MOLECULAR ABUNDANCES IN IRC +10216

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ABSTRACT

The observed molecular column-densities in IRC +10216 can be matched by chemical-equilibrium calculations for $T \sim 1250^{\circ}K$, $P \sim 100$ dyn cm^{-2} and no graphite grain formation. Condensation of silicon carbide into grains may explain the low observed abundances of SiO and SiS.

INTRODUCTION

The infra-red object IRC +10216 is a barely visible, cool carbon star, surrounded by an expanding, dusty, molecular envelope, and has $T \sim 2230$ K, $L \sim 5 \times 10^4$ $L_{\odot}$ (Cohen 1979). The temperature of graphite dust is estimated to be 600 K at 10 R_*, falling to 350 K at 60 R_* (Crabtree and Martin 1979). SiC grains are also known to be present from an 11 emission feature (Treffers and Cohen 1974). The molecules CO and HCN are observed out to 4000 R_* and 1200 R_* respectively, while the other 15 molecules identified in IRC +10216 are unresolved. Molecular line widths indicate a terminal velocity of 15 km/s (McCabe et al. 1979, and references therein).

We wish to determine whether the relative abundances of all 17 molecules can be explained by a "freeze-out" model: this supposes that chemical equilibrium holds close to the central star's photosphere, but that as the temperature and density fall in the circumstellar wind molecular reaction rates drop rapidly enough that molecular abundances are "frozen" near their equilibrium abundances at some point near the star. The ratio of the chemical timescale to the expansion timescale is proportional to the distance from the star for bimolecular exchange reactions and a steady wind. This implies a possible freeze-out for $n(total) < 10^{10} cm^{-3}$ (cf. 10^{15} at the photosphere).

The comparison of abundances is tricky because column densities have been derived from infra-red absorption and radio emission lines. Only CO and HCN have been observed in both, and some of the column-

densities are model-dependent. We merged the two abundance sets by scaling to the absorption figures to allow for dilution in the larger radio beam (60" compared with 3"). We have adopted abundances relative to CO for comparison with equilibrium calculations. In total there are 12 molecules with measured column-densities and known equilibrium constants.

Table 1. A comparison of molecules observed in IRC +10216 with calculated equilibrium abundances. The adopted relative abundances are with respect to CO = $10^{20} cm^{-3}$ and are taken from the underlined entries. The equilibrium abundances correspond to log P = 2, log T = 3.1.

| Molecule | Column density (cm^{-2}) | | Adopted relative abundance | Expansion (kms^{-1}) velocity | $\log\left(\dfrac{\text{observed abundance}}{\text{equilibrium abundance}}\right)$ |
	Emission (mm)	Absorption (μm)			
CO	2×10^{17} 4×10^{17}	5×10^{19} $\underline{10^{20}}$	1	15-16	0 (by definition)
CS	$\underline{1.8 \times 10^{15}}$ $CO/CS \approx 10^{4}$	-	1.8×10^{-5}	13	+0.6
CN	10^{15} $CN/CO = 2.8 \times 10^{-3}$ $CN/CS \gtrsim 8$	-	2.8×10^{-3}	14	+6.5
C_3N	$10^{14} \rightarrow 8 \times 10^{14}$	-	2.5×10^{-6}	13	+0.3
HCN & HNC	$CO/HCN \gtrsim 150$ $CO/HCN \gtrsim 60$ $HCN/CN \gtrsim 3$	$\geq \underline{1.5 \times 10^{18}}$	0.015	-	−0.3
HC_3N	$\underline{1.8 \times 10^{15}}$	-	1.8×10^{-5}	13	−0.3
HC_5N	4×10^{14}	-	-	-	-
HC_7N	2×10^{14}	-	-	-	-
C_2H	$\underline{3 \times 10^{14} \rightarrow 2 \times 10^{15}}$	-	10^{-5}	15	+0.2
C_2H_2	-	$\geq \underline{3 \times 10^{19}}$	0.3	-	−0.1
SiO	$\underline{4.1 \times 10^{14}}$	-	4.1×10^{-6}	10	−3.3
SiS	$\underline{1.6 \times 10^{15}}$	-	1.6×10^{-5}	13	−2.9
CH_3CN	Detection only	-	-	-	-
CH_4	-	$\underline{2.5 \times 10^{17}}$	2.5×10^{-3}	-	−0.8
C_4H	$\underline{4 \times 10^{14} \rightarrow 3 \times 10^{15}}$	-	1.2×10^{-5}	-	−0.7
NH_3	-	$\underline{10^{16} - 10^{17}}$	$10^{-5.5}$	14	+4.0

CALCULATIONS

The calculations involve 164 molecules containing 25 elements. The 14 IRC +10216 molecules with known equilibrium constants are included. The set of equations for the conservation of each element

is solved by Newton–Raphson iteration to give the number density of
free neutral atoms for each element (Wyckoff and Clegg 1977). The
input parameters are: 1250 K < T < 2800 K, 10^{-5}< P< 10^3 dyn cm^{-2} and
C/O = 1.76 and 5, typical of conditions expected to exist in carbon
star atmospheres. O/H is derived from the CO/H$_2$ ratio (Kwan and Hill
1977) and other abundances are assumed to be solar. Graphite grains
are allowed for in one set of calculations by setting p(C) (the partial
pressure of monatomic carbon) equal to p$_v$ (C) (the vapour pressure of
monatomic carbon over graphite) for p(c) > p$_v$(C). An accuracy of around
1 order of magnitude is expected, allowing for 0.3 eV uncertainties in
the dissociation energies.
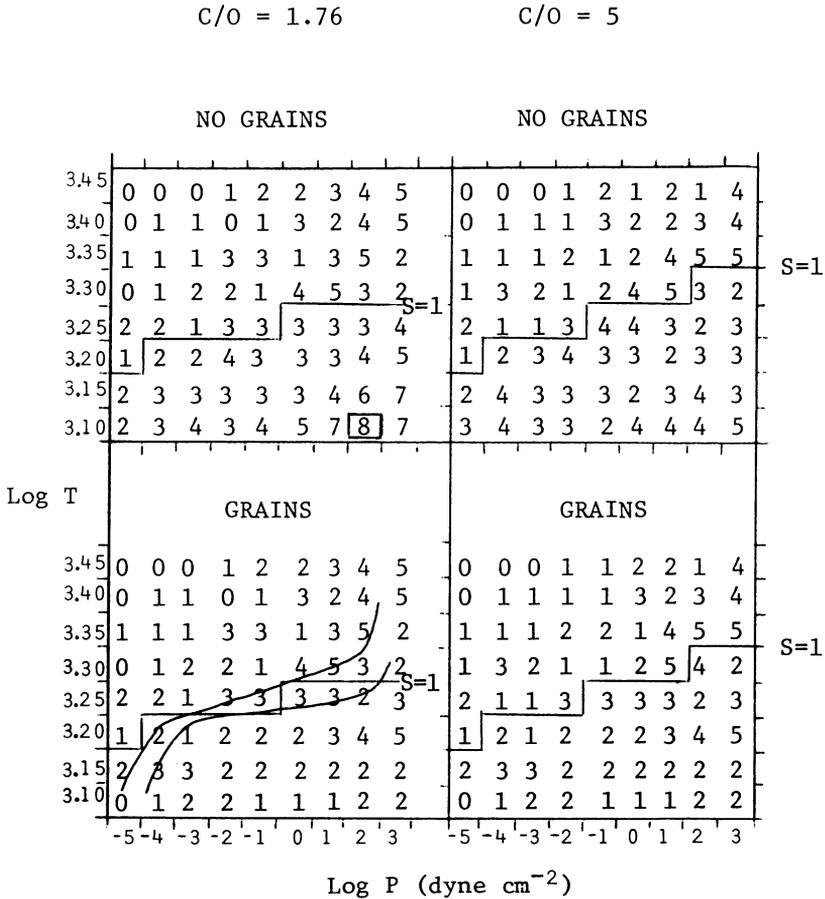
Figure 1. The number of molecules in IRC +10216 agreeing with
equilibrium calculations to within an order of magnitude. A total
of 12 molecules was considered.

RESULTS

The best agreement occurs for

a) $T \simeq 1250$ K, $P \sim 100$ dyn cm^{-2}
b)   C/O$\sim$1.76
c)   no graphite grains present

Under these circumstances 8 out of 12 molecules agree to within an order of magnitude. Of the other four:

d)   SiS and SiO are below the equilibrium abundance by a factor of about 10^3.
e)   CN and NH$_3$ are above the equilibrium abundance by factors of about 10^6 and 10^4 respectively.

DISCUSSION OF RESULTS (a) TO (e)

(a)   Such a P-T combination does not fit the Lucy model for cool carbon stars (Lucy 1976) in which the expanding atmosphere is driven primarily by radiation pressure on graphite grains. The P-T relations for that model are shown as the curves in the lower left of Fig. 1. However it is possible to get agreement for 5 molecules at $T \sim 2000$ K, $P \sim 10$ dyn cm^{-2}. Variation of the parameters in the model, in particular the grain composition (see (d)), does not alter this conclusion. A $1/r^2$ density distribution does fit the best-fit conditions if the ideal gas law is obeyed. In that case a model with a heated shock region near the photosphere is more appropriate (Willson 1976).

(b)   The C/O ratios in carbon stars are uncertain. IRC +10216 has a high carbon index in Cohen's 1979 classification. Our results suggest C/O < 5, so an intermediate value seems appropriate.

(c)   C$_2$H$_2$ and HCN agree over a wide range of pressures and temperatures but give poor agreement when graphite grains are present. However the supersaturation ratio $S(C) = p(C)/p_V(C) \sim 30$ when no grains are present, and such a value normally implies the condensation of grains. There already exists evidence that grains do not form until $r = 5R_*$ (Sutton et al. 1979).

(d)   The low abundance of SiO and SiS suggests that SiC grains condense out before graphite. This might happen for a number of reasons:

(i)   For C/O < 1.05, $P \sim 10$ dyn cm^{-2} the supersaturation ratio of SiC [$S(SiC) = p(SiC)/p_V(SiC)$] is greater than $S(C)$.

(ii) $S(SiC)$ rises more sharply than $S(C)$ as the temperature is lowered and may reach some critical value first.

(iii)   The stellar radiation tends to inhibit graphite grain

formation and promote SiC grain formation (Woolf 1975) – the inverse greenhouse effect.

Efficient SiC grain formation is required, a reasonable proposition in view of estimated graphite and SiC grain masses in the envelope, $3 \times 10^{-7} M_\odot$ and $4 \times 10^{-9} M_\odot$ respectively (Cohen 1979, Treffers and Cohen 1974). Further, the depletion factor of 10^3 implies initial condensation of SiC at around 1500 K, an acceptable temperature.

(e) The CN/CO ratio is particularly sensitive to temperature. Both CN and NH_3 may well be formed on grain surfaces.

FURTHER POINTS

(1) The abundances of large molecules, e.g. C_2H_4, C_2H_6, C_6H_6, not included in the equations, were found from the atomic abundances. Their inclusion would not affect the calculations.

(2) In the freeze-out model we expect the ratio HCN/HNC to be about 300 from the difference in binding energy between the two molecules. This is consistent with our estimated value from observations by Zuckerman (personal communication).

(3) Crude estimates for the equilibrium constants of HC_5N and HC_7N give a large uncertainty in the values for HC_5N/HC_3N and HC_7N/HC_5N. For a freeze-out at $T \sim 1000$ K the observed values lie within the margins of error (Clegg 1979).

ACKNOWLEDGEMENTS

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DISCUSSION FOLLOWING McCABE

Herbst: The JANAF tables are often in error!

McCabe: Updating of equilibrium constants in our calculations has
never altered the relative abundances by significant amounts. We require
an order of magnitude accuracy, typical of the estimated errors in the
observations.

Tatum: In order to compare the results of different equilibrium
calculations, there is a need for us all to use a "standard" set of
equilibrium constants, without necessarily trying to up-date them in the
light of more recent data. For diatomic molecules, for example, one
could calculate "standard" equilibrium constants from the data in the
recent book by Huber and Herzberg.

McCabe: A standard set of equilibrium constants upon which calcu-
lations can be based is certainly desirable. For those molecules which
are included in the Tsuji 1964 chemical equilibrium calculations, it has
been possible to compare results over part of the p-T range in the
C/O=5 case. The agreement is found to be adequate for our purposes.
It would, of course, be useful for others to repeat our calculations.

Huebner: Assuming non-equilibrium in your calculations is a very
important advance in stellar atmosphere modelling. Do you have all the
reverse reactions in your program to check if chemical equilibrium is
indeed a good starting condition?

McCabe: Our calculations are for *chemical equilibrium* only. The
individual reactions involved are therefore irrelevant and do not enter
into the program. Crude estimates of reaction rates suggest that to a
first approximation we can consider there to be an abrupt transition
from chemical equilibrium to no reactions at all. Our fit to observed
abundances is based on this "freeze-out" assumption. We are not
attempting to do time-dependent calculations.