

Understanding the chemical complexity in Circumstellar Envelopes of C-Rich AGB stars: The case of IRC +10216

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Abstract The circumstellar envelopes of carbon-rich AGB stars show a chemical complexity that is exemplified by the prototypical object IRC +10216, in which about 60 different molecules have been detected to date. Most of these species are carbon chains of the type C_nH , C_nH_2 , C_nN , HC_nN . We present the detection of new species (CH_2CHCN , CH_2CN , H_2CS , CH_3CCH and C_3O) achieved thanks to the systematic observation of the full 3 mm window with the IRAM 30m telescope plus some ARO 12m observations. All these species, known to exist in the interstellar medium, are detected for the first time in a circumstellar envelope around an AGB star. These five molecules are most likely formed in the outer expanding envelope rather than in the stellar photosphere. A pure gas phase chemical model of the circumstellar envelope is reasonably successful in explaining the derived abundances, and additionally allows to elucidate the chemical formation routes and to predict the spatial distribution of the detected species.

Keywords astrochemistry · circumstellar matter · molecular processes · AGB stars · IRC +10216

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1 Introduction

IRC +10216 was discovered in the late sixties as an extremely bright object in the mid infrared (Becklin et al. 1969). Since then and with the development of radioastronomy during the seventies it was recognized as one of the richest molecular sources in the sky together with some others such as the Orion nebula, Sagittarius-B2 and the Taurus molecular cloud complex.

IRC +10216 consists of a central carbon-rich AGB star, i.e. $C/O > 1$ in the photosphere, losing mass at a rate of $2\text{--}4 \times 10^{-5} M_{\odot} \text{ yr}^{-1}$ in the form of a quasi-spherical wind that produces an extended circumstellar envelope (CSE) from which most of the molecular emission arises. To date, some 60 different molecules have been detected in this source, most of which are organic molecules consisting of a linear and highly unsaturated backbone of carbon atoms. Among these species there are cyanopolyynes ($HC_{2n+1}N$) and their radicals ($C_{2n+1}N$), polyynes radicals (C_nH), carbenes (H_2C_n), radicals ($HC_{2n}N$) as well as S-bearing (C_nS) and Si-bearing (SiC_n) species (Glassgold 1996; Cernicharo et al. 2000).

It is nowadays accepted that the formation of these molecules occurs either under chemical equilibrium in the dense ($n > 10^{10} \text{ cm}^{-3}$) and hot ($T_k \sim 2000 \text{ K}$) vicinity of the stellar photosphere or in the colder and less dense outer envelope when the interstellar UV field photodissociate/ionize the molecules flowing out from the star producing radicals/ions which undergo rapid neutral-neutral and ion-molecule reactions (Lafont et al. 1982; Millar et al. 2000). This picture of circumstellar photochemistry resembles that occurring in cold dense clouds ($T_k = 10 \text{ K}$, $n \sim 10^4 \text{ cm}^{-3}$) such as TMC-1 (Kaifu et al. 2004). In both places organic molecules are mostly unsaturated, which is typical of low temper-

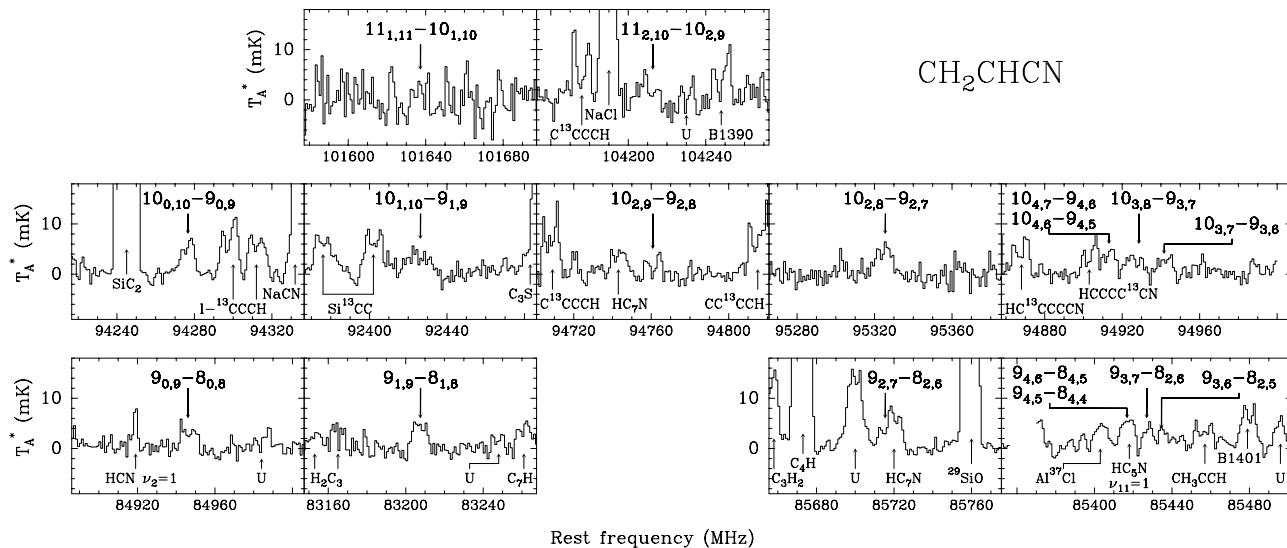


Fig. 1 Rotational lines of CH_2CHCN detected toward IRC +10216 with the IRAM 30m telescope.

ature non-equilibrium chemistry and simply reflects the trend of gas phase bimolecular reactions in ejecting an hydrogen atom and the low reactivity of H_2 with most hydrocarbons.

In this contribution we report on the detection toward IRC +10216 of the partially saturated C-bearing species CH_2CHCN , CH_2CN and CH_3CCH ; the S-bearing molecule H_2CS and the oxygen-carbon chain C_3O . All these species are known to exist in cold dense clouds (Matthews & Sears 1983; Irvine et al. 1988; Irvine et al. 1981; Irvine et al. 1989; Brown et al. 1985). Thus, their detection in IRC +10216 stress the similarity between the chemistry taking place in cold dense clouds and in the CSEs of C-rich AGB stars.

2 Observations

The observations of CH_2CHCN , CH_2CN , H_2CS and CH_3CCH were achieved with the IRAM 30m telescope (see e.g. Fig. 1) while C_3O was observed with both the IRAM 30m and ARO 12m telescopes.

The IRAM 30m observations were carried out during several sessions from 1990 to 2005, most of them after 2002 in the context of a λ 3 mm line survey of IRC+10216 from 80 to 115.75 GHz (Cernicharo et al., in preparation). Two 3 mm SIS receivers with orthogonal polarizations were used in single-sideband mode with image sideband rejections >20 dB. The standard wobbler switching mode was used with an offset of $4'$. The back end was a 512 two-pole filter with half-power widths and spacings equal to 1.0 MHz.

The ARO 12m observations were done in several runs between 2003 and 2005. The receivers were dual-channel cooled SIS mixers at 2 and 3 mm, operated in

single-sideband mode with ~ 18 dB rejection of the image sideband. The back ends were two 256 channel filter banks with 1 and 2 MHz resolutions, configured in parallel mode (2×128 channels) for the two receiver channels. A millimeter auto correlator spectrometer with 2048 channels of 768 kHz resolution was operated simultaneously to confirm features seen in the filter banks. Data were taken in beam switching mode with $\pm 2'$ sub-reflector throw.

3 Molecular column densities

The number of CH_2CHCN , CH_2CN and C_3O lines detected was large enough to allow us to construct rotational temperature diagrams (see e.g. Fig. 2). The rotational temperatures derived (see table 1) are within the range of other shell distributed molecules in IRC +10216: 20-50 K (Cernicharo et al. 2000). For CH_3CCH and H_2CS we observed only a few transitions with similar upper level energies and it was not possible to constrain the rotational temperature which was assumed to be 30 K.

In Table 1 we give the column densities¹ (averaged over the IRAM 30m beam, $\theta_{MB}=21-31''$ at λ 3 mm) of the species detected for the first time (in bold) as well as values or upper limits derived for other related species. The column densities of the new species are in the range 10^{12} - 10^{13} cm^{-2} . Note for example that both CH_3CN and CH_3CCH have very similar column densities although the lines of CH_3CCH are some 30 times weaker

¹ For CH_2CN and H_2CS , the two molecules which have two interchangeable nuclei with non zero spin, we have assumed an ortho-to-para ratio 3:1 when deriving their column densities.

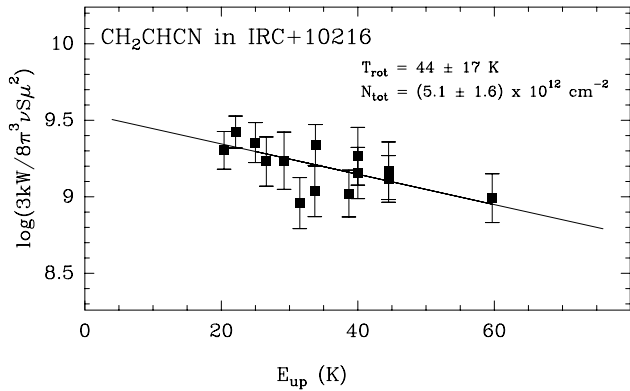


Fig. 2 Rotational temperature diagram of CH₂CHCN.

than those of CH₃CN mostly because the different electric dipole moments (0.780 D vs. 3.925 D). The two related species CH₃CN and CH₂CN have similar column densities which may indicate a common chemical origin (see Sec 4). The carbon-rich nature of IRC +10216 makes oxygen-bearing species to have a low abundance. For example thioformaldehyde is more abundant than formaldehyde despite the cosmic abundance of oxygen being 50 times larger than that of sulphur.

4 Molecular synthesis in the outer envelope

In order to explain how the detected species are formed we have performed a detailed chemical model of the outer envelope. The chemical network consists of 385 gas phase species linked by 6547 reactions, whose rate constants have been taken from the astrochemical databases UMIST99 (Le Teuff et al. 2000) and osu.2003 (Smith et al. 2004), recently revised². The temperature and density radial profiles as well as other physical parameters are taken from Agúndez & Cernicharo (2006). The resulting abundance radial profiles for CH₂CHCN, CH₂CN, CH₃CCH, H₂CS and related species are plotted in Fig. 3. The model predicts that these four molecules together with C₃O (not plotted in Fig. 3, see Tenenbaum et al. (2006) for a detailed discussion) are formed with an extended shell-type distribution ($r \sim 20''$) via several gas phase reactions.

Vinyl cyanide (CH₂CHCN) is formed by the reaction between CN and ethylene (C₂H₄), which is most likely the main formation route in dark clouds (Herbst & Leung 1990). Fortunately, the reaction has been studied in the laboratory and has been found to be very rapid at low temperature (Sims et al. 1993) and to produce vinyl cyanide (Choi et al. 2004). The predicted

Table 1 Column densities of some molecules in IRC +10216

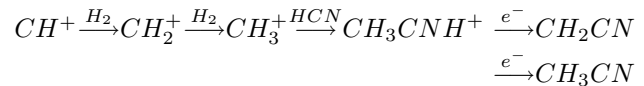
Molecule	T _{rot} (K)	N _{tot} (cm ⁻²)		
		observed	calculated	
			This Work	MI00
CH₂CHCN	44	5.1(12)	1.4(13)	2.2(11)
CH ₃ CN	40	3.0(13)	6.3(12)	6.8(12)
CH₂CN	49	8.4(12)	4.6(12)	1.4(13)
CH ₃ C ₃ N	30 ^a	<1.3(12)	1.2(11)	1.4(12)
CH₃CCH	30 ^a	1.6(13)	1.1(12)	8.0(12)
CH ₃ C ₄ H	30 ^a	<9.7(12)	8.2(12)	9.0(12)
H ₂ CO	28	5.4(12) [6]	2.8(12)	–
H₂CS	30 ^a	1.0(13)	1.3(12)	4.4(11)
C ₂ O	30 ^a	<7.0(12) [19]	7.0(11)	–
C₃O	27	2.6(12) [19]	2.8(12)	–
C ₄ O	30 ^a	<6.0(12) [19]	–	–
C ₅ O	30 ^a	<3.0(12) [19]	–	–

Notes: a(b) refers to $a \times 10^b$. The total column density across the source N_{tot} is twice the radial column density N_{rad}. A superscript "a" indicates an assumed value.

References: (MI00) Chemical model of Millar et al. (2000).

column density agrees reasonably well with the observational value.

In our model both CH₂CN and CH₃CN are mostly formed (>90 %) through the dissociative recombination (DR) of CH₃CNH⁺



whereas the major destruction process (>90 %) for both species is photodissociation. The branching ratios in the DR of CH₃CNH⁺ are not known and are assumed to be equal. Assuming, as we do, that the photodissociation rate of CH₃CN and CH₂CN are equal, the observed CH₃CN/CH₂CN ratio suggests branching ratios in the DR of CH₃CNH⁺ of 0.8 for the (CH₃CN + H) channel and 0.2 for (CH₂CN + H₂ or 2H). This estimate will be strongly affected if the photodissociation rates of CH₃CN and CH₂CN are very different but not if, as has been suggested by Herbst & Leung (1990) and Turner et al. (1990), CH₂CN does indeed react with atomic oxygen, the abundance of which is too low at the radius where CH₂CN is present.

The synthesis of CH₃CCH involves ion-molecule reactions with the dissociative recombination of the C₃H₅⁺ and C₄H₅⁺ ions as the last step. The model underproduces it by an order of magnitude, probably due to uncertainties and/or incompleteness in the chemical network, which affect the formation rate of the last step species C₃H₅⁺ and C₄H₅⁺. The heavier chain CH₃C₄H is also predicted with a column density even higher than

² See <http://www.udfa.net> and <http://www.physics.ohio-state.edu/~eric/research.html>

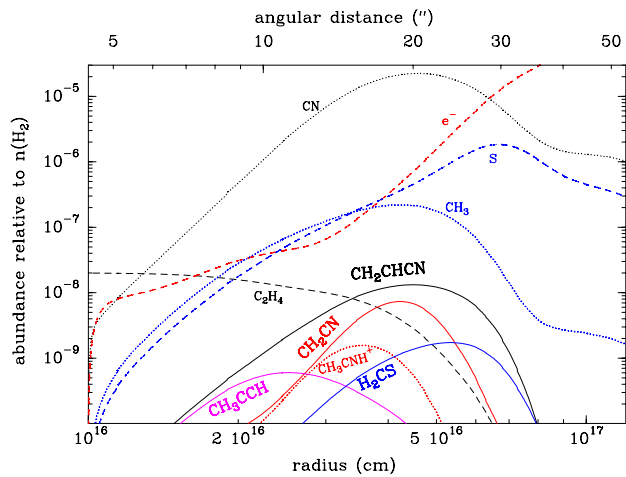


Fig. 3 Abundances of CH_2CHCN , CH_2CN , CH_3CCH and H_2CS (solid lines) and related species (dotted and dashed lines) given by the chemical model, as a function of radius (bottom axis) and angular distance (top axis) for an assumed stellar distance of 150 pc.

that of CH_3CCH . The larger rotational partition function works against lines being detectable, but the higher dipole moment (1.21 D vs. 0.78 D) could result in line intensities similar to those of CH_3CCH .

Thioformaldehyde is formed by the reaction $\text{S} + \text{CH}_3$ and in less extent through the DR of H_3CS^+ (see Agúndez & Cernicharo 2006 for a detailed discussion). The order of magnitude of discrepancy between model and observations reduces to a factor 4 with further non-local non-LTE radiative transfer calculations. We note, however, that a significant fraction of both H_2CO and H_2CS could be formed in grain surfaces by hydrogenation of CO and CS respectively.

The detection of C_3O in IRC +10216 (Tenenbaum et al. 2006), only previously detected in the dark clouds TMC-1 (Brown et al. 1985) and Elias 18 (Trigilio et al. 2007), stress both the similarity between dark clouds and C-rich CSEs chemistries and also the non-negligible oxygen chemistry taking place in C-rich CSEs. Actually astrochemical networks consider that C_3O is formed through DR of the molecular ions $\text{H}_n\text{C}_m\text{O}^+$ (see Fig. 4). However, the C_3O column density derived in IRC +10216 is an order of magnitude higher than calculated which could imply additional chemical routes for its formation, e.g. neutral-neutral reactions of atomic oxygen with carbon chain radicals such as those suggested in Fig. 4.

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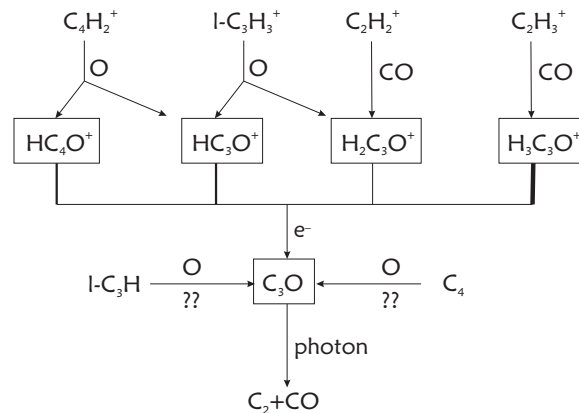


Fig. 4 Scheme showing the main chemical formation routes to C_3O . From Tenenbaum et al. (2006).

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