CONDENSATION AND MOLECULAR ABUNDANCES IN STELLAR ATMOSPHERES

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ABSTRACT. Equilibrium calculation containing 211 species of 22 elements has been used to study the effect of condensation on molecular abundances as a function of temperature (T) and pressure (P). The condensation of 162 species are tested and 65 species in solar composition and 64 in a C-rich composition have been found to condense. The calculations show the expected result that the abundances of molecules containing condensable elements like Si, Al, Mg, Fe, Zr and Ti in solar composition and C together with above elements in carbon rich composition reduce significantly with condensation. Surprisingly, the abundances of molecules containing S, F and Cl in solar composition and O, S, F and Cl in carbon rich composition are enhanced with condensation but abundances of molecules containing CO like H_2CO, HCO in carbon rich composition hardly varies.

1. INTRODUCTION

A large number of calculations with varying complexity exists on condensation temperatures of elements and molecules for (T,P) relevant to stellar atmospheres (cf. Hoyle and Wickramasinghe 1962; Kamijo 1963; Lord 1965; Donn, Wickramasinghe, Hudson and Stecher 1968; Fix 1969; Gilman 1969; Anders 1971; Lewis 1972; Grossman and Larimer 1974; Barshay and Lewis 1976). Of late condensation in stellar wind has been explored (cf. Gail and Sedlmeyer 1986 and references therein). However, none of these authors studied the effect of condensation on molecular abundances for temperature and density relevant to stellar atmospheres, except perhaps by Hoyle and Wickramasinghe (1968) who have shown that the gas phase abundances of species decrease steeply with decreasing temperature after condensation temperature. The other work which appears to be more extensive than that of Hoyle and Wickramasinghe (1968) is by Ames, Fullerton and Huebner (1976) but exists in abstract form only. Here we determine equilibrium molecular abundances as a function of (T,P) including condensation. Such a calculation is necessary for two reasons: (i) for comparison of theoretical molecular abundances with observations in the atmosphere of cool stars and (ii) as

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molecular abundances with condensation provide more realistic relative abundances for frozen and/or initial abundance needed for circumstellar study.

2. DETAILS OF CALCULATION AND RESULTS

The calculation assumes that the gas is in thermal equilibrium. Then one can write partial pressure $P(A_\alpha B_\beta C_\gamma)$ of a molecule $A_\alpha B_\beta C_\gamma$, where A,B,C denotes elements and α,β,γ their respective numbers in the molecule as

$$P(A_\alpha B_\beta C_\gamma) = P_A^\alpha P_B^\beta P_C^\gamma K(A_\alpha B_\beta C_\gamma),$$

where P_A, P_B, P_C are partial pressures of A, B, and C respectively and $K(A_\alpha B_\beta C_\gamma)$ the equilibrium constant of the molecule $A_\alpha B_\beta C_\gamma$. If the total pressure P and abundances η_A, η_B, η_C of A, B, C relative to hydrogen are known, one can write n equations of the form

$$P = P_A + P_B + P_C + P(A_\alpha B_\beta C_\gamma) + \dots\dots$$

$$\eta_A P_H = \alpha P(A_\alpha B_\beta C_\gamma) + \dots\dots\dots\dots\dots$$

$$\eta_B P_H = \gamma P(A_\alpha B_\beta C_\gamma) + \dots\dots\dots\dots\dots$$

$$\eta_\gamma P_H = \gamma P(A_\alpha B_\beta C_\gamma) + \dots\dots\dots\dots\dots$$

for n elements A, B, C..... Here P_H is the fictitious pressure of hydrogen nuclei. Supplementing above n equations with equation of charge neutrality, one gets n+1 equations for n+1 unknown $P_A, P_B, P_C\dots$ and electron pressure P_e. A solution of these equations give partial pressures P_A, P_B, P_C of elements A, B, C, use of which leads to partial pressure of any molecule. If any of these partial pressures are larger than the corresponding vapour pressure of that molecule, the physical state of that species is favourable for condensation. Whether condensation occurs and how much of a given species goes into the condensation is not fully understood. I have, therefore, assumed that

(i) the condensation occurs whenever partial pressure of a species is larger than its vapour pressure, and

(ii) molecules condense till partial pressure becomes equal to its vapour pressure. This has been done by reducing the element in the molecule with least relative abundances. As for example when Al_2O_3 condenses, the abundance of Al has been reduced to make partial and vapour pressures of Al_2O_3 equal. Abundance of oxygen, of course, has been reduced proportionately. This provides the amount of depletion of Al and molecular composition when condensation of Al_2O_3 takes place.

The calculation considers 211 ionic, atomic and molecular species of 22 elements with two relative elemental abundances: (i) solar and (ii) solar except enhanced carbon to give C/O = 2. We have checked 162 species, many of which are not in the detailed calculations, for condensation and found that 65 molecules condense in the range of $1000 \leqq T \leqq 2000$, $-5 \leqq \log P_H \leqq 5$ for the solar composition and 64 molecules condense in the carbon rich composition. The details of equilibrium constant and vapour pressure data used and the determined partial pressures of various species as functions of (T,P) including amount of condensation will be published elsewhere. Figures 1 and 2 summarise the effect of condensation on molecular abundances.

Figure 1 shows the variation of abundances as a function of T at $\log P_H = 3.0$ for solar composition with (continuous line) and without (dashed line) condensation. It shows that:

(i) some molecules like CO, H_2O, OH, H_2CO are uneffected due to condensation. This arises as these molecules are not effected by condensation of molecules involving elements like Si, Al with lower relative abundances than the elements like H, C and O.

(ii) Gas phase abundances of molecules which condenses like Al_2O_3, ZrO_2, Fe and those like SiO, SiS, FeS containing condensing elements decrease with condensation. This is the result of condensable elements being in the solid phase and just not available for molecules.

(iii) The abundances of some molecules, however, enhance in presence of condensation. Molecules bearing S, F and Cl fall in these category. This is the result of these elements becoming free from molecules, a constituent of which condenses. As an example, S is generally bound as SiS. When Si condenses as Mg_2SiO_4 or $MgSiO_3$, abundance of SiS(g) reduces due to reduction of Si(g). This releases S to enhance sulphur bearing molecules like CS, SO, SO_2, HS, H_2S, etc. Same is true for Cl which is in the form of AlCl besides being in the form of HCl with no condensation. When Al condenses, Cl, which was in AlCl, is released to increase Cl bearing molecules like HCl.

Figure 2 shows similar plot for $\log P_H = 3.0$ for carbon enhanced composition. It shows the three properties found in solar composition except that oxygen bearing molecules together with S, F and Cl bearing molecules enhance when condensation is included in the calculation. Moreover, the molecules containing CO as a constituent like H_2CO, HCO and CO itself remain uneffected due to condensation of carbon into graphite. On the other hand CO_2 increases and CH_4 and CH decreases. This is due to CO binding being stronger than that of C into graphite.

The results presented above are in a way expected. It shows however that one need to be careful in inferring molecular abundances with condensation from those without, as increase of some molecules and constancy of H_2CO in presence of condensation would have been difficult to anticipate.

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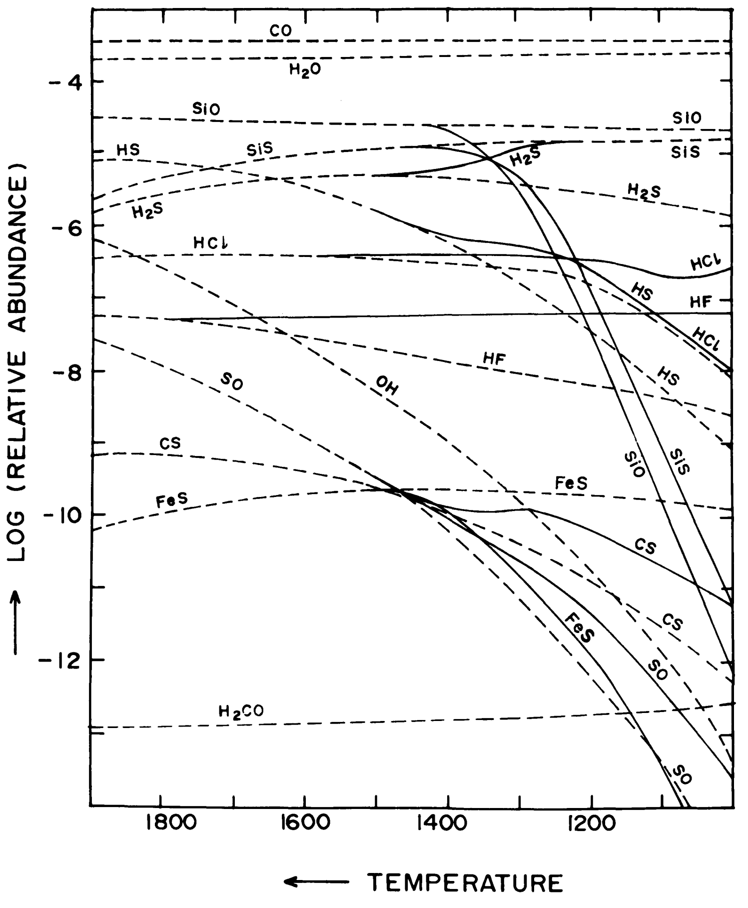

Figure 1: Variation of relative gas phase molecular abundances with temperature at log P_H = 3.0 for solar composition with (continuous line) and without (dashed line) condensation.

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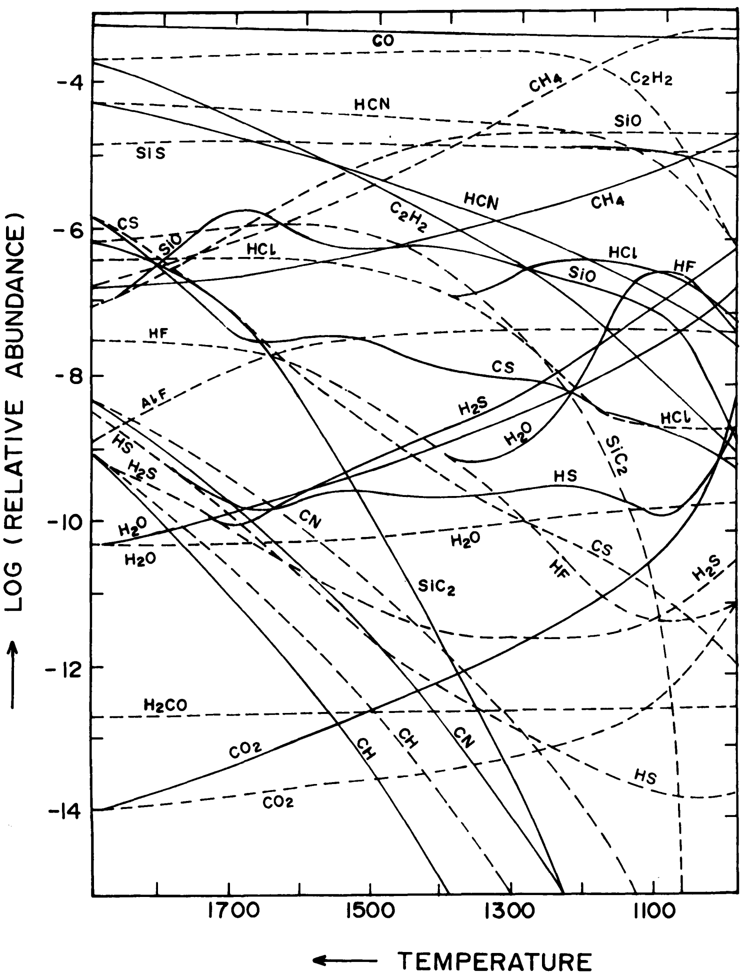

Figure 2: Variation of relative gas phase molecular abundances with temperature at log P_H = 3.0 for carbon enhanced composition with (continuous line) and without (dashed line) condensation.

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DISCUSSION

OMONT: What kind of solids did you include in C-rich stars?
TARAFDAR: 162 species were checked for condensation in C-rich atmospheres of which 64 were found to condense. The important among these are ZrC, graphite, TiC, SiC, ZrN, Zr, TiN, Fe_3C, Si, Fe, V, Ti and AlN. At low temperatures and high pressures species which condense in solar composition like $MgSiO_3$, Mg_2SiO_3 and Fe_2SiO_4 also condense.

HUEBNER: We had done similar calculations about 10 years ago. If I recall correctly, our abundance curves showed much sharper changes at the condensation temperatures (Ames, Fullerton, Huebner). Also Sieber had done similar calculations for a much more limited set of molecules (Thesis: Bonn, FRG).
TARAFDAR: Thanks for this information. However, it is difficult to comment on the differences without knowing the differences in the input in the two cases.

P.A. FELDMAN: Your calculations indicate that SiC_2 is markedly reduced (by 4 orders of magnitude) via condensation of grains in IRC+10°216. Yet Thaddeus et al. found SiC_2 to be an abundant species in the circumstellar envelope of this star. Are we to conclude that condensation of SiC grains did not occur? Of course, we know it did because the 11 μm SiC feature is really quite strong in this source.
TARAFDAR: The amount of decrease of SiC_2 depends on the temperature and pressure. Figure that I showed is for log P_H = 3.0, and there the decrease varies between zero to seven orders in the range $2000 \geqq T \geqq 1300$°K. Whether we will observe appreciable SiC_2 in presence of SiC condensation depends on temperature and pressure of the atmosphere from which material is expelled to form circumstellar gas and on changes undergone by this expelled gas on its outward journey. You can get relative abundance of SiC_2 with respect to hydrogen of 10^{-8} inspite of SiC condensation if you expell gas at log P_H = 3, T = 1700 °K and freeze it.

TATUM: I believe the condition that the partial pressure of a molecule in the gaseous phase is greater than the vapour pressure of the solid may not be sufficient to ensure condensation. A condensation nucleus is necessary to start it off.
TARAFDAR: I agree that it is a necessary but not sufficient condition and one needs some condensation nuclei . The charge particles present even at low temperatures and/or produced by cosmic rays may provide the necessary nuclei.

SAXENA: Would you please tell me why CO_2 increases on condensation of C in your last figure?
TARAFDAR: In presence of condensation, partial pressure of carbon in C-rich atmosphere is reduced, at a given temperature and pressure. As all oxygen is in the form of CO, the partial pressure of oxygen increases with condensation to keep CO constant. This increases CO_2 abundance.

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