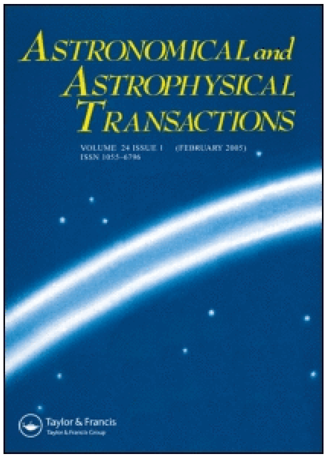

Astronomical & Astrophysical Transactions
The Journal of the Eurasian Astronomical Society
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713453505

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Online Publication Date: 01 July 1997
To cite this Article: Shmeld, I. (1997) 'The influence of dust condensation on the molecular abundances of the carbon star circumstellar envelope', Astronomical & Astrophysical Transactions, 13:4, 255 - 259
To link to this article: DOI: 10.1080/10556799708202967
URL: http://dx.doi.org/10.1080/10556799708202967

Astronomical and Astrophysical Transactions, 1997,
Vol. 13, pp. 255–259
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Session 4 : Interstellar Medium and Star Formation

THE INFLUENCE OF DUST CONDENSATION ON THE MOLECULAR ABUNDANCES OF THE CARBON STAR CIRCUMSTELLAR ENVELOPE

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(Received December 11, 1995)

Calculations of chemical equilibrium in the circumstellar envelope of carbon star IRC+10216 are performed. In order to account for the amount of C and Si lost by gas phase due to C and SiC dust condensation the variations of concentration of C and Si in this phase were used and the problem of chemical equilibrium in the gas phase was solved. Our calculations lead to the conclusion that if C/O changes from 2 to 1.1 the abundances of such C-bearing molecules as HCN, CH_4 and C_2H_2 change by about two orders and, if dust formation stops when C/O $\leq$ 1.1, the assumption of chemical equilibrium can explain the observable abundances of C_2H_2, CH_4, HCN, and HC_3N in the inner envelope of the star. The SiC dust formation in the envelope can explain the observable deficiency of some silicon-containing molecules, namely SiO and SiC_2 when Si depletion is about 70%. The upper limit of SiC_2 abundance given by Gensheimer *et al.* (1995) is in accordance with our equilibrium calculations. The calculated abundances of sulphur-containing molecules are briefly discussed.

KEY WORDS Circumstellar envelopes-carbon stars, IRC+10216

1 INTRODUCTION

One of the most interesting stages of the evolution of asymptotic giant branch (AGB) stars is the phase of superwind and fast mass loss with the formation of a well-developed circumstellar envelope (CSE). For some of those stars the mass-loss rates may reach $10^{-4} M_{\odot}$ yr^{-1} and the star radiates generally in the IR. The high density and low temperature of such envelopes mean that most of the material in them is in a molecular form and a strong process of grain formation takes place.

Currently there are many theoretical investigations into the chemical composition of these objects.

Most of them have been directed at investigating the well-studied extreme carbon star IRC+10216. This is the richest circumstellar source of molecular line emission, known to day. According to the present notion the chemical composition of the CSE near the star is forming under chemical equilibrium and most of the molecules with saturated valences, such as CO, HCN, C_2H_2, SiS, CS are formed in such way. In the outer layers, where interstellar UV is not shielded, the photochemical ion-molecular reactions are most important and a lot of additional molecules are formed from these parent species (see McCabe *et al.*, 1980; Lafont *et al.*, 1982; Huggins *et al.*, 1988; Millar and Herbst, 1994, for instance).

In the region where the gas cools to temperatures near 1000 K carbon-and silicon-containing dust (mainly C and SiC) condensation occurs and the molecular abundances may be affected by depletion of C and Si. The observational deficiency of some silicon-containing molecules such as SiO, SiC_2 in comparision with calculations of thermochemical equilibrium in the region near the star is believed to be due to Si depletion resulting from grain formation (see McCabe *et al.*, 1979; Bieging and Tafalla, 1993; Gensheimer *et al.*, 1995). Calculations of chemical equilibrium made under an assumption that gaseous carbon-and silicon-containing molecules are in equilibrium with the solid phase lead to results that are not consistent with observational abundances (McCabe *et al.*, 1979; Lafont *et al.*, 1982).

It is more likely that only a part of the carbon or silicon is incorporated into grains due to radiative acceleration of the medium and a considerable decrease in density which stops the grain formation. In this context it is worthwhile to investigate the abundances of some silicon-and carbon-containing species in the CSE near the star under the assumption of chemical equilibrium and partial depletion of C and Si due to dust formation.

2 METHOD AND ASSUMPTIONS

In order to investigate the influence of incorporation of carbon and silicon into grains on the abundances of carbon-and silicon-containing molecules in the inner part of the CSE of a carbon AGB star, sequences of calculations of chemical equilibrium for the CSE of IRC+10216 with gradually decreasing silicon and carbon abundances have been made.

Chemical elements H, O, C, N, Si, S and 94 more important species have been taken into account. The initial elemental abundances in the CSE were taken as solar except C for which we took $C/O = 2$ which is not too great for the extreme object IRC+10216 in our opinion. The calculations were carried out for $T = 1250$ K and $p = 3 \times 10^{-5}$ dyn cm^{-2}, close to the dynamical model of Lucy (1976). When scaling of the observational abundances was necessary to compare our calculations with observations we chose the arbitrary distance 200 pc to the star (Bieging and Tafalla, 1993). When fractional abundance was given we used $H_2/CO \approx 10^3$ to obtain the relative abundance to CO.

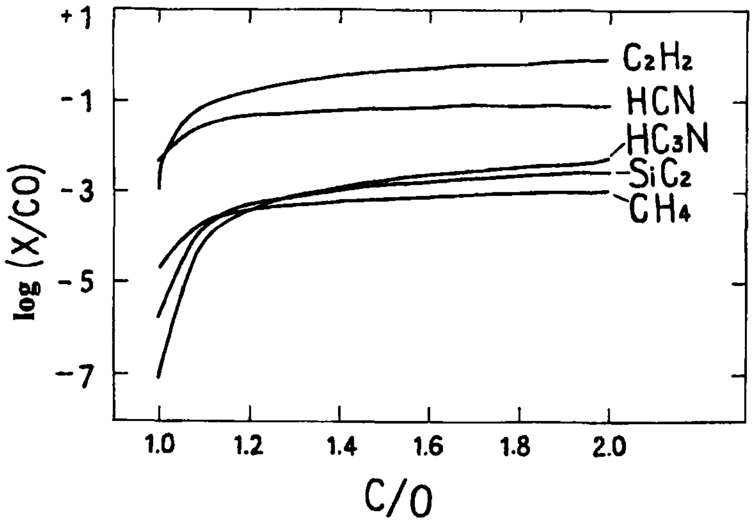

Figure 1 The calculated abundances of carbon-containing molecules dependent on C/O.

3 RESULTS AND DISCUSSION

The results of our calculations for C depletion are shown in Figure 1. They show that if C/O changes from 2 to 1.1 the abundances of such C-bearing molecules as HCN, CH_4 and C_2H_2 change by about two orders.

For the molecule CH_4 Lafont *et al.* ((1982) gave $CH_4/CO = 2 \times 10^{-3}$. Omont (1993) reported this to be about 10^{-4}.

One of the most abundant molecules in the envelopes of carbon stars is C_2H_2. In accordance with McCabe *et al.* (1979), Lafont *et al.* (1982), and Omont (1993) one can conclude that $C_2H_2/CO \approx 10^{-1}$.

Williams and White (1992) reported that $HCN/CO = (5-9) \times 10^{-3}$ for the inner envelope of IRC+10216. Omont (1993) reported this to be about 10^{-2}.

If $C/O \approx 1.1$ our calculations give $CH_4/CO \approx 10^{-4}$, $C_2H_2/CO \approx 10^{-1}$ and close to 10^{-2} for HCN/CO.

It is worthwhile examining the abundance of HC_3N in the inner layers of the envelope. Generally, this molecule forms in the outer layers of the envelope and its distribution has a shell-like structure (Bieging and Tafalla, 1993; Audinos *et al.*, 1994). The general opinion is that the concentration of HC_3N is very small in the inner layers of the CSE but Audinos *et al.* (1994) found that the observable abundance of this species can depend on the spectral line used for the observations. They obtain a fractional abundance of HC_3N of about 6×10^{-8} at a distance of about 10^{15} cm from the central star for IRC+10216 which also corresponds to a C/O of about 1.1. The relative concentration of HC_3N at this distance given by Bieging and Tafalla (1993) (10^{-9}) requires a C/O of about 1.05.

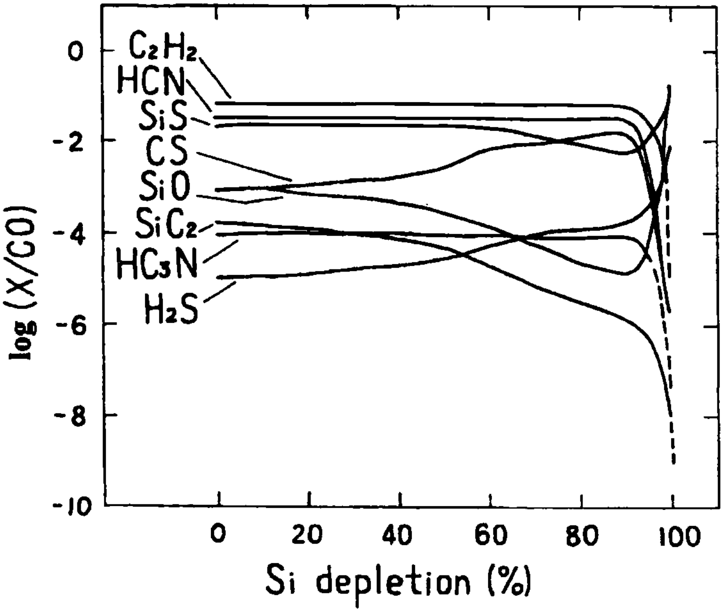

Figure 2 The calculated abundances dependent on silicon depletion.

So if the dust formation process ends when C/O $\leq$ 1.1 an assumption of chemical equilibrium can explain the observational amounts of such C-bearing molecules as CH_4, C_2H_2, HCN and HC_3N.

The calculations for silicon depletion were carried out for C/O = 1.1 according to our calculations with C/O variation. For the molecules of interest our results are shown in Figure 2. The fraction of silicon, incorporated into the dust is on the x axis and log(X/CO) on the y axis. Our conclusions are given below.

- SiC_2 – according to our calculations if silicon is depleted by more than 50% then the fractional abundance of this molecule is less than the upper limit of this abundance in the inner region of the CSE given by Gensheimer *et al.* (1995) (5×10^{-8}).

- SiO – according to Nyman *et al.* (1993) its fractional abundance is somewhat dependent 10^{-6}–10^{-7} (SiO/CO = 10^{-3}–10^{-4}) on the spectral line used. This corresponds to Si depletion of $\leq$ 70%.

- SiS – according to the same paper SiS/CO is about 10^{-3} which is about 1.5 orders less than our calculations give.

According to Williams and White (1992) the CS/CO in the inner envelope of IRC+10216 is about 10^{-3}, which is about half order less than is given by our calculations if the silicon depletion is about 60%.

It is worthwhile underlining that the depletion of Si leads to an increase of the abundance of H_2S. According to Omont (1993) the H_2S/CO is about 5×10^{-6} in the envelope of IRC+10216. We cannot explain the observational deficiency of H_2S in terms of our model. However Goebel (1993) argues the possibility that at lower temperatures the catalytic reaction $SiC_{solid} + H_2S_{gas} \rightarrow SiS_{2solid} + H_{2gas}$ takes place and the abundance of H_2S drops. He also suggests the reaction $SiC_{solid} + CS_{gas} \rightarrow SiS_{2solid}$ which could affect the observational abundance of CS.

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