlands

*Received 1993 November 2; accepted 1994 March 3*

## ABSTRACT

The first molecule containing Na has been detected in the outer circumstellar envelope of IRC 10216, by means of four rotational transitions in the 3 and 2 mm spectral regions. Observations are well fitted by a low rotation temperature of 11 K, typical of the outer envelope. The column density and fractional abundance depend on the distribution assumed for NaCN, the abundance varying between $6 \times 10^{-9}$ and $1 \times 10^{-7}$ for distributions corresponding to $HC_3N$ (outer plus intermediate envelope) and $HC_7N$ (outer envelope only). The fraction of cosmic Na in the form of NaCN is probably several percent, so that significant amounts of Na escape incorporation into grains, unlike the fraction ($<0.002$) that applies for Si. If IRC 10216 is typical, relative abundances of Na and Si as observed in the diffuse interstellar medium are consistent with rates of ejection in the gas phase from circumstellar envelopes.

*Subject headings:* ISM: abundances — ISM: molecules — stars: mass loss

## 1. INTRODUCTION

Mass loss from evolved stars is the major source of heavy elements in the interstellar medium (ISM). The refractory elements are thought to be mainly condensed into grains in the inner envelopes of evolved circumstellar shells (CSEs), and assuming that they are coated with mantles of organic compounds, the grains are unlikely to be photoeroded in the ISM to the refractory element layers before being incorporated into dense molecular clouds. Therefore, an explanation of the observed gas-phase refractory elements in the diffuse ISM (which themselves are accreted efficiently onto grains) requires an understanding of how refractory elements are lost in the gas phase from CSEs (see Turner 1991 for a review).

The situation regarding Si is relatively well understood. The detections in the outer envelope of IRC 10216 of $SiC_2$ (Thaddeus, Cummins, & Linke 1984) and SiN (Turner 1992a), when compared with earlier studies of the amounts of SiS and SiO which reach the outer envelope (Morris 1975), led to the conclusion (Turner 1992a) that only a fraction $10^{-4}$ to $10^{-3}$ of all Si escapes to the ISM in gaseous form from IRC 10216. Thus, the traditional idea that the interstellar gas/dust ratio of $\sim 100$ represents the condensation of essentially all refractory elements in evolved stellar envelopes needed no revision.

The recent detection of MgNC (Kawaguchi et al. 1993) in the outer envelope of IRC 10216 is understandable in view of Tsuji's (1973) prediction that gas-phase Mg should remain atomic under thermochemical equilibrium in the dense inner envelope and the expectation (Turner 1991) that Mg, being less refractory than Si, should condense less completely and later in the outflow than Si. Thus, appreciable quantities of Mg reach the outer envelope in reactive form ($Mg^+$).

Other refractory elements detected as molecules in IRC 10216 are NaCl, KCl, AlCl, and AlF (Cernicharo & Guelin 1987). These are all predicted (Tsuji 1973) to be the predominant forms under thermochemical equilibrium in O-rich CSEs, while NaCN would be the dominant Na compound in C-rich CSEs (Tsuji 1992; see Turner 1992b). Because these detected species occur only in the innermost envelope (Cernicharo & Guelin 1987), they give no information as to the fraction of Na or Al that reach the outer envelope and hence the ISM.

Just as MgNC can be argued as the likely Mg compound in the outer envelope if Mg appears there as $Mg^+$, so can NaCN be argued for as the most likely outer envelope compound of Na if sodium occurs there as $Na^+$. Thus, NaCN is a likely outer envelope constituent by reason of either in situ formation or transportation as NaCN from the dense inner envelope. Observed profiles can distinguish inner from outer envelope location. A comparison of the NaCN abundance in the outer envelope with the cosmic Na abundance can indicate the efficiency with which Na is incorporated into grains in the CSE outflow.

The question of detecting refractory element compounds in interstellar objects remains open. In view of the widespread presence of Si molecules in warm massive star-forming regions, Turner (1991) predicted that compounds of Mg, Na, and possibly Fe should also be seen. We have conducted a sensitive search for NaCN in several interstellar sources.

We report here the successful detection of NaCN in the outer envelope of IRC 10216. NaCN was not seen in interstellar clouds.

## 2. SPECTROSCOPY OF NaCN

NaCN (NaNC) is a T-shaped molecule in the ground vibronic state, with the Na nucleus lying along a line that intersects near the midpoint of the CN bond and forms an angle of $\sim 86°$ with that bond. We have predicted transition frequencies and intensities using the spectroscopic parameters derived

---

[1] Operated by Associated Universities, Inc., under cooperative agreement with the National Science Foundation.

from the molecular beam electron-resonance spectroscopy studies of van Waals, Meerts, & Dymanus (1984). Each rotational level is split into 12 hyperfine components by the N ($I = 1$) and Na ($I = 3/2$) nuclear electric quadrupole interaction. For all relevant rotational levels ($4_{04}$ and higher), the spread in energy of the 12 components is an approximately constant 12 MHz, and the pattern is very similar. Thus, the strong $\Delta F = \Delta N$ transitions are nearly coincident. Since $\Delta F = \Delta N$ transitions decrease in relative intensity with increasing N, the $5_{05}$–$4_{04}$ transition has the largest intrinsic linewidth, 83% of its intensity occurring within a width of 0.9 MHz and 100% within a width of 1.6 MHz. We estimate the accuracy of the rotational frequencies to be ~1 MHz or better, by use of the sextic centrifugal distortion constants given by van Waals et al. (1984). In Table 1 we present only the center frequencies for each rotational transition and the pure rotational line strength. The *a*-type dipole moment, which lies along the Na-(CN) axis, is calculated as 3.6 debye (Klein, Goddard, & Bounds 1981).

## 3. OBSERVATIONS AND RESULTS

Observations were made with the NRAO 12 m telescope in 1993 October, at 77836.7 MHz ($5_{05}$–$4_{04}$), 93206.1 MHz ($6_{06}$–$5_{05}$), 108472.0 MHz ($7_{07}$–$6_{06}$), and 138652.1 MHz ($9_{09}$–$8_{08}$). At both 3 and 2 mm, dual channel SIS junction receivers were used, tuned for single-sideband operation. Telescope main-beam efficiencies $\eta_c$ and beamwidths $\theta_B$ are, respectively, (0.645, 81″), (0.625, 68″), (0.61, 58″), and (0.56, 45″). Measured intensities $T_R^*$ (calibrated by the usual chopper vane method) are converted into brightness temperatures via $T_B = \eta_c^{-1}[1 + (\theta_B/\theta_s)^2]$, where $\theta_s$ is the assumed source angular diameter. Beam-switching (4′ throw) was used for IRC 10216, frequency-switching (±1.2 MHz) for TMC 1, and position switching for other sources. Except for TMC-1, 1 MHz spectral resolution was used, corresponding to a velocity resolution of 3.85, 3.22, 2.76, and 2.16 km s$^{-1}$ at the four frequencies, respectively. For TMC-1, 24 kHz resolution gave 0.092 km s$^{-1}$ resolution at the single observed frequency of 77.836 GHz. Figure 1 shows the observed spectra toward IRC 10216. At 77.8 GHz, the observed line is both stronger than its expected LTE value and wider than is compatible with the calculated hfs. S. Takano (1993, private communication) has pointed out that the $5_{05}$–$4_{04}$ transition is blended with the $C_4H$, $v_7 = 1$, $^2\pi_{3/2}$, 17/2–15/2(e) transition at 77833.1 MHz. This transition has never been observed, but from IRAM 30 m observations of adjacent-*J* transitions (Yamamoto et al. 1987), we estimate it will contribute $T_R^* = 14$ mK, 9.4 mK, and 7.8 mK at the 12 m telescope for $C_4H$ source diameters of 36″, 18″, and 6″, respectively. The intrinsic NaCN linewidth is then reduced from 16 MHz (Fig. 1) to 12.4 MHz. As indicated in Table 1, the observed velocity width (to zero intensity) decreases uniformly from 47.7 km s$^{-1}$ at 77 GHz to the expected value of 30 km s$^{-1}$ for IRC 10216 at 108 GHz. This is consistent with our calculated hyperfine patterns.

Line shapes are not well determined by our observations. The lines at 77, 108, and 139 GHz suggest cusps (with one cusp weaker than the other, as occurs in many IRC 10216 species), while the line at 93 GHz is flat-topped. Cusped profiles indicate spatially resolved, optically thin lines, while flat-topped profiles indicate unresolved optically thin lines. Since NaCN is surely unresolved in the 12 m beams, we conclude that all lines are flat-topped within the noise. There is no evidence for parabolic-shaped profiles, indicative of unresolved, optically thick lines.

To determine the location of NaCN within the envelope, we assume all four lines have a single rotational temperature $T_{\rm rot}$. A simple LTE calculation then gives the value of $T_{\rm rot}$ as a function of the assumed value of $\theta_s$. We consider $\theta_s$ values of 36″ (the size of $HC_3N$, $J = 2$–1; Wootten, Truang-Bach, & Rieu 1993; Bell 1993), 18″ (the size of $HC_7N$ [Wootten et al. 1993]), 12″ (the size of SiS), and 1″ (roughly the size within which thermochemical equilibrium is expected). Because the ratio of $T_B$ for higher *J* lines to $T_B$ for lower *J* decreases as $\theta_s$ is decreased, we require a *lower* value of $T_{\rm rot}$ to fit all four lines as $\theta_s$ is decreased. This efect is small: $T_{\rm rot} = 12$ K for $\theta_s = 36''$, and 10 K for $\theta_s = 12''$. A value $T_{\rm rot} \simeq 11$ K is entirely consistent with the range 10–15 K found for several outer envelope species (Bell 1993; Bieging & Rieu 1988; Bieging & Tafalla 1993; Wootten et al. 1993) and establishes NaCN as an outer envelope species.

TABLE 1

OBSERVED PARAMETERS OF NaCN

| Transition | Frequency[a] (MHz) | $E_l/k$ (K) | $S_{ij}$ | Source | $T_R^*$ (mK) | $\Delta v$[b] (km s$^{-1}$) | $T_B$[c] (mK) |
|---|---|---|---|---|---|---|---|
| $5_{05}$–$4_{04}$.......... | 77836.7 | 7.50 | 4.996 | IRC 10216 | (9.0, 13.6, 15.2)[d] | 47.7 | (85, 346, 1098) |
| | | | | TMC-1 | <10 | (0.5) | <38.4[e] |
| | | | | W51M | <10 | (14.5) | <1030[f] |
| $6_{06}$–$5_{05}$.......... | 93206.1 | 11.23 | 5.994 | IRC 10216 | 10.7 | 37.6 | (79, 212, 573) |
| | | | | W51M | 10? | 14.5 | 765?[f] |
| $7_{07}$–$6_{06}$.......... | 108472.0 | 15.70 | 6.990 | IRC 10216 | 12.5 | 30.4 | (74, 198, 506) |
| | | | | Sgr B2OH | <10 | (18.0) | <62[g] |
| $9_{09}$–$8_{08}$.......... | 138652.1 | 26.86 | 8.981 | IRC 10216 | 9.7 | 25.9 | (43.7, 117, 255) |
| | | | | TMC-1 | <35 | (0.5) | <62[h] |

[a] Centroid frequency (hfs not included), calculated from molecular constants of van Waals et al. (1984).

[b] Full width to zero intensity for IRC 10216; FWHP otherwise. Values in parentheses are assumed.

[c] Entries for IRC 10216 refer respectively to the assumed NaCN distributions: (1) of $HC_3N$ ($J = 2$–1); (2) of $HC_7N$; (3) of SiS. See text.

[d] Calculated by deconvolving the contribution from $C_4H$ ($v_7 = 1$) for $C_4H$ source diameters of 36″, 18″, and 6″, respectively (see text).

[e] No assumed beam dilution. The hyperfine dilution factor is 2.56.

[f] Source diameter $\theta_s = 10''$ assumed.

[g] $\theta_g = 35''$ assumed.

[h] No assumed beam dilution and no hyperfine dilution factor.

1994ApJ...426L..97T

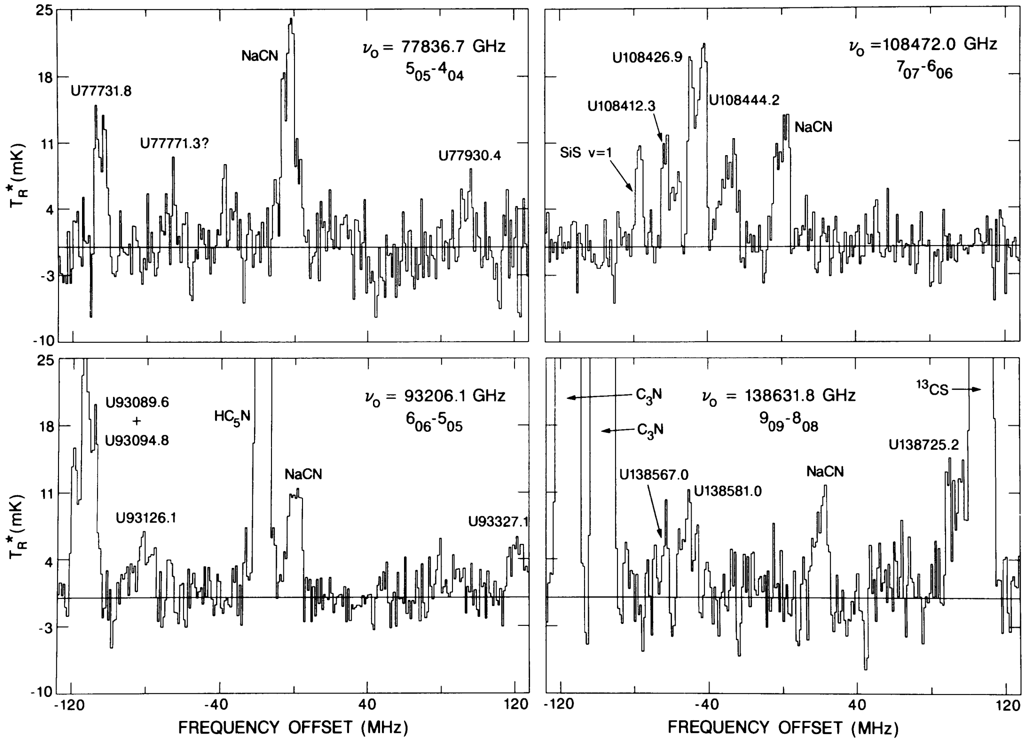

FIG. 1.—Four observed transitions of NaCN in IRC 10216. Band center frequency is indicated in each panel and coincides with the calculated frequency for all cases except the $9_{09}$–$8_{08}$ transition, whose frequency is 138652.1 GHz. The narrow $v = 1$ line of SiS at 108.395 GHz arises from within the inner acceleration zone.

## 4. DISCUSSION

### 4.1. *Interstellar Sources*

The observed position in TMC-1 is that of the cyanopolyyne peak, where HCN also peaks. An LTE calculation using $T_{\rm rot}$ = 8 K and our observed upper limit of $T_B < 38$ mK (no beam dilution and a hyperfine dilution factor of 2.5 when convolved with a 24 kHz spectral resolution) gives a limiting column density of $N$(NaCN) $\leq 1.3 \times 10^{11}$ cm$^{-2}$. If we adopt a total column density $N$(H$_2$) = $1 \times 10^{23}$ cm$^{-2}$, then the fractional abundance is $X$(NaCN) $\leq 1.3 \times 10^{-12}$.

Until recently, the only refractory elements observed in molecular form in (warm) interstellar objects were Si and P. In the cold TMC-1 object, sensitive limits have been established for SiO (Ziurys, Friberg, & Irvine 1989) and for PN (Turner et al. 1990) and PO (Turner 1993). Recently, Bell, Avery, & Watson (1993) have tentatively detected MgNC toward TMC-1, but there is presently some discrepancy between observed and measured frequencies (Suenram & Steimle 1993). There is consequently no knowledge at present of the depletion of the refractory elements in the cold, dense ISM. Such depletions are important in understanding the life cycle of grains and molecules in the ISM. While NaCN is an expected, if not major, carrier of Na in C-rich CSEs (§ 4.2), the carrier of Na in cold dense interstellar clouds is unknown because gas-phase Na may not be in the form Na$^+$ (which reacts with HCN) and because thermochemical equilibrium is obviously not relevant. We conclude only that gaseous NaCN accounts for less than $2 \times 10^{-7}$ of the total cosmic Na in TMC-1.

Negative results for star-forming molecular clouds such as Sgr B2OH and W51M (Table 1) are not surprising, since they are O-rich. Our upper limits for $X$(NaCN) are ~4 times larger than for TMC-1. NaO and NaH are also not seen in these regions (Turner 1991) but are thought likely for O-rich systems. The prevalence of Si species, and the fact that Si is more refractory than Na, implies that Na species should be detectable, though in as yet unknown compounds.

### 4.2. *IRC 10216*

To derive column densities and fractional abundances for NaCN, we consider three distributions for NaCN. (1) The distribution of HC$_3$N ($J$ = 2–1) is roughly a Gaussian whose intensity falls off inside a radius of 3″.5 and approaches zero at a radius of 36″ (Wootten et al. 1993). It illustrates a species formed in both the outer and intermediate envelope but not the inner envelope. Taking $\theta_s = \sim 36''$, we find $N$(NaCN) = $(2.0 \pm 0.3) \times 10^{13}$ cm$^{-2}$. Assuming a constant mass-loss rate of $4.8 \times 10^{-5}$ $M_\odot$ yr$^{-1}$, the density distribution is $n(r) = 2 \times 10^{37}/r^2$ ($r$ in centimeters). A distance of 200 pc is adopted. Integrating over the HC$_3$N region gives $N$(H$_2$) = 3.5 × $10^{21}$ cm$^{-2}$, or $X$(NaCN) = $5.8 \times 10^{-9}$. (2) The distribution of HC$_7$N is annular, with half-power intensities occurring at radii of 18″ ± 5″. It is typical of a species formed solely in the outer envelope. An approximate convolution of such an annulus with the 12 m telescope beams yields $N$(NaCN) = $(3.8 \pm 0.3) \times 10^{13}$ cm$^{-2}$. Integrating over this region gives $N$(H$_2$) = $4.5 \times 10^{20}$ cm$^{-2}$, or $X$(NaCN) = $1.2 \times 10^{-7}$. (3) SiS is roughly Gaussian distributed with intensity approaching zero at a radius of 6″ (Bieging & Rieu 1988). It is formed solely in the inner envelope and photodissociated beyond 6″. We find $N$(NaCN) = $(1.5 \pm 0.1) \times 10^{14}$ cm$^{-2}$. Integration of $n(r)$ gives $N$(H$_2$) = $3.1 \times 10^{23}$ cm$^{-2}$, or $X$(NaCN) = $4.8 \times 10^{-10}$. If the distance to IRC 10216 is less than 200 pc, values of $X$(NaCN) will be larger.

The cosmic fractional abundance of Na is $1.7 \times 10^{-6}$.

Therefore, a fraction $3 \times 10^{-4}$ to $7 \times 10^{-2}$ of Na is in the form of NaCN, with the higher value applying if NaCN is confined to the outer envelope as we believe. Since NaCN will be quickly photodissociated in the diffuse ISM, the rate of ejection of gas-phase Na to the diffuse ISM is $5 \times 10^{-12}\ M_{\odot}\ \mathrm{yr}^{-1}$. The fraction NaCN/Na is at least an order of magnitude larger than the fraction of all Si in the half-dozen Si species predicted by Herbst et al. (1989) to harbor all of the gas-phase Si. Even if there are no other Na molecules comparable in abundance to NaCN, we conclude that no more than 93% of all Na is incorporated in grains, as compared to over 99% of all Si. Na appears considerably less refractive than Si, as expected (Turner 1991). The interstellar gas/dust ratio may not be well explained for the more volatile refractory elements on the usual hypothesis that they are fully incorporated into grains.

There is presently some disagreement as to whether outer envelope molecules in IRC 10216 are excited predominantly by IR radiation (Bieging & Tafalla 1993) or predominantly by collisions (Wootten et al. 1993). NaCN is similar to several other molecular species in having a single value of $T_{\mathrm{rot}}$ independent of $J$. Different species appear to have somewhat differing $T_{\mathrm{rot}}$ [e.g., $T_{\mathrm{rot}}(\mathrm{HC_3N}) \simeq 15$ K]. These characteristics might suggest that IR excitation is dominant, especially since collisional rates are much less than the Einstein $A$ rates for each transition of NaCN. IR rates (and hence $T_{\mathrm{rot}}$) would differ from species to species, since the IR flux is strongly wavelength dependent. The IR spectrum of NaCN is unknown. Conversely, collisional excitation might produce a $J$-dependence for $T_{\mathrm{rot}}$, since the collision rates are less than the Einstein $A$ values, which vary by a factor of 5.8 over the four observed transitions of NaCN. These arguments are not definitive, especially since they imply that the equality between $T_{\mathrm{rot}}$ for NaCN and the gas kinetic temperature as deduced by Truong-Bach, Morris, & Rieu (1991) is a coincidence.

To assess the chemistry of NaCN in IRC 10216, we note that different types of reactions dominate inner, intermediate, and outer envelopes. Tsuji (1992) has predicted that NaCN is the dominant carrier of Na under the thermochemical equilibrium conditions of the inner envelope. Assuming a constant mass-loss rate, the fractional abundance of NaCN in the inner envelope (equal to that of gaseous Na itself) should be preserved by the outflow. Our value of $X$(NaCN) for the outer envelope is much smaller than the cosmic value, indicating that NaCN is significantly lost to grains in either the thermochemical equilibrium zone or during the outflow. In any case, line profiles should show evidence of the unresolved optically thick NaCN transitions from the innermost region, which would dominate the total column density. The 93.2 GHz is clearly inconsistent, although the other lines are less certain. In the intermediate envelope, neutral-neutral reactions are possible, e.g., reaction of Na with HCN, $\mathrm{CH_3CN}$, $\mathrm{(CN)_2}$. Such reactions are endothermic. On the other hand, the reaction Na + CN may be exothermic, but is likely to be very slow. Therefore, NaCN is best explained by ion-molecule reactions in the outer envelope, where Na is efficiently ionized by interstellar UV radiation (ionization potential 5.1 eV). There are few studies of $\mathrm{Na^+}$ reactions. Leung, Herbst, & Huebner (1984) predict that $\mathrm{Na^+ + H_2 \rightarrow NaH_2^+} + h\nu$ is slow. Applying the arguments of Kawaguchi et al. (1993) for the MgNC chemistry to the present case, we suggest that $\mathrm{Na^+ + HCN \rightarrow NaCN^+ + H}$ is endothermic. The most likely reaction is $\mathrm{Na^+ + HCN \rightarrow NaCNH^+} + h\nu$, followed by electron dissociative recombination to produce NaCN. The principle destruction mechanism would be reaction of NaCN with $\mathrm{He^+}$ or $\mathrm{C^+}$, whose rates are $\sim 1.0 \times 10^{-8}\ \mathrm{cm^{-3}\ s^{-1}}$ (Leung et al. 1984), much larger than the formation rate. This scheme is therefore consistent with the low values of $X$(NaCN) observed. The derived value of $N$(NaCN) is about a factor of 2 larger than that derived by Kawaguchi et al. (1993) for MgNC if we assume the same angular size ($\sim 24''$) for each species. This difference could disappear if MgCN (not yet searched) has an abundance similar to MgNC, a reasonable possibility since the two forms differ in energy by only $\sim 0.2$ eV. By comparison, the cosmic abundance of Mg is $\sim 17$ times larger than Na. The suggested ion-molecule rates could be much faster for Na than for Mg, or Na could be much less depleted than Mg onto grains during the outflow. The latter possibility is consistent with Na being less refractory than Mg.

We are indebted to Shuro Takano for pointing out the blend of NaCN $5_{05}$–$4_{04}$ with $\mathrm{C_4H}$, $v_7 = 1$, $J = 17/2$–$15/2(e)$ and also for the identifications of U77731.8 with CCS ($6_6$–$5_5$), U93089.6, and U93094.8 with $\mathrm{C_5H}$ ($^2\pi_{1/2}$, $J = 39/2$–$37/2$), and U138725.2 with $\mathrm{C_3S}$ ($J = 24$–$23$).

## REFERENCES

Bell, M. 1993, ApJ, 417, 305
Bell, M., Avery, L. & W., Watson, J. G. K. 1993, in preparation
Bieging, J. H., & Rieu, N.-Q. 1988, ApJ, 329, L107
Bieging, J. H., & Tafalla, M. 1993, AJ, 105, 576
Cernicharo, J., & Guelin, M. 1987, A&A, 183, L10
Herbst, E., Millar, T. J., Wlodek, S., & Bohme, D. K. 1989, A&A, 222, 205
Kawaguchi, K., Kagi, E., Hirano, I., Takano, S., & Saito, S. 1993, ApJ, 406, L39
Klein, M. L., Goddard, J. D., & Bounds, D. J. 1981, J. Chem. Phys., 75, 3909
Leung, C. M., Herbst, E., & Huebner, W. 1984, ApJS, 56, 231
Morris, M. 1975, ApJ, 197, 603
Suenram, R. & Steimle, T. C. 1993, private communication
Thaddeus, P., Cummins, S. E., & Linke, R. A. 1984, ApJ, 283, L45
Truong-Bach, Morris, M., & Rieu, N.-Q. 1991, A&A, 249, 435
Tsuji, T. 1973, A&A, 23, 411
———. 1992, private communication
Turner, B. E. 1991, ApJ, 376, 573
———. 1992a, ApJ, 388, L35
———. 1992b, in Astrochemistry of Cosmic Phenomena, ed. P. D. Singh (Dordrecht: Kluwer), p. 181
———. 1993, in preparation
Turner, B. E., Tsuji, T., Bally, J., Guelin, M., & Cernichar, J. 1990, ApJ, 365, 569
van Waals, J. J., Meerts, W. L., & Dymanus, A. 1984, Chem. Phys., 86, 147
Wootten, H. A., Truong-Bach, & Rieu, N.-Q. 1993, in preparation
Yamamoto, S., Saito, S., Guelin, M., Cernicharo, J., Suzuki, H., & Ohishi, M. 1987, ApJ, 323, L149
Ziurys, L. M., Friberg, P., & Irvine, W. M. 1989, ApJ, 343, 201

*Note added in proof.*—We have detected a fifth transition of NaCN in IRC 10216, the $6_{16}$–$5_{15}$ line at 90.39439 GHz. The line has $T_R^* = 11.4 \pm 2$ mK and $\Delta v = 37.5\ \mathrm{km\ s^{-1}}$ full width to zero intensity. These parameters agree perfectly with the other lines detected. The line is flat-topped or perhaps slightly cusped like the other lines.