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Letter to the Editor

Detection of the SiNC radical in IRC+10216

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Abstract. Following discovery of the free radical SiCN in the C-star envelope IRC+10216, we report the detection in the same source of its isomer SiNC. The microwave spectra of SiNC and SiCN were studied in the laboratory and their rotational transition frequencies are accurately known. The ground fine structure state of SiNC, $^2\Pi_{1/2}$, gives rise to a series of rotational transitions, spaced by 12.8 GHz, each with Λ-doubling. Five weak lines are detected with the IRAM 30-m telescope at the frequencies of the $J = 6.5 \rightarrow 5.5$ (e), $7.5 \rightarrow 6.5$ (f), $8.5 \rightarrow 7.5$ (f) and $10.5 \rightarrow 9.5$ (e) and (f) rotational transitions. Other SiNC lines from these or adjacent rotational transitions are found to be blended with stronger lines from known molecules.
The lines assigned to SiNC have a cusped shape, characteristic of species confined to a hollow shell in the outer circumstellar envelope. They are twice weaker than their SiCN counterparts, which have the same shape, and presumably arise in the same region of the envelope. SiNC and SiCN have about the same abundance in IRC+10216, $\sim 4 \times 10^{-9}$ with respect to H_2. This contrasts with HCN, HC_3N and HC_5N, for which the cyanide to isocyanide abundance ratio is >100.

Key words. stars: circumstellar matter – stars: AGB and post-AGB – stars: individual: IRC+10216 – ISM: molecules – radio lines: stars

1. Introduction

Millimeter-wave spectral line surveys of the molecular envelope of IRC+10216 have yielded more than 60 molecules, many containing refractory elements (Cernicharo et al. 2000, hereafter CGK). These include the metallic compounds AlCl, AlF, KCl, NaCl, MgCN and MgNC, the silicon compounds SiO, SiS, SiC, SiC_2, SiC_3, SiC_4, and the recently detected radicals SiCN (Guélin et al. 2000, hereafter GMC) and AlNC (Ziurys et al. 2002).

Although many refractory molecules are observed close to the central star of IRC+10216, others, such as SiC, SiC_2 and MgNC, are only detected in the outer envelope and are thought to form in situ (Guélin et al. 1993, hereafter GLC). The formation of refractory molecules in a cold, tenuous medium is poorly understood: it may be the result of gas-phase reactions between molecules and radicals or ions, or of reactions on dust grains (see GLC and the review of Glassgold 1996). To clarify this question, the study of additional refractory molecules is highly desirable.

The detection of refractory species in space is hampered by their low abundances and the lack of accurate spectroscopic data. Four years ago, Apponi et al. (2000) observed in a laboratory discharge three Si-bearing isoelectronic radicals, SiCCH, SiCN and SiNC, and measured their microwave spectra. These measurements led almost at once to the detection of SiCN in IRC+10216 (GMC). In this Letter, we report the detection in this source of its isomeric rearrangement SiNC.

2. Observations

Like SiCN and SiCCH, SiNC is linear and has a regular $^2\Pi$ electronic ground state. Its rotational spectrum consists of nearly harmonic Λ doublets each split by 11–13 MHz, separated by twice the rotational constant: 12.8 GHz. Each rotational transition is further split by magnetic hyperfine structure, but for the large J transitions studied here that is unresolved, and the spectrum reduces to the Λ doublets, the two components of which are denoted e and f. By analogy with SiCN, which has a similar moment of inertia and dipole moment[1], the rotational lines of SiNC in IRC+10216 are expected to peak in intensity at wavelengths between 3 mm and 2 mm.

The present observations of SiNC were made with the IRAM 30-m telescope. Two dual-polarization SIS-mixer receivers were used to observe the 3-mm and 2-mm rotational transitions; the receivers were tuned to a single sideband, with rejections of the image (upper) sideband >25 dB at 3-mm and >13 dB at 2-mm. (The rejection level was measured against a

[1] The permanent dipole moments SiCCH, SiCN, and SiNC are μ_0 = 1.4 D, 2.9 D and 2.0 D, respectively, according to ab initio calculations – see references in Apponi et al. (2000).

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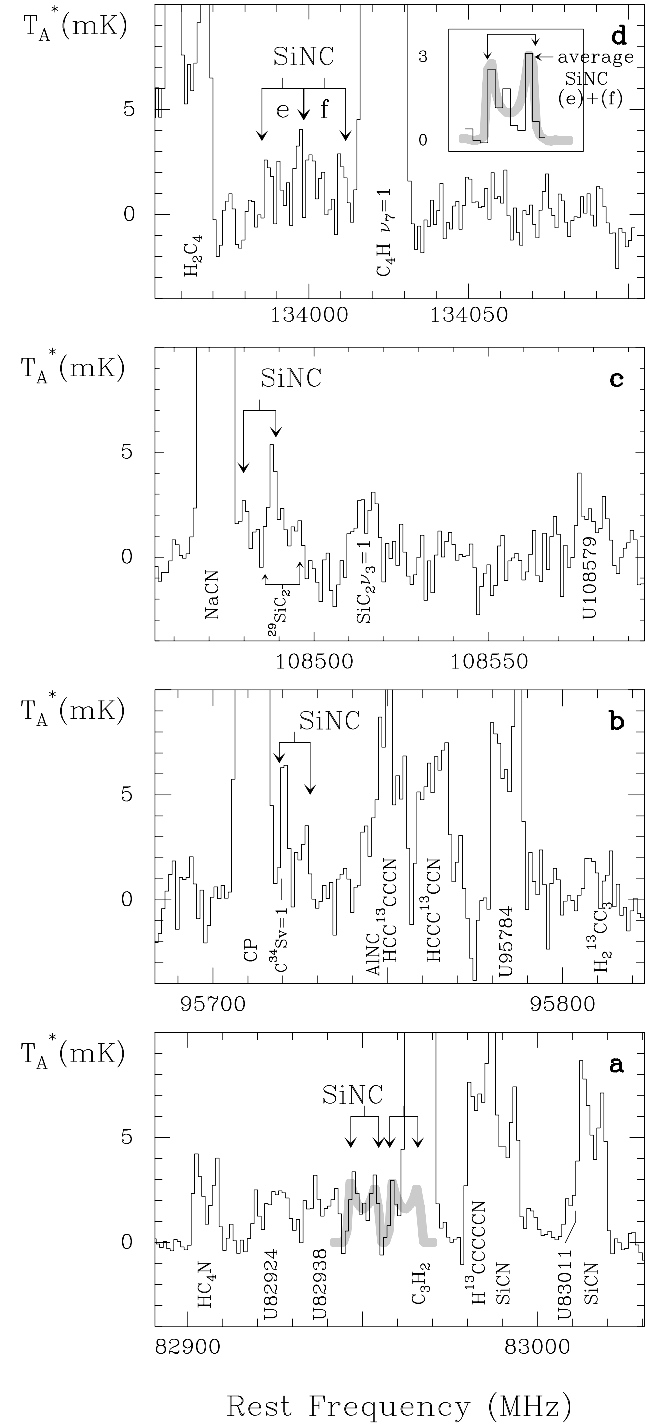

Fig. 1. Spectra of four rotational transitions of SiNC observed with the 30-m telescope. Most lines in IRC+10216 are cusped in shape and have widths of 29 km s^{-1}, like the $2\nu_7, 14 \rightarrow 13$ line of C_4H, whose profile, scaled down by a factor of 60, is shown as a thick grey line in the insert in Fig. 1d. The rest frequencies of the SiNC Λ-doublet components are indicated by short vertical lines and the edges of the 29 km s^{-1}-wide cusped lines by vertical arrows. Six SiNC line components, corresponding to the $J = 6.5 \rightarrow 5.5$ (e and f), $7.5 \rightarrow 6.5$ (f), $8.5 \rightarrow 7.5$ (f), and $10.5 \rightarrow 9.5$ (e and f) rotational transitions of SiNC are detected. The thick grey lines in Fig. 1a show a fit to the SiCN $6.5 \rightarrow 5.5$ lines. The thin line profile in the insert in Fig. 1d represents the average of the SiNC $10.5 \rightarrow 9.5$ (e) and (f) lines: this average profile is well fitted by the C_4H line profile scaled down by a factor of 60.

frequency-modulated load and checked by recording the intensity of strong astronomical lines from the image sideband.) The system noise temperature was 100–200 K.

Data were taken in the balanced wobbler-switching mode, with a wobbling frequency of 0.5 Hz and a throw of 1.5–2′. Zero to third-order baselines were removed across the 0.5 GHz-wide band of the spectrometer. The channel resolution was 1 MHz. The telescope pointing and focus were checked by monitoring the intensity and shape of the strongest lines lying in the IF band and, every 1–2 h, by observing a nearby planet or the continuum source OJ287.

3. Results

Four rotational transitions of SiNC in IRC+10216, $J = 6.5 \rightarrow 5.5, 7.5 \rightarrow 6.5, 8.5 \rightarrow 7.5$, and $10.5 \rightarrow 9.5$, are shown in Fig. 1. The millimeter lines in this source generally have sharp edges and a constant width of 29 km s^{-1}, making them fairly easy to identify (see e.g. Fig. 2 of GMC and CGK). The typical cusped profile of a line arising in the outer envelope of IRC+10216 is shown in the insert in Fig. 1d, where the thick grey line represents the $2\nu_7, l = 0, N = 14 \rightarrow 13$ line of C_4H (133 862 MHz) at a scale 1/60.

In Fig. 1, we have marked by a short vertical line the laboratory-derived rest frequencies of the SiNC transition components, and by two vertical arrows the positions predicted for the edges of the SiNC lines (these arrows are at ± 14.5 km s^{-1} from the center of the line). Both components of the $10.5 \rightarrow 9.5$ doublet, although weak, are detected. This can be better seen on the insert in Fig. 1d where we have shown the average profile of both doublet components (scale 1/1) superimposed on the C_4H line, scaled down by a factor of 60. Similarly, the high-frequency components (f) of the $J = 7.5 \rightarrow 6.5$ and $8.5 \rightarrow 7.5$ rotational doublets are clearly detected (Figs. 1c and 1b). The low-frequency components (e) of the latter doublets are unfortunately blended with much stronger lines of CP and NaCN and are not visible. Finally, the (e) component of the $J = 6.5 \rightarrow 5.5$ doublet is also detected (Fig. 1a), as is the low-frequency wing of the (f) component (see the thick grey line near 82 960 MHz) – the rest of which is blended with a strong line of C_3H_2.

Although the density of lines in IRC +10216 at the 2 mK level is fairly large, there is little doubt that the six lines in Fig. 1 are produced by SiNC. Rest frequencies of the components agree with the laboratory frequencies to within 1 MHz, or about 10% of a linewidth, and relative intensities agree well with those expected (see Table 1). We have searched for alternate assignments (in both the observed and the image receiver sidebands) in the standard catalogs of molecular transitions of astrophysical interest, as well as in a line catalog specifically assembled for IRC+10216 (see CGK). The transitions of known molecules that are likely to be present in Fig. 1, even at very weak levels, are indicated on the figure: none of them coincides to better than 4 MHz with our six SiNC lines. The density of lines that remain unidentified in IRC+10216 at the present sensitivity is typically two per 100 MHz (see GMC and Cernicharo et al. 2004), making it highly unlikely that the six SiNC lines in Fig. 1 are the result of chance coincidence.

Among the identified lines of other molecules in Fig. 1, we note the $J = 36 \rightarrow 35$ lines of three ^{13}C isotopomers of HC_5N and the $J = 7.5 \rightarrow 6.5$ Λ-doublet of SiCN. The latter doublet has already been reported by GMC, but at a lower signal-to-noise. The line at 82 905 MHz is identified by Cernicharo et al. (2004) as the high-frequency component of the $N, J = 18, 19 \rightarrow 17, 18$ rotational transition of the linear isomer of the HC_4N radical.

4. Discussion

In spite of the low signal-to-noise, the SiNC lines of Fig. 1 appear to have the same cusped shape as the lines of SiCN and of many carbon chain molecules and radicals (Fig. 2 of GMC). Guélin et al. (1993, 2000) have shown by interferometric observations that the cusped lines in IRC+10216 are caused by the concentration of molecules in a thin shell of radius ≃15″. One of the best examples is the abundant SiCC molecule (Lucas et al. 1994).

Molecules in this thin shell have mm-line intensities which agree with those expected for a Boltzmann distribution of the rotational populations (see e.g. Kawaguchi et al. 1995 and CGK) – probably an indication of collisional excitation and a fairly uniform shell. Rotational temperatures of molecules with moments of inertia and dipole moments similar to those of SiNC are all in the range 15–30 K. For SiCN, the $J = 6.5 \rightarrow 5.5$ through $9.5 \rightarrow 8.5$ lines yield $T_{\rm rot} = 22$ K – possibly an underestimate since the lines are weak and since the highest energy lines that are observed originate from a level with $E_{\rm u}/k = 27$ K.

For SiNC here, we derive $T_{\rm rot} = 18$ K, even more uncertain because of the weakness of the lines (owing largely to the 40% smaller dipole moment of SiNC relative to that of SiCN).

Assuming that the rotational temperature of SiNC is 18 K, we derive a column density (twice the radial column density accross the shell) of $\simeq 2 \times 10^{12}$ cm^{-2}, about equal to that of SiCN (GMC). For both SiCN and SiNC, the population in the $^2\Pi_{3/2}$ ladder, which lies well above the $^2\Pi_{1/2}$ ground ladder, has been assumed to be negligible. The column densities of SiNC and SiCN are similar to that of MgCN (Ziurys et al. 1995) and are ≃20 times smaller than those of SiC (Cernicharo et al. 1989) and MgNC. On the assumption of a thin shell, the abundances of SiNC, SiCN and MgCN, relative to H_2, are $\sim 4 \times 10^{-9}$.

Despite a dedicated search for its $J = 9.5 \rightarrow 8.5$ rotational transition, we have failed to detect SiCCH. The 3σ upper limit for the integrated intensity of this line, 38 mK km s^{-1}, yields an upper limit to the SiCCH column density which is close to the value of the detected lines of SiCN and SiNC (on the assumption that $T_{\rm rot} = 20$ K). This failure is hardly surprising: although MgNC and AlNC are readily detected in IRC+10216, MgCCH and AlCCH have not been found.

It has been argued by GMC that SiCN may be formed in IRC+10216 by the radiative association of Si^+ with HCN, leading to $SiNCH^+$ and $SiCNH^+$, followed by dissociative recombination – a path similar to that proposed by Glassgold et al. (1986) for the formation of SiC_2. The radiative association of Si^+ with HCN had been previously considered by Herbst et al. (1989) in their study of silicon chemistry in interstellar clouds. These authors derived a rather large reaction rate from laboratory measurements in high pressure ternary conditions ($6 \times 10^{-15}\,(T/300)^{-1.5}$ cm^3 mol^{-1} s^{-1}). The dissociative recombination of $SiNCH^+$ would yield SiNC. SiCN could also be formed from parallel reactions of Si^+ with HNC, but this isomer is 1000 times less abundant than HCN in the outer envelope and is thus unlikely to play a significant role.

Table 1. Observed line parameters.

Obs. freq. MHz	Obs.-cal. MHz	Species	Transition $J \rightarrow J'$	$\int T_A^* dv$ mK km s^{-1}
SiNC:				
82 951 (1)	.4	SiNC	6.5–5.5 (e)	69 (10)
82 962 (1.5)^b	.2	SiNC	6.5–5.5 (f)	60 (20)
95 723 (1)^b	.4	SiNC	7.5–6.5 (f)	81 (20)
108 484 (1)^b	–0.5	SiNC	8.5–7.5 (f)	47 (15)
133 991 (1)	–0.8	SiNC	10.5–9.5 (e)	49 (10)
134 006 (2)	1	SiNC	10.5–9.5 (f)	42 (10)
SiCN:				
82 990.8^b (4)	.33	SiCN	7.5–6.5 (e)	160 (8)
83 015.7 (1)	.1	SiCN	7.5–6.5 (f)	155 (12)
94 056.6 (1)	.2	SiCN	8.5–7.5 (e)	159 (23)
94 081.7 (3)	.3	SiCN	8.5–7.5 (f)	127 (23)
105 121.7^b (3)	–.3	SiCN	9.5–8.5 (e)	128 (30)
105 146.8 (2)	.1	SiCN	9.5–8.5 (f)	140 (15)
Other:				
(MHz)	(MHz)			mK km s^{-1}
82 924	–	U	–	60
82 938	–	U	–	55
83 011	–	U	–	50
95 784	–	U	–	230
108 579	–	U	–	57
Upper limits:				
–	103 067.4	SiCCH	9.5–8.5 (e)	<38
–	103 098.4	SiCCH	9.5–8.5 (f)	<38

Notes: the number in parenthesis are 1σ uncertainties on the last digit, derived from least square fits; they do not include the 5% calibration uncertainty. The upper limits quoted for the SiCCH line intensities correspond to 3σ. ^{b} Denotes a partly blended line.

SiC_2 and SiCN could also be formed through neutral gas phase reactions involving free radicals. Recently Canossa et al. (2001) have measured in the gas phase, the reaction:

$$\mathrm{Si + HCCH \rightarrow SiCC + H_2}\quad \text{(most probable product)},$$

and find it proceeds efficiently at low temperatures (rate 3.5×10^{-10} cm^3 mol^{-1} s^{-1} at 15 K). They suggest that this is the main route for forming SiC_2 in IRC+10216.

Neutral Si atoms may react also with HCN which is highly polar:

$$\begin{aligned}\mathrm{Si + HCN} &\rightarrow \mathrm{SiCN + H}\\ &\rightarrow \mathrm{SiNC + H.}\end{aligned}$$

This reaction has not yet been studied and its energetics and its rate at low temperatures are not known. The branching ratio between SiCN and SiNC is also not known. It could, however, approach unity because of the large size of the Si atom. We note in this respect that MgNC is more stable and more abundant than its isomer MgCN.

Alternately, these silicon molecules could be synthesized on the surface of Si-rich grains. It is known that SiC, SiC_2 and Si_2C are abundant in certain stellar atmospheres, and that they condense quickly onto grains when they are expelled into space. The reaction of Si atoms with HCN on silicon substrates has been studied in the laboratory, and is found to proceed efficiently at 12 K, yielding both SiNC and SiCN (but with an unknown branching ratio: Maier et al. 1998). These molecules, once formed, may be released into the gas when the grains are exposed to interstellar UV radiation. According to GLC, the similarity of the spatial distributions of species as different as C_4H, SiC_2, MgNC, and, probably SiCN and SiNC, is better explained by grain chemistry than by gas phase reactions.

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