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Molecular Structure in the Envelopes of Metal-Rich Red Giants

S.F.C. ROSSI *and W.J. MACIEL*

Instituto Astronômico e Geofísico, Universidade de São Paulo, Caixa Postal 30.627, São Paulo, 01051, SP, Brasil

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Abstract In this work we obtain molecular and atomic abundances in metal-rich red giant envelopes, based on the dissociation equilibrium theory. Number densities of H, and SiO, and other parameters are also estimated in order to check SiO maser pumping models in circumstellar envelopes.

1. INTRODUCTION

Expanding circumstellar envelopes around red giant stars have been Interpreted as a consequence of mass loss from the stars[1,2,3]. From the observational standpoint, such phenomenon is indicated, forexample, by blueshifts of metallic lines in absorption[4].

Several mechanisms have been proposed to explain the observed mass loss rate[3,4,5]. According to Maciel[6,7], when the observed infrared excess is not strong - which is the case of some late *M*-type variables - there is an indication of low grain density, and the radiation pressure on molecular bands of CO, H_2O and OH can be important as a mass ejection mechanism. The concentrations of molecular speciesformed by H, C, N and O were obtained[7] considering the supersonic region of the flow and radiation pressure on molecular bands. In a later work[8], several model envelopes have been calculated with mass loss caused by the radiation pressure on grains and molecules. It was then assumed that the velocity was constant throughout the envelope and as a consequence the decrease of the gas temperature was slow near the base of the envelope ($r = R \simeq R_*$ where R is the base of the envelope and R_* is the stellar radius). Therefore, a continuous decrease in the molecular concentrations was obtained (see figure 2 of reference 8), and the obtained column densities were interpreted as lower limits.

In the present work, we study the molecular structure of a red giant envelope according to the model developed by Maciel[6,7], con-

sidering a total of 53 molecular species composed of H, C, N, O, S, Si, Fe and Mg; special emphasis is given to the SiO molecule, for which we estimate the column density and some parameters relevant for the determination of the pumping mechanism responsible for the observed maser emission. Finally, the possibility of nucleation of some atomic and molecular species is also considered

2. MOLECULAR STRUCTURE

The physical structure of the envelope is poorly known, since the observed quantities - such as the gas velocity - are not sufficient to uniquely determine all the physical parameters.

The variation of the gas temperature and velocity with the position r/R_* in the inner regions of the envelope is obtained by solving numerically the flow equations[6,7]. A parabolic least-square fit of the density ρ (g cm^{-3}) as a function of the temperature $T(K)$ shows that

$$\rho = (a_0 + a_1 T + a_2 T^2) \times 10^{-16} \qquad (1)$$

where $a_0 = -3.5153$, $a_1 = 4.9727\times10^{-3}$, $a_2 = -6.2210\times10^{-7}$, with an error lower than 3%. It should be stressed that equation (1) refers to the *envelope* structure, which is clearly much less dense than the stellar atmosphere. By placing the base of the envelope at $r = R \simeq R_*$ it is implicitely assumed that the gas density reaches typical envelope values ($\sim 10^8$ cm^{-3}) in a small fraction of the envelope radius. As shown by more recent calculations[9], this is a reasonable hypothesis even if a moderately warm chromosphere stands behind the cool envelope. On the other hand, given the low ($\sim$ 10 km/s) gas velocity, a gas density of the order of 10^{-16} g cm^{-3} is necessary to explain the observed range of the mass loss rate (10^{-6} - 10^{-8} $M_\odot$/year).

In order to determine the molecular abundances we assume that the inclusion of the new species does not change sensibly the dynamical structure of the envelope. In other words, the mass loss rate ($\dot{M} \sim 10^{-7}$ $M_\odot$ yr^{-1}), the variation of ρ and T with position, and indirectly the relation $\rho(T)$ given by equation (1) are not strongly modified by the inclusion of the new molecules. As we discuss later in this section, such hypothesis is approximately valid.

The equilibrium molecular densities can be obtained through the dlssociatlon equllibrium, and the dissoclation constants used in the calculations have been recently calculated[10]. In view of our interest in the study of the nucleatlon of some compounds inthestellar envelope, a metal rich chemlcal composition. is adopted[11], which favours particle formation. We further consider the average value[12] N(Fe)/N(H) $\simeq 1.1\times10^{-5}$ iind N(S)/N(H) $\simeq 5.9\times10^{-5}$ (Si/S $\simeq$ 1.6).

The results are shown in Figures la-d. Figure la shows the densitles (cm^{-3}) of the most abundand species in the region $1.0 \leq r/R_* \leq 1.22$, and can be dlrectly compared with published results[7], except for the inclusion of SiO. The position $r/R_* \simeq 1.22$ corresponds to the "critical radius", where the terminal velocity is attained. The molecular density profiles are practically indistinguishable from the original curves, showing the agreement between the (independent) numerlcal methods used by Maciel[7] and in this study. The main difference occurs in the CO profile, which undergoes a decrease of the srder of 0.3 in log n, or of a factor 2 in number density. Naturally, this is due to the fact that part of the oxygen atoms are consumed in forming SiO molecule, which was not included in the original work. It is difficult to estimate the effect of such reduction in the mass loss rate without calculating the complete envelope structure. On the other hand, the maintenance of the gas density (n_H, n_H) variations, the size of the envelope and the (observed) final velocities, indicate that the main physical parameters of the envelope are retained. Therefore, the observed difference in the CO profile does not *strongly* affect the envelope structure, and the hypothesis made at the beginning of this section remains valid, at least in an approximate way.

We should note that the abundance calculations presented heredo not take into account condensation effects. The nucleation of any species would change the behaviour of the curves in Figure 1, and for this particular species the partia1 pressure would be limited to the saturatlon pressure. Such possibility was checked by considering as candidates For the nucleation process the species C, SiC, Si, SiO_2, Fe and Mg [13,14,15]. As we can see from Figure 2, none of them attains the saturation pressure over the temperature.range ($1200 \lesssim T(K) \lesssim 2000$, $r/R_* \lesssim 1.2$). In fact, Draine[16] concluded that the formatlon of silicate grains in a oxygen-rich envelope (O/C $\sim$ 2.0) occurs at $r > 2R_*$. Fur-

thermore, the flrst condensates to occur in such regions are probably sillcates, aluminates etc., which are generally heavier than the species considered in this work.

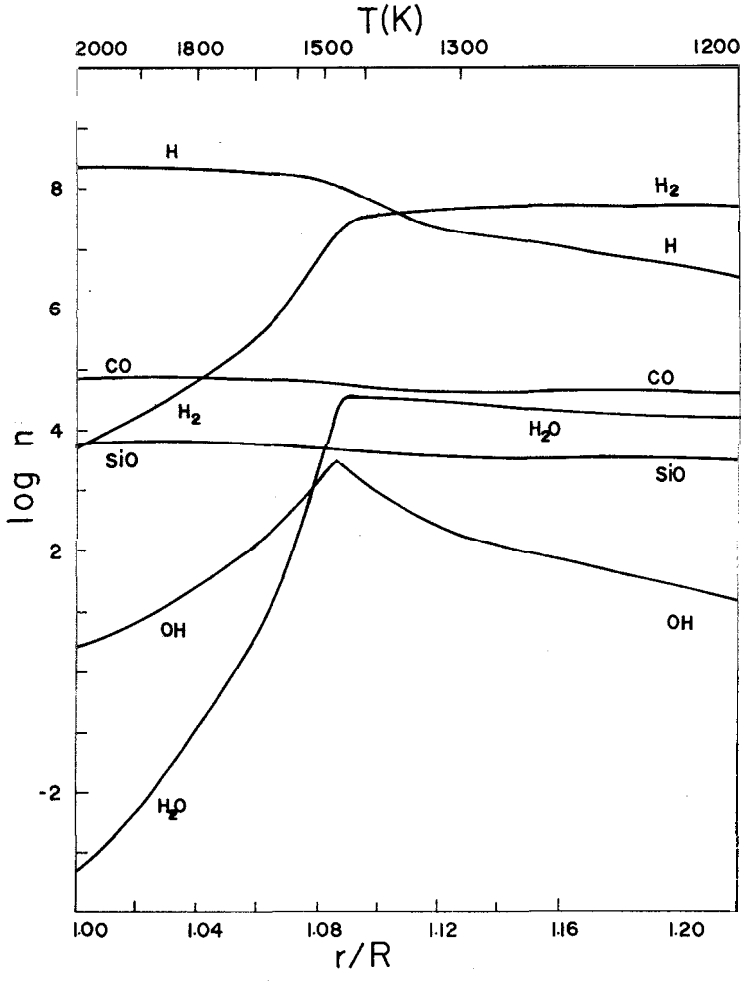

Fig. 1a

Fig.1 - Atomic and molecular abundances (cm^{-3}) as functions of position (r/R_*) and temperature (K) in the envelope.

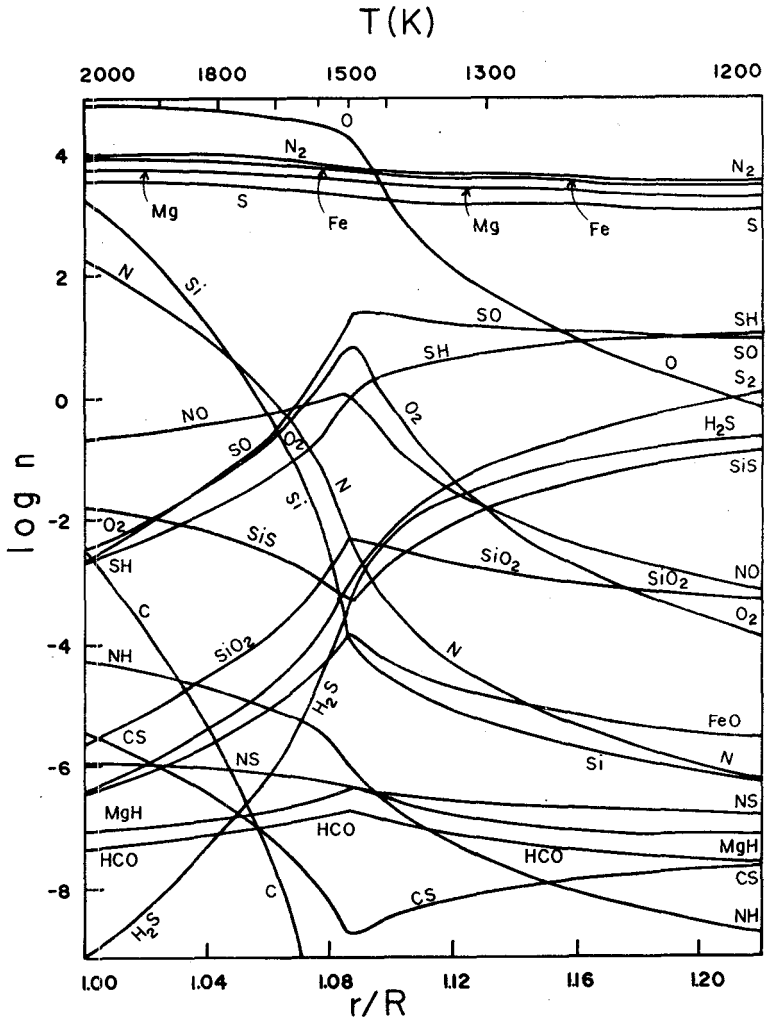

Fig. 1b

Fig. 1 - Atornic and molecular abundances (cm^{-3}) as functions of position (r/R_*) and temperature (K) in the envelope.

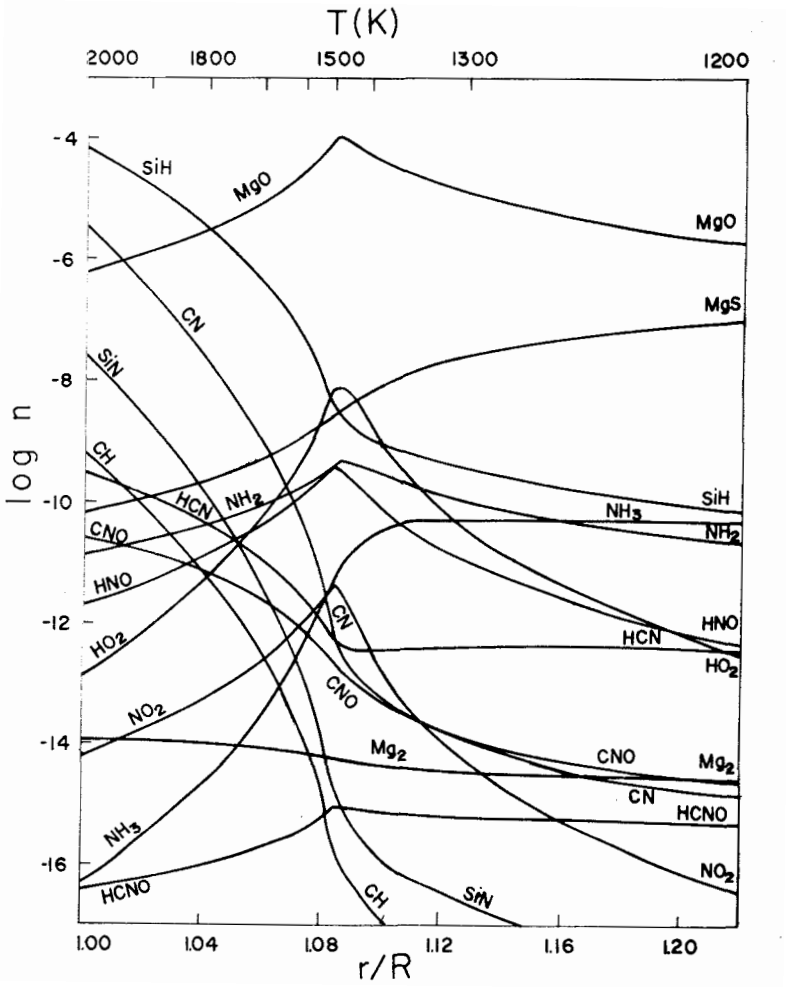

Fig. Ic

Fig.1 - Atomic and molecular abundances (cm^{-3}) as functions of position (r/R_*) and temperature (K) in the envelope.

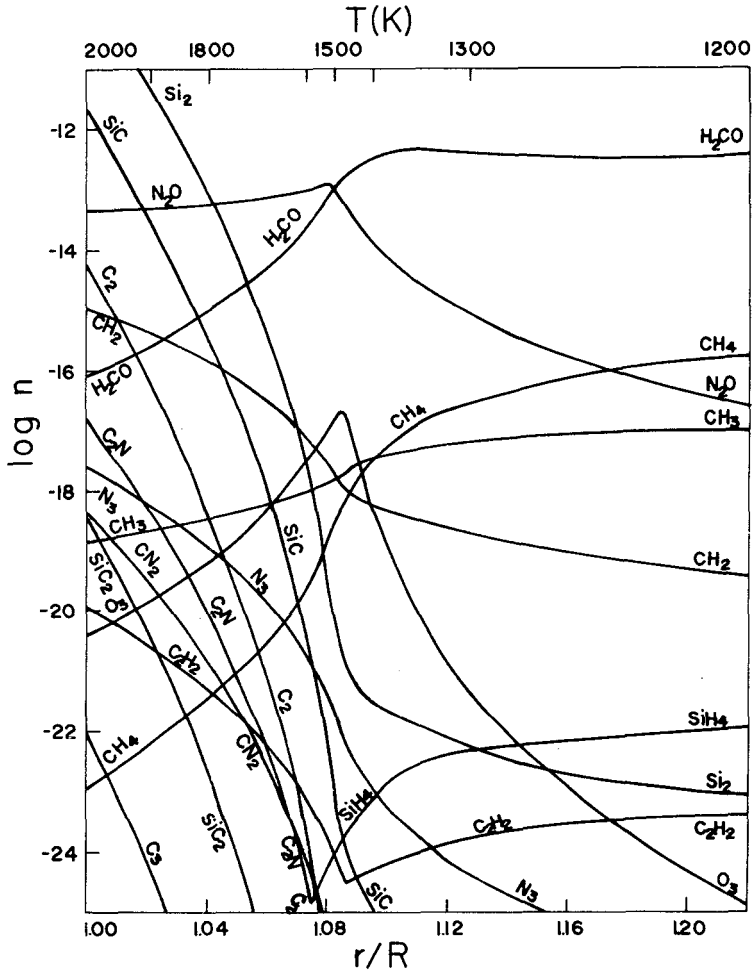

Fig. 1d

Fig.1 - Atomic and molecular abundances (cm^{-3}) as functions of position (r/R_*) and temperature (K) in the envelope.

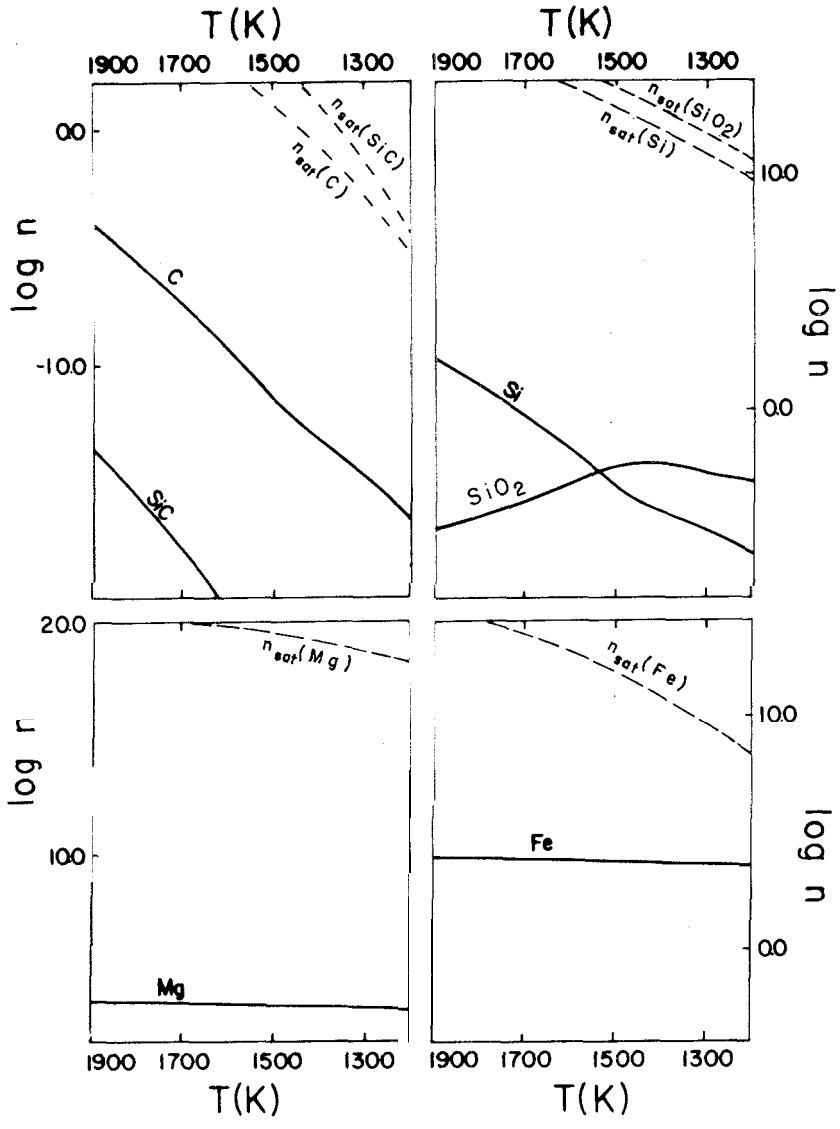

Fig.2 - Saturation (n_{sat}) and partial densities of C, SiC, Si, SiO_2, Mg and Fe in the circurnstellar envelope.

3. SiO IN CIRCUMSTELLAR ENVELOPES

Since the detection of SiO maser radiation (vibrational level $v=1$)[17], several mechanisms have been proposed to explain the inversion of the low rotational levels of the excited vibrational levels of this molecule. Kwan and Scoville[18] have considered the stellar radiation as source of excitation from $v=0$ to $v=2$, and the inversion of the level $v=1$ is obtained by cascades from $v=2$. On the other hand, Elitzur[19] proposed that the maser emission takes place in the inner shells of the atmosphere. The levels of the v-state are collisionaly pumped from the fundamental state, decaying radiatively to v-1. Bujarrabal and Nguyen-Q-Rieu[20] have studied both collisional and radiative mechanisms. Although the calculations indicate that the collisions can invert the SiO transitions, this mechanism is criticized since it is strongly dependent on vibrational and rotational cross sections which are not well known. They have suggested that the maser pumping in the v-state operates by absorption of infrared stellar radiation (8μ) from v-1 and optically-thick radiative decay. This mechanism becomes effective in the inner regions of the envelope.

The physical conditions found in these models are given in Table 1 (R and C stand for "radiative" and "collisional", respectively). It is interesting to discuss some parameters related to the SiO molecule as derived in the present work. A similar discussion on H_2O and OH molecules was given earlier[7].

First, the total SiO column density is $\sim 3.5\times10^{17}$ cm^{-2} close to the value (5×10^{17} cm^{-2}) estimated without taking into account the gas acceleration at the base of the envelope[8]. This is due to the factthat the SiO behaves in a way similar to CO, contrary to earlier expectations[8].

The mass loss rate implicitely assumed in this paper isafactor 10 lower than obtained in model 3 (see Table 1) and within the range considered by Elitzur[19]. From earlier calculations[8] we can infer that an increase in M by a factor 10 implies an increase of the gas density by the same factor.

The position r/R_*, in Table 1 corresponds to the region of maximum amplification, and only models 2(C) and 3(C) are in agreement with the interval considered in this study. The SiO concentration does not

Table 1

Pararneter \ Model	1† (R)	2 (C)	3 (R)	3 (C)	This Work
$\dot{M}$ ($M_\odot$/year)	10^{-5}	10^{-6}-10^{-7}	10^{-6}	10^{-6}	10^{-7}
R_*(cm)	5.8×10^{13}	3×10^{13}	10^{14}	10^{14}	6.96×10^{13}
r/R_*	3.5	$\lesssim$1.004	1.5	1.1	1.0 - 1.2
T_e (K)	2000	2000	2000	2000	2000
T (K)	300	2000-2500	1000	2000	2000-1200
$n(H_2)$ (cm^{-3})	10^9	$\lesssim 10^{12}$	10^9	10^{10}	$\lesssim 10^8$
$n(SiO)/n(H_2)$	4×10^{-5}	4×10^{-5}	4×10^{-5}	4×10^{-5}	7×10^{-5} (1.2 R_*)
$n(SiO)$ (cm^{-3})	4×10^4	4×10^7	4×10^4	4×10^5	7×10^3 (1.02 R_*)
Flux (erg cm^{-2} s^{-1} H_2^{-1})	-	-	10^{-5}-10^{-6}	-	1.7×10^{-6}

†Model 1: Kwan and Scoville (1974)[18]. Model 2: Elitzur (1980)[19]. Model 3: Bujarrabal and Nguyen-Q.Rieu (1981)[20].

show any peak in the circumstellar envelope as we can see from Figure 1a: at $r \sim 9R_*$, $n(SiO)$ is decreased by a factor 100, and at $r \sim 30$ R the density is reduced by a factor 1000. On the other hand, the inclusion of a hot chromosphere above the photosphere[3,9] could move the region of molecular formation by an unknown factor which could reach a considerable fraction of the stellar radius. In the case of pulsating variable stars, the pulsation could have an analogous effect because the induced shockwave could change the adiabatic behaviour in the studied region. Thus, the region of formation/maximum abundance of molecules would be closer to the models 1(R) and 3(R) (see Table 1). According to Figure 1, in the region 1.0 R_* - 1.06 R_* the velocity gradient is $\simeq 10^{-13}$ km s^{-1}/cm and $r\frac{dv}{dr} \sim 0.5$ km s^{-1}, which is lower than the observed line width ($\sim$ 1 km s^{-1}) in maser transition[17]. Therefore, the maser amplification in the radial direction could be viable if the population inversion mechanism were efficient.

The molecular hydrogen density is $\lesssim 10^8$ cm^{-3} and $n(H_2) \sim 5\times10^7$ cm^{-3} at the "critical point". According to Bujarrabal and Nguyen-Q-Rieu[20], if $n(H_2)$ à 10^{10} cm^{-3} (radiative mechanism) the maser emission

ceases, as the collisional de-excitation of v=1 surpasses the radiative one ("quenching"). The same occurs for $n(H_2) \gtrsim 10^{11}$ cm^{-3} in the collisional case. At $T \gtrsim 1400$ K, the hydrogen is essentially atomic and $n(H)$ is always lower than 10^{10} cm^{-3}. The parameter $n(H_2)$ is limited by the total density at $r = R_*$, which is related to the mass loss rate.

The $n(SiO)/n(H_2)$ ratio is constant from 1.2 R_*, where $n(SiO)/n(H_2) = 7\times10^{-5}$ and agrees with the values of the other models. We must note that the condensation of silicate grains tends to decrease this ratio, since most of the available silicon is in atomic form.

At $r \sim R_*$, the black body flux at 8μ calculated in our model is $\simeq 1.7\times10^{-6}$ erg s^{-1} cm^{-2} Hz^{-1}. The observed infrared excess was not taken into account, but it can be counterbalanced by the decrease of the stellar continuum caused by molecular absorption[21]. On the other hand, in order to assure the efficiency of the radiative pumping, the number of photons emitted at 8μ must be greater than or equal to the observed rate of SiO photons[20]:

$$N_\nu(8\mu) \gtrsim N(SiO) \simeq 10^{43} \text{ photons s}^{-1}$$

For the estimated black body flux we obtain $N_\nu(8\mu) \sim 1.5\times10^{44}$ photons s^{-1} for $\Delta\nu/\nu \sim 10^{-5}$. This rate does not exclude the radiative pumping model even if the effective infrared flux is effectively reduced by a factor 3[21].

As we have seen the parameters calculated in this work (including also effective temperature T_e and gas temperature T), adopting local thermodynamic equilibrium, are not in general very different from those considered in the pumping models of SiO maser. A comparison of the results does not allow us to make a clearcut definition of physical process operating in red giants, although those of Kwan and Scoville[18] and Elitzur[19] seem to be incompatible with our calculations. Consequently, the results obtained favour the mechanism proposed by Bujarrabal and Nguyen-Q-Rieu[20], specially the radiative ($3R$) pumping mechanism.

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Resumo

Neste trabalho são calculadas abundâncias moleculares e atômicas em envelopes de estrelas gigantes vermelhas ricos em metais, com base na teoria do equilíbrio de dissociação. São estimados alguns parâmetros relativos à molécula SiO, com o objetivo de testar os modelos existentes de bombeamento do maser observado nestes envelopes.