Understanding the chemical complexity in Circumstellar Envelopes of C-Rich AGB stars: The case of 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 $2-4\times10^{-5}$ $M_\odot$ 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), polyyne radicals (C$_n$H), carbenes (H$_2$C$_n$), radicals (HC$_{2n}$N) as well as S-bearing (C$_n$S) 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$>10^{10}$ cm$^{-3}$) and hot ($T_K$~2000 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 K, n$\sim10^4$ cm$^{-3}$) such as TMC-1 (Kaifu et al. 2004). In both places organic molecules are mostly unsaturated, which is typical of low temper-
nature 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 to-
ward IRC +10216 of the partially saturated C-bearing
species CH$_2$CHCN, CH$_2$CN and CH$_3$CCH; the S-bearing
molecule H$_2$CS and the oxygen-carbon chain C$_3$O. 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 be-
tween the chemistry taking place in cold dense clouds
and in the CSEs of C-rich AGB stars.

2 Observations

The observations of CH$_2$CHCN, CH$_2$CN, H$_2$CS and
CH$_3$CCH were achieved with the IRAM 30m telescope
(see e.g. Fig. 1) while C$_3$O 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 $\lambda$ 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 $\sim$18 dB rejection of the image sideband. The back ends were two 256 channel filter banks with 1 and 2 MHz resolutions, configured in parallel mode (2$\times$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$_2$CHCN, CH$_2$CN and C$_3$O lines de-
tected was large enough to allow us to construct rota-
tional temperature diagrams (see e.g. Fig. 2). The ro-
tational 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$_3$CCH
and H$_2$CS we observed only a few transitions with sim-
ilar upper level energies and it was not possible to con-
strain the rotational temperature which was assumed
to be 30 K.

In Table 1 we give the column densities (averaged
over the IRAM 30m beam, $\theta_{MB}=21-31''$ at $\lambda$ 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$_3$CN and CH$_3$CCH have very similar column densities although the lines of CH$_3$CCH are some 30 times weaker

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1 For CH$_2$CN and H$_2$CS, 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.
than those of CH$_3$CN mostly because of the different electric dipole moments (0.780 D vs. 3.925 D). The two related species CH$_3$CN and CH$_2$CN have similar column densities which may indicate a common chemical origin (see Sec II). 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 revised. The temperature and density radial profiles as well as other physical parameters are taken from Agúndez & Cernicharo (2006). The resulting abundance radial profiles for CH$_2$CHCN, CH$_2$CN, CH$_3$CCH, H$_2$CS and related species are plotted in Fig. 3. The model predicts that these four molecules together with C$_2$O (not plotted in Fig. 3) have an extended shell-type distribution ($r\sim$20") via several gas phase reactions.

Vinyl cyanide (CH$_2$CHCN) is formed by the reaction between CN and ethylene (C$_2$H$_4$), 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 column density agrees reasonably well with the observational value.

In our model both CH$_2$CN and CH$_3$CN are mostly formed (>90\%) through the dissociative recombination (DR) of CH$_3$CNH$^+$

\[
CH^+ + H_2 \rightarrow CH_2^+ \quad H_3^+ + CH_3 \quad CH_3C NH^+ \quad e^- \rightarrow CH_2CN \\
- \rightarrow CH_3CN
\]

whereas the major destruction process (>90\%) for both species is photodissociation. The branching ratios in the DR of CH$_3$CNH$^+$ are not known and are assumed to be equal. Assuming, as we do, that the photodissociation rate of CH$_3$CN and CH$_2$CN are equal, the observed CH$_3$CN/CH$_2$CN ratio suggests branching ratios in the DR of CH$_3$CNH$^+$ of 0.8 for the (CH$_3$CN + H) channel and 0.2 for (CH$_2$CN + H$_2$ or 2H). This estimate will be strongly affected if the photodissociation rates of CH$_3$CN and CH$_2$CN are very different but not if, as has been suggested by Herbst & Leung (1990) and Turner et al. (1990), CH$_2$CN does indeed react with atomic oxygen, the abundance of which is too low at the radius where CH$_2$CN is present.

The synthesis of CH$_3$CCH involves ion-molecule reactions with the dissociative recombination of the C$_3$H$_5^+$ and C$_4$H$_2^+$ 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 C$_3$H$_5^+$ and C$_4$H$_2^+$. The heavier chain CH$_3$C$_4$H is also predicted with a column density even higher than

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Table 1: Column densities of some molecules in IRC +10216

| Molecule | T$_{rot}$ (K) | N$_{tot}$ (cm$^{-2}$) |
|----------|--------------|----------------------|
|          | observed     | calculated           | This Work | M00  |
| CH$_2$CHCN | 44          | 5.1(12)              | 1.4(13) | 2.2(11) |
| CH$_3$CN  | 40          | 3.0(13)              | 6.3(12) | 6.8(12) |
| CH$_2$CN  | 49          | 8.4(12)              | 4.6(12) | 1.4(13) |
| CH$_3$C$_2$N | 30$^a$   | <1.3(12)             | 1.2(11) | 1.4(12) |
| CH$_3$CCH | 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)              | 2.8(12) | –     |
| H$_2$CS   | 30$^a$     | 1.0(13)              | 1.3(12) | 4.4(11) |
| C$_2$O    | 30$^a$     | <7.0(12)             | 7.0(11) | –     |
| C$_3$O    | 27         | 2.6(12)              | 2.8(12) | –     |
| C$_4$O    | 30$^a$     | <6.0(12)             | –     | –     |
| C$_5$O    | 30$^a$     | <3.0(12)             | –     | –     |

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: (M00) Chemical model of Millar et al. (2000).

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2 See [http://www.udfa.net](http://www.udfa.net) and [http://www.physics.ohio-state.edu/~eric/research.html](http://www.physics.ohio-state.edu/~eric/research.html)
that of CH$_3$CCH. 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$_3$CCH.

Thioformaldehyde is formed by the reaction $S + CH_3$ and in less extent through the DR of H$_3$CS$^+$ (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$_2$CO and H$_2$CS could be formed in grain surfaces by hydrogenation of CO and CS respectively.

The detection of C$_3$O 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$_3$O is formed through DR of the molecular ions H$_2$C$_m$O$^+$ (see Fig. 4). However, the C$_3$O 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. 3](chart.png)

**Fig. 3** Abundances of CH$_3$CHCN, CH$_3$CN, CH$_3$CCH and H$_2$CS (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.

![Fig. 4](chart.png)

**Fig. 4** Scheme showing the main chemical formation routes to C$_4$O. From Tenenbaum et al. (2006).