

CIRCUMSTELLAR CHEMISTRY : THEORETICAL STUDIES

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ABSTRACT. The different chemical processes responsible for the observed molecular abundances in massive circumstellar shells are examined : freezing-out of chemical equilibrium, radical and ion reactions, grain and shock processes, photochemistry, etc...

1. INTRODUCTION

Detailed studies of the chemical composition of the circumstellar envelopes of late type stars are indispensable in deriving element and isotopic ratios there, which are direct witnesses of nucleo-synthesis and of dredge-up mechanisms from the interior to the surface of the star. A good knowledge of the chemical mechanisms is also important to afford information on topics such as UV radiation field, ionization, dust formation and processing, the dynamics of the envelopes, and eventually their evolution.

As discussed by Zuckerman in these proceedings, the physical conditions in the external parts of the envelopes are very similar to those in the interstellar medium. However, completely different conditions prevail in the very internal layers close to the photosphere ; and the circumstellar medium is characterized by the extreme rapidity of its evolution, with typical time constants of the order of 10^3 years. Accordingly, the chemistry is highly time dependent and out of equilibrium, and the abundances of the most stable and abundant species can be frozen out through the whole envelope from the dense and hot layers near the photosphere where they were in thermal equilibrium. Besides, compared to the interstellar medium, the circumstellar envelopes present a whole range of elemental abundances which produce a wide variety in the abundances and the nature of the molecules observed. In particular the carbon-rich envelopes contain a wealth of carbon molecules, which are nearly absent in oxygen rich envelopes.

Since the chemistry in circumstellar envelopes has been recently reviewed (Glassgold and Huggins 1985 (GH), Omont 1985), we will emphasize here its main features and we will pay particular attention to the more recent developments. We will begin by a brief outline of the

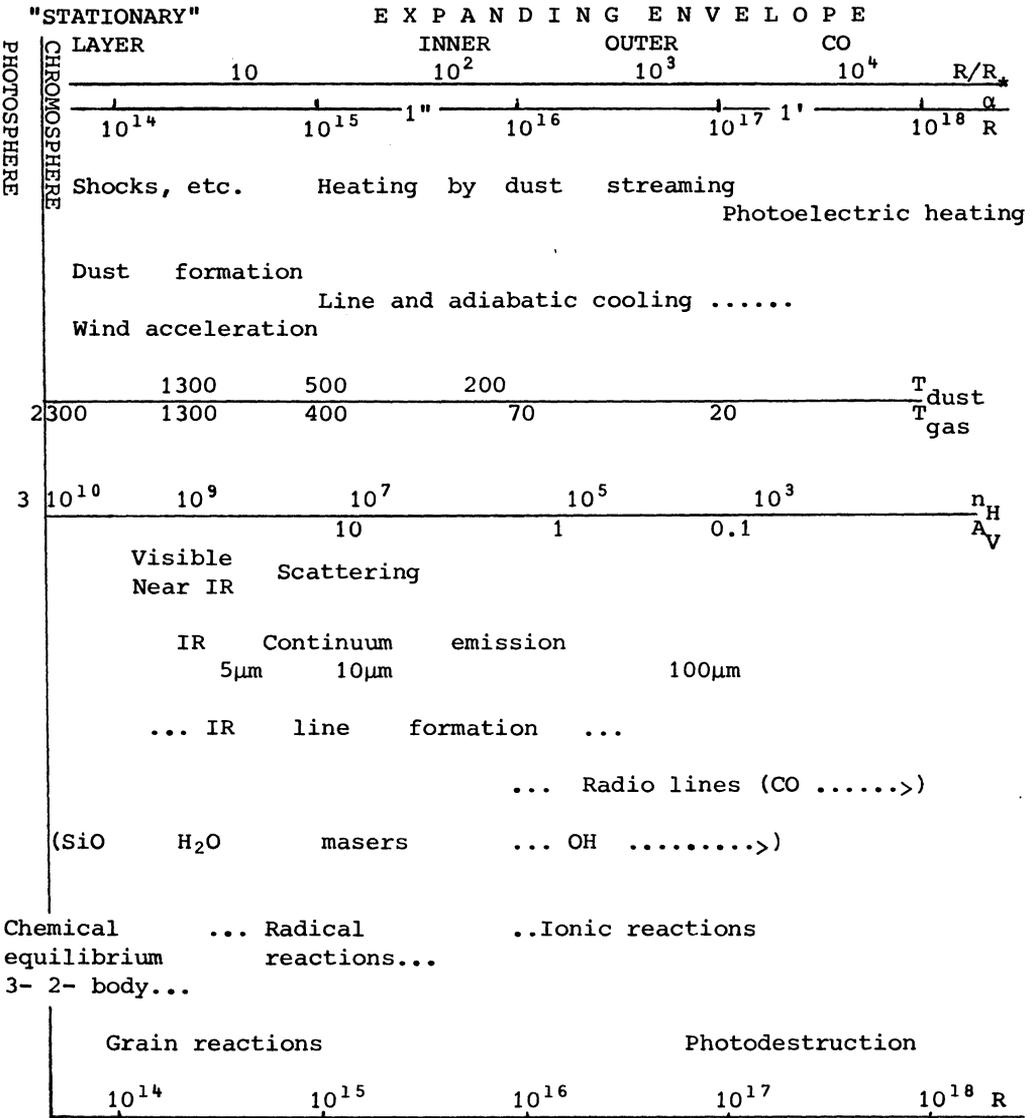


Figure 1. Structure of a massive envelope (IRC+10216). Assumed parameters : $d = 200$ pc, $R_* = 1000 R_\odot = 7 \cdot 10^{13}$ cm, $\dot{M} = 4 \cdot 10^{-5} M_\odot/\text{yr}$. In the outer envelope : $n_H = 5 \cdot 10^{37} \text{ r}^{-2} \text{ cm}^{-3}$,

$A_V = 2.5 \cdot 10^{-22} N_H$. The range of maser emission is indicated for similar O-rich envelopes, it is obviously irrelevant for C-rich shells such as IRC+10216.

(From Omont (1985) in Mass-Loss from Red Giants. Eds. M. Morris and B. Zuckerman. D. Reidel)..

physical parameters which govern the behaviour of the chemical processes, and of the main features of the observed molecular abundances that chemical modelling should explain.

2. PHYSICAL CONDITIONS

The physical structure of circumstellar envelopes is reviewed with some details in Omont (1985). Hence, we will give here only a brief account of the general characteristics of the different physical parameters relevant for the discussion of the chemical processes. A schematic picture of the structure of a massive envelope is given in figure 1 (reproduced from Omont 1985). The numerical values of the different parameters which appear there, refer to a model of the envelope of IRC+10216 by Keady et al. (1986), and they give a reasonable account of the order of magnitude of the physical parameters in the different parts of similar envelopes. The relatively "stationary" layer just above the photosphere is a somewhat complicated and certainly confused region. The physical parameters are rather uncertain there, as well as the physical processes : turbulent motions, shocks, wind formation, dust formation, (and possibly presence of a stellar companion), etc. On the other hand, in objects such as IRC+10216, the structure of the outer layers appears remarkably smooth with a nearly perfect spherical symmetry, and almost constant expansion velocity and mass-loss rate. The huge expanding envelopes typically span three orders of magnitude in radius, and hence six in density. A distinction between different regions there refers mainly to chemical processes (photochemistry) or to the formation of spectral lines with different opacities and excitation conditions. The O- or C-rich character of the envelope does not seem to fundamentally affect its physical structure. On the other hand, only massive envelopes such as IRC+10216 are well shielded against UV photodissociation, and hence are mostly molecular. Molecules are much less extended in less massive envelopes, which can even be completely permeated by galactic (and possibly chromospheric) UV radiation. As discussed by Zuckerman (1980, and in these proceedings), the massive envelopes are likely to be the progenitors of planetary nebulae, and some of them are probably already at the pre-planetary-nebula stage (CRL 2688, CRL 618, etc.), with a well developed (bipolar) nebulosity, and direct evidence of shocks (H_2 emission, etc...).

As already stated, the values of the density n and of the temperature T , and the velocity field in the very internal layers are very uncertain. The value of the expanding velocity V_e in the outer envelope generally lies in the range 10-20 km/s (with indications of high velocity flows in bipolar objects). Such values are compatible with radiation driving the expansion (Jura, Zuckerman in these proceedings), although the mechanism of wind acceleration remains uncertain (see e.g. Holzer 1985), and appears related in some way to the presence of pulsations (Jura in these proceedings).

The mass-loss rates \dot{M} can be relatively accurately determined (when the distance is known) from CO (Knapp and Morris 1985), OH (Wamsley in these proceedings) or IR observations. If \dot{M} is constant, the density

obeys a r^{-2} dependence,

$$n_H = \frac{C}{r^2} = \frac{3 \cdot 10^{37}}{r^2} \frac{M_H}{10^{-5} M_\odot / Y_r} \frac{10 \text{ km/s}}{V_e}$$

where n_H is the total number of H nuclei per cm^3 and \dot{M}_H is the hydrogen mass-loss rate.

In the external envelope, heating is achieved mainly by grains streaming through the gas at a few km/s, and possibly by the photoelectric effect with galactic UV radiation in the very external regions. Cooling occurs by adiabatic expansion and through the rotational lines of abundant molecules : mainly CO and possibly H_2O , H_2 , HCN, etc... It is very difficult to infer the temperature directly from line observations because most of the molecular lines are excited by IR pumping (Morris 1975). Accordingly, most of our knowledge of the temperature relies on theoretical estimates (Goldreich and Scoville 1976, Kwan and Hill 1977, Kwan and Linke 1982). They lead to temperature laws typically decreasing as $r^{-0.7}$. However, it is clear that photoelectric heating raises the temperature again in the very external layers when $n \lesssim 10^3 \text{ cm}^{-3}$. But this effect has not yet been properly modelled because of uncertainties in dust properties.

3. OBSERVED ABUNDANCES

Most of the information on the chemical processes in the circumstellar shells comes from the observed molecular abundances. Their general characteristics are reviewed by Zuckerman in these proceedings, Olofsson (1985), Glassgold and Huggins (1985) (GH) and Omont (1985).

The derivation of the abundances from infra-red or radio observations is not simple. Even the notion of a mean abundance \bar{x}_i of a species i can be misleading when the local abundance $x_i(r)$ strongly varies with the position because of active chemical processes. The mean abundances \bar{x}_i are nevertheless useful to give a rough description of the amount of the considered species in an envelope. When it is properly defined, \bar{x}_i generally refers to the abundance in the relatively external molecular shells in the case of radio observations, and in the region of infra-red continuum emission or just above in the case of infra-red line observations.

A list of observed molecules in IRC+10216 is given in table I where we have reproduced the estimated abundances of GH (see also Omont 1985) with slight modifications and additions. As mentioned by GH, uncertainties in these values are large and can reach an order of magnitude.

The ultimate goal of chemical modelling is to explain each of these abundances. However, in the present state of observations and understanding, one has to consider more modest objectives and to try to explain the main features, e.g. : how the main species (CO, C_2H_2 , HCN) reflect the abundance of the elements in the gas phase, the presence of an appreciable fraction of carbon not in CO and not in the grains, the large abundance of carbon chains especially cyanopolyynes, the presence of radicals, the mild depletion of S- and Si-species, the absence of ions, etc...

Other C-rich envelopes (e.g. CRL 2688 see Table 1) present similar

TABLE I. Observed abundances in IRC+10216 adapted from Table I of GH (see also Omont 1985). All abundances are uncertain by factors $\gtrsim 3$. $x(\text{CO})/(\text{H}) \approx 3 \cdot 10^{-4}$. Molecules also detected in CRL 2688 are underlined.

$\bar{x}(i)/x(\text{CO})$	Species	$\bar{x}(i)/(\text{H})$
		10^{-5}
10^{-2}	<u>HCN</u> , C_2H_2	
		10^{-6}
		<u>CN</u>
10^{-3}	<u>NH₃</u>	
	CH_4 , C_2H_4	<u>HC₃N</u> , <u>C₂H</u>
	<u>CS</u> , <u>SiS</u>	<u>HC₅N</u> , <u>C₄H</u>
		C_3N , <u>SiC₂</u>
10^{-4}		<u>HC₇N</u>
	SiO	<u>C₃H₂</u>
	<u>HNC</u>	$\text{HC}_{1,1}\text{N}$
		10^{-8}
10^{-5}		C_3H
	SiH ₄	
	CH_3CN	
		10^{-9}

characteristics, with significant differences (see e.g. Sopka et al. 1986, Guilloteau et al. 1986). The presence of a huge abundance of atomic C in CRL 2688 (Beichman et al. 1983), if confirmed, is obviously of fundamental importance for the chemistry. The variety of observed molecules is less rich in O-rich envelopes, the main feature of which is the presence of masers (OH, H₂O, SiO, see Wamsley in these proceedings). However, in addition to CO, thermal SiO, H₂S and NH₃, very recent observations have shown the presence there of HCN (Deguchi and Goldsmith 1985, Deguchi et al. 1986, Jewell 1985) and of SO₂, SO and H¹³CN (Lucas et al. 1986, Guilloteau et al. 1986), especially in the massive bipolar envelope OH 231.8+4.2.

4. CHEMISTRY IN THE INNER REGIONS

4.1. Time constants of chemical processes

The chemical structure of circumstellar envelopes is essentially determined by the physical conditions and by the relative values of the different reaction rates and time constants. The most important characteristic time is just the "dynamical time" $t_{\text{dyn}} = r/v$. Its inverse has to be compared to the different rates of the main chemical processes (Fig. 2 and Omont 1985) : chemical reactions with closed shell molecu-

cules, radicals or ions, photodestruction by the shielded UV radiation, and reactions with grains.

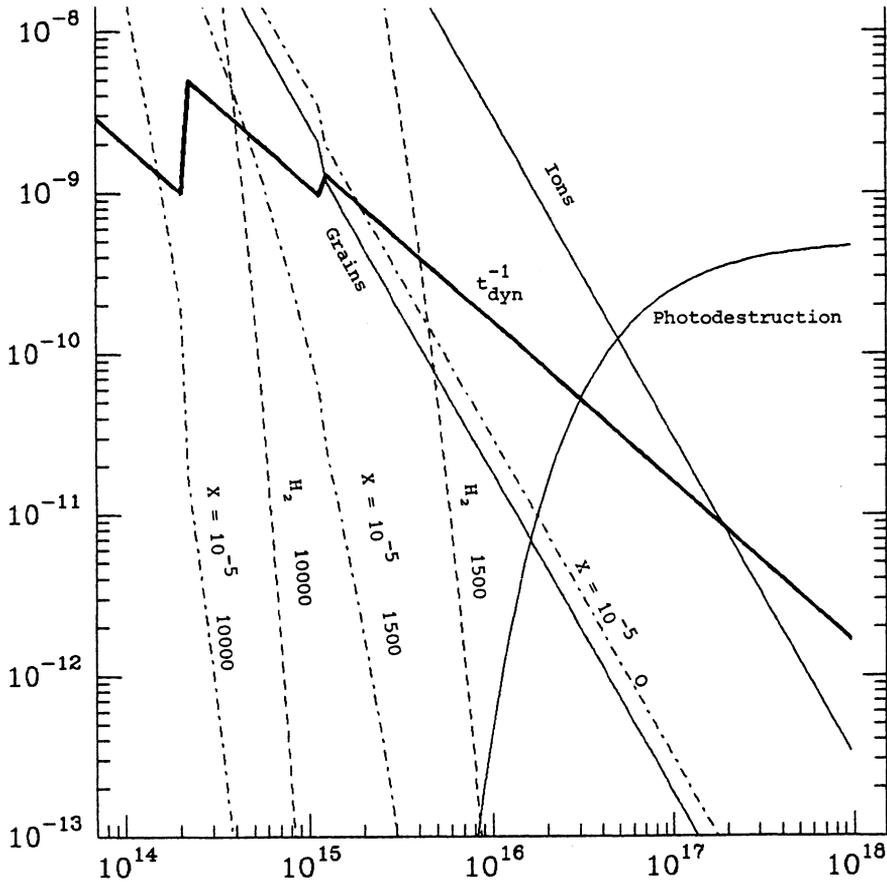


Figure 2. Time constants and reaction rates (sec^{-1}) in the envelope of IRC+10216 with the model of Figure 1. The assumed typical rates are the following : photodissociation $5 \cdot 10^{-10} \exp(-7 \cdot 10^{16}/r)$; grains $6 \cdot 10^{-17} n_{\text{H}}$; ions $10^{-9} X n_{\text{H}}$ with $X = 10^{-5}$; reactions with H_2 $5 \cdot 10^{-12} n_{\text{H}} \exp(-T/T_{\text{B}})$ with $T_{\text{B}} = 1500$ and 10000 K ; reactions with other abundant species (e.g. C_2H_2) $10^{-11} X n_{\text{H}} \exp(-T/T_{\text{B}})$ with $X = 10^{-5}$ and $T_{\text{B}} = 0, 1500$ and 10000 K.

Figure 2 displays the variations with r of τ_{dyn}^{-1} and of characteristic examples of the different rates in IRC+10216 with the model of Figure 1 (Keady et al. 1986). The comparison of these quantities with τ_{dyn}^{-1} shows that in such envelopes one can clearly distinguish between the chemical processes important in the inner dense and warm layers where chemical reactions and grain processes can be faster than τ_{dyn}^{-1} , and the ones to be considered (photodissociation and possibly ionic reactions) in the external envelope. However, the situation has to be carefully examined for every type of envelope. For instance, in much less

massive envelopes photochemistry can interest most of the envelope. On the other hand, there are massive envelopes where the regions of photo-destruction and of radical reactions overlap, when the density of radicals is particularly large : OH in OH-IR stars (Scalo and Slavsky 1980, Slavsky and Scalo, 1985) and possibly H in different types of envelopes, and C in C-rich objects such as CRL 2688.

4.2. Thermal equilibrium, freezing out and radical reactions in the inner shells

In the very dense layers in the photosphere and above, chemical equilibrium is probably a good approximation if effects of UV radiation are negligible (see Clegg et al. 1983 for a discussion of situations such as α Ori where this condition is not met). The computation of molecular abundances is then relatively easy and involves only the abundances of the elements and the thermochemical data (ΔG_f°) of the different molecules (see Tsuji 1964, for photospheres, McCabe et al. 1979 and Lafont et al. 1982 for models of internal envelopes, and the review by GH).

Because of the overwhelming abundance of hydrogen, the boundary of the region of full chemical equilibrium probably coincides with the point where the rates of three-body reactions with two hydrogens equals t_{dyn}^{-1} . More precisely, the critical process is the freezing-out of three-body formation of H_2 , which occurs for $n_H \sim 10^{11} \text{ cm}^{-3}$. This process and the resulting abundance of atomic hydrogen have been discussed in detail by Glassgold and Huggins (1983) and by GH. The corresponding values of H/H_2 critically depends on the physical conditions in the upper stellar atmosphere and are always relatively high, $\gtrsim 10^{-3}$. However, it is not clear at all whether this value remains frozen out in the subsequent layers or can be completely altered by processes such as catalytic radical reactions (Lafont et al. 1982), grain processes or shocks (Section 3.3.). Although the sensitivity of the observational searches of atomic hydrogen by the 21 cm line is not very high, they have shown that $x_H < 10^{-2}$ at least in some objects (IRC+10216 (Zuckerman et al. 1980), Knapp and Bowers 1983).

In the colder regions above the photosphere when $T \lesssim 1000\text{--}1500 \text{ K}$, two-body reactions between two closed shell species rapidly freeze out because of their high activation energies. This is also the case with very exothermic reactions such as most collisional dissociations. Gas phase chemistry is then dominated by radical reactions. The most important are by far those involving H such as $AH + H \rightleftharpoons A \cdot + H_2$ (e.g. $A \cdot = OH, O, C_2H, CN, SH, S, \text{ etc.}$). The ratio A/AH is then at equilibrium with H/H_2 .

Accordingly, all radicals with a binding energy to H, larger than that of H_2 , 4.5 eV, (e.g. CN and C_2H) have a very rapidly decreasing abundance when T decreases. On the other hand, the hydrides with a low binding energy such as SH_2 or NH_3 (Slavsky and Scalo 1985) are rapidly destroyed if H is present.

Such reactions have typical activation energies in the range 1000–3000 K. Accordingly, they freeze out for temperatures lower than a few hundred K (Figure 2). However, other radical reactions with abundant species such as $C_2H + C_2H_2 \rightarrow C_4H_2 + H$, have lower activation energy,

and can proceed a little further out.

Thus, it is clear that the assumption of freezing out of thermodynamical chemical equilibrium is completely irrelevant for radical and subordinated species. The evaluation of their abundance requires a complete solution of the time dependent network of chemical reactions (see e.g. Goldreich and Scoville 1976, Scalo and Slavsky 1980, Slavsky and Scalo 1985) with the appropriate reactions rates, which can be relatively well known for the main O-, N- and S- species (Slavsky and Scalo 1985), but which are often highly uncertain especially for carbon species.

4.3. Grain and shock processes

As for the interstellar medium, when discussing the chemistry of circumstellar gas, it should always be kept in mind that the amounts of heavy elements in the gas and in grains are comparable. Grains play a major role in depleting the gas of most of the elements, and possibly in injecting in the gas new species. Exchanges between the gas and grains are important in the region of grain formation ($T \lesssim 1500\text{--}1000\text{ K}$) and growth ($t_{\text{gr}} \lesssim t_{\text{dyn}}$, Figure 2). As the grain processes are discussed elsewhere (see e.g. Jura and Tarafdar in these proceedings, Omont 1985), they will not be discussed again here. It is nevertheless worth recalling that most of them (condensation, accretion, surface reactions, grain collisions, etc...) are very uncertain, and that this problem plagues any theoretical modelling of circumstellar chemistry, especially in the inner layers where these processes are active.

The problem is somewhat similar with shocks. They are certainly very frequent in the very internal layers, and they can interest very extended regions at least in some objects such as bipolar nebulae where H_2 emission (see references in GH) and even Herbig-Haro like objects (Cohen et al. 1985) are observed. The main effects of shocks on the chemistry are probably the dissociation of molecules such as CO or N_2 (and H_2) otherwise inactive, and, if the density is low enough and the cooling rapid, the stabilization in the cold and low density gas of species formed in the high temperature shock. It is not impossible that such processes could explain the observation of species such as SH_2 or NH_3 , hardly predicted by the radical reactions, or (e.g. HCN in O-rich stars) requiring large amounts of atoms such as C not locked in very stable molecules such as CO. However, our knowledge of these circumstellar shocks is still very uncertain, and they clearly depend on the objects and their geometry.

5. PHOTOCHEMISTRY IN THE OUTER SHELL

As reviewed in detail by GH to which we refer the reader, photodissociation by the ambient UV galactic radiation limits the radial extent of the molecules and is probably the major source of radicals in dense envelopes. There exist now numerous detailed models of this photodissociation : e.g. Goldreich and Scoville (1976), Scalo and Slavsky (1980), GH, Laffont et al. (1982), Huggins et al. (1984), Glassgold et al. (1986).

The main observational evidence of this photodissociation is the large extent of OH maser emission (Goldreich and Scoville 1976). In IRC+10216 there is evidence of both a very large extent of CN (Wootten et al. 1982, Truong-Bach et al. 1986), and of a limited extent of HCN (Olofsson et al. 1982, Bieging et al. 1984). Accordingly, it seems likely that most of the observed CN is created by photodissociation of HCN.

In massive envelopes the generated radicals of abundant species can efficiently enter further reactions, mainly with abundant atoms or radicals. Thus, photochemistry creates significant amounts of new species in the external shells. Such processes are probably of marginal importance in C-rich envelopes (except for reactions with atomic C if it is as abundant as found by Beichman et al. (1983) in CRL 2688). But they can be very efficient in O-rich envelopes because of the very large abundance of OH. Modelling of the photochemistry there has been performed in detail by Slavsky and Scalco (1985). They predict in particular a very large abundance of SO₂ (and SO). Accordingly, the low abundance of SO₂ reported by Lucas et al. (1986) in most of the O-rich envelopes could imply a sulfur depletion in the gas phase. On the other hand, the high abundance of SO₂ in the extreme envelope OH 231.8+4.2 (and in OH 26.5 + 0.6) and the detection of SO there (Guilloteau et al. 1986) implies an abundance of SO₂ comparable with the cosmic abundance of sulfur in line with the model of Slavsky and Scalco.

For some species such as C₂H₂, photodestruction can produce ions such as C₂H₂⁺ with branching ratios of several tenths. Furthermore, the successive photodestruction chain of every carbon containing molecule terminates with the production of C⁺ (e.g. C₂H₂ → C₂H + C₂ → C + C⁺ or CO + C → C⁺). The production of these ions (except CO photodissociation) occurs in regions ($r \lesssim 10^{17}$ cm) where the density is still large enough to allow condensation reactions that form carbon chains. Formation of C₃H from reaction between C⁺ and C₂H has thus been modelled by Nejad et al. (1984) and Glassgold et al. (1986). Reactions of C₂H₂⁺ with HCN and C₂H could well explain the observed abundances of the cyanopolynes and C₄H (Glassgold et al. 1986, Mamon et al. 1986). In the internal layers where UV radiation does not penetrate, the major source of ions is probably ionization of H₂ by cosmic rays as in interstellar clouds. This process has been also discussed by Glassgold et al. (1986). Almost every H₂ ionization is successively processed into H₃⁺, then into HCO⁺ and then into H₂CN⁺ and C₂H₃⁺. The case of HCO⁺ is of particular interest because it has been actively searched for in IRC+10216 (Johansson et al. 1984, Lucas et al. 1986). Its non detection, with a limit four times smaller than the predictions of the standard model of Glassgold et al. (1986), should imply a relatively large abundance of electrons in the external shells, and could be partially explained by the large rates of ionic reactions with HCN at low temperature (Mamon et al. (1986).

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DISCUSSION

ZUCKERMAN: In your calculation of intensity of HCO^+ in IRC+10°216 what distance did you assume for the star and what happens if you change the distance, say to 100 pc?

OMANT: 200 pc. If we change the distance, we have to be careful as we need to change other distance dependent parameters as well.

TURNER: Ziurys and I have observed the ground state and (0,1,0), (0,2,0) transitions of HCN in IRC+10°216 and find that both the line widths and line shapes are identical for all three of the $J = 3-2$ transitions. The shapes suggest all three are optically thick, and do not indicate any anomalous effects such as possible masering, as one possibility for your $J = 1-0$ result.