

Letter to the Editor
On the formation of warm molecular layers
P. Woitke, Ch. Helling, J.M. Winters, and K.S. Jeong

Institut für Astronomie und Astrophysik, TU Berlin, Sekr. PN 8-1, Hardenbergstrasse 36, D-10623 Berlin, Germany (woitke@physik.tu-berlin.de)

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Abstract. The levitation of the outer atmospheres of AGB stars by pulsations is proposed as possible mechanism to form “warm molecular layers”. We compare the amounts of CO, H₂O, CO₂ and SO₂ molecules found in an oxygen-rich dynamical model atmosphere with the values derived from recent ISO observations. In the model, the molecules are present in a layered structure behind shock waves which leads to a substantial increase of the column densities in comparison with static models. By additional non-LTE investigations, we calculate the vibrational and rotational excitation temperatures of these molecules and discuss the respective deviations from the kinetic gas temperature in view of the interpretation of the observations.

Key words: infrared: stars – molecular processes – hydrodynamics – stars: late-type – stars: circumstellar matter

1. Introduction

Recent ISO observations in the “thermal infrared” spectral region (about 2... 16 μm) have revealed new constraints on the outer atmospheres of oxygen-rich AGB stars. The physical conditions present in these layers close to the photosphere are of special interest concerning various long-standing astrophysical problems, as for example the occurrence of chromospheres and shock waves, the formation of molecules and dust, the acceleration of stellar winds, and how these phenomena are related to each other.

Free from the disturbances of the Earth’s atmosphere, new molecular absorption and/or emission features have been detected in several O-rich AGB stars including Miras and semi-regular variables which appeared quite different from what could be expected from standard model atmospheres. The magnitude and the spectral shapes of the bands attributed to CO₂, SO₂ and H₂O can be used to probe the physical and chemical conditions in these outer atmospheres (Table 1). The discovery of the excess absorption/emission features led several authors to the conclusion that rather dense, quasi-static molecular envelopes at temperatures of 500... 2000 K exist around these stars – termed as “warm molecular layers”. These layers are clearly distinct from the much cooler circumstellar envelopes already known from radio observations.

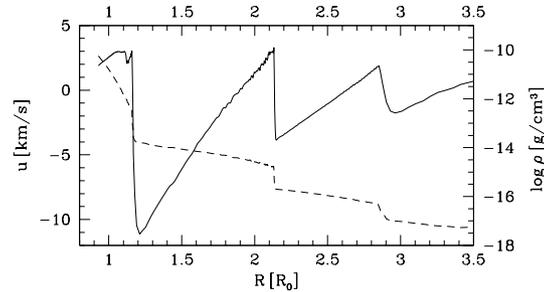


Fig. 1. Radial structure of an oxygen-rich time-dependent model at one instant of time (full line: velocity u , dashed line: gas density ρ). Model parameters: $T_* = 2800$ K, $L_* = 10^4 L_\odot$, $M_* = 1 M_\odot$, $C/O = 0.43$, piston amplitude $\Delta u = 2 \text{ km s}^{-1}$, pulsation period $P = 650$ d.

In this letter, we report on clues to the origin of such molecular layers based on hydrodynamical model calculations. This is in contrast to previous works, which have assumed the temperature and density of these layers in order to obtain agreement with the observations and allowed for the first quantitative interpretations. In a simple, but quantitative model, where dust formation is not taken into account, we demonstrate the contribution of the pulsation to the formation of such layers.

2. Time-dependent model atmosphere

A time-dependent model of the dynamical atmosphere of an AGB star with solar element abundances has been calculated by means of the CHILD-code developed by Fleischer et al. (1992). The code solves the coupled equation system describing time-dependent hydrodynamics, radiative transfer, chemistry, and dust formation in a self-consistent way. However, the model shown in Fig. 1 turns out to be dust-free. Consequently, the pure effect of the stellar pulsation (as simulated by the piston approximation) is studied. The composition of the gas is calculated by assuming chemical equilibrium and the radiative transfer problem is solved in grey approximation. In contrast to Fleischer et al. (1992), Planck mean gas opacities have been used, based on the line data for TiO, CO, H₂O and SiO beside several continuum opacity sources. The stellar parameters have not been chosen to describe any specific star, but just represent a typical model.

Since radiation pressure on molecules fails to accelerate the gas substantially ($a_{\text{rad}}/g < 0.3$), no further disturbances

Table 1. Observed molecular bands and derived quantities for various O-rich AGB stars including Miras and semi-regular variables. The excitation temperatures T_{exc} are deduced from the shape (i. e. the rotational fine-structure) of the bands. Consequently, T_{exc} reflects the rotational temperature of the lower vibrational state in case of an absorption feature, and of the upper vibrational state in case of an emission feature.

molecule	band [μm]	object	appearance	T_{exc} [K]	col. density [10^{17} cm^{-2}]	total number [10^{44}]	R [R_*]	n_{H_2} [cm^{-3}]	ref.
CO	4.6	SW Vir	em.	2160	1000	–	2	10^{11}	(1)
H ₂ O	2.7	β Peg	abs.	1250	70	–	2	–	(1)
	2.7	30g Her	abs.	1250	200	–	2	–	(1)
	2.7	SW Vir	abs.	1250	300	–	2	–	(1)
CO ₂	4.2	SW Vir	abs.	1250	1.2	–	2	–	(1)
	4.2	S Vir	abs.	1250	15	–	2	–	(1)
	4.2	RT Vir	abs.	1000	3	–	2	–	(1)
	13.5 – 16.2	(O-rich AGB)	abs./em.	650 – 1250	–	–	–	–	(2)
	13.9	R Crt	em.	650	–	350*	a few	–	(3)
	13.9	R Dor	em.	650	–	48*	a few	–	(3)
	15.0	R Crt	em.	160	–	12*	several 100	–	(3)
	15.0	R Dor	em.	150	–	0.97*	several 100	–	(3)
	15.0	R Cas	abs./em.	150	–	5.9*	several 100	–	(3)
	13.5 – 16.2	(O-rich AGB)	em.	600 – 700	10 – 100	~ 100	several	$10^{10} - 10^{12}$	(6),(5)
	13.5 – 16.2	W Hya	em.	1250	–	–	–	–	(6)
15.0	(O-rich AGB)	abs./em.	(different)	–	–	–	–	(6)	
SO ₂	7.3	UX Cyg	abs.	600	–	750	1.8	$> 4.4 \cdot 10^9$	(4)
	7.3	<i>o</i> Cet	em.	600	–	300	4.6	$> 1.0 \cdot 10^8$	(4)
	7.3	T Cep	abs./em.	600	–	1400 – 6800	4 – 5.8	$> 8.5 \cdot 10^8$	(4)

abs.: absorption feature, em.: emission feature, –: not stated, *: total number of molecules in the excited vibrational state. (1): Tsuji et al. (1997), (2): Justtanont et al. (1998), (3): Ryde et al. (1999), (4): Yamamura et al. (1999), (5): de Jong (1999), (6): Cami et al. (1997).

are introduced into the velocity field and the model exhibits a rather simple saw-tooth-like velocity structure and a step-wise decreasing density profile (see also Fleischer et al. 1992, Höfner et al. 1998). Due to the propagating shocks caused by the pulsation, a considerable time-dependent levitation of the atmosphere is achieved, i. e. the density is much larger than in the initial hydrostatic model (see top panels of Fig. 2).

The analysis of the composition of the gas in chemical equilibrium (Fig. 2, r.h.s.) reveals two distinct regions with enhanced molecular particle densities: a region close to the star ($1 \dots 1.2 R_0$) and a region further out ($1.6 \dots 2.1 R_0$, slightly dependent on the considered molecule). The second maximum is not present in the static model (l.h.s.) and is situated in a post-shock region. The polyatomic molecules are more strongly affected by the levitation since their concentrations depend on a larger power of the density. In comparison to the static model, the total amounts of molecules have increased by about 2% for CO, 25% for SiO, but by factors of about 5, 50, and 300 for CO₂, H₂O, and SO₂, respectively.

3. Molecular excitation temperatures

Based on the results of the time-dependent model (velocity field, gas density and temperature), several molecular excitation temperatures have been calculated. The non-LTE calculations are performed in a similar way as described by Woitke et al. (1996), but have been extended to polyatomic

molecules and improved in order to include the ro-vibrational pumping effect.

Detailed level energies and transition probabilities have been deduced from the HITRAN-database (Rothman et al. 1987), yielding 5000 ... 10 000 ro-vibrational levels and $\sim 30\,000$ lines for H₂O, CO₂ and SO₂ each. The radiative data for CO have been kindly provided by Jørgensen (1997, priv. comm.). The collisional rates for vibrational and rotational (de-)excitation are calculated by analytical formulae (Millikan & White (1964) and Hollenbach & McKee (1979), respectively) with more recent data for CO and H₂O. The code calculates two excitation temperatures (T_{rot} and T_{vib}) in order to achieve constancy in time of the total respective energies contained in the molecule in form of rotational and vibrational excitation, as demanded by the non-LTE statistical equations. The continuous background radiation field is assumed to be given by a radially diluted Planckian of stellar temperature, i. e. the outer atmosphere is assumed to be optically thin *in the continuum*. Optical depth effects in the lines are accounted for by applying Sobolev theory according to the local velocity gradient present in the model. More details will be described in a forthcoming paper.

Fig. 3 shows the results obtained for CO, H₂O, CO₂ and SO₂. The figure indicates that LTE ($T_{\text{g}} = T_{\text{vib}} = T_{\text{rot}}$) only holds very close to the star. As the gas density decreases with increasing distance from the star, first the vibrational temperatures T_{vib} decouple from T_{g} as soon as the gas density approaches a critical

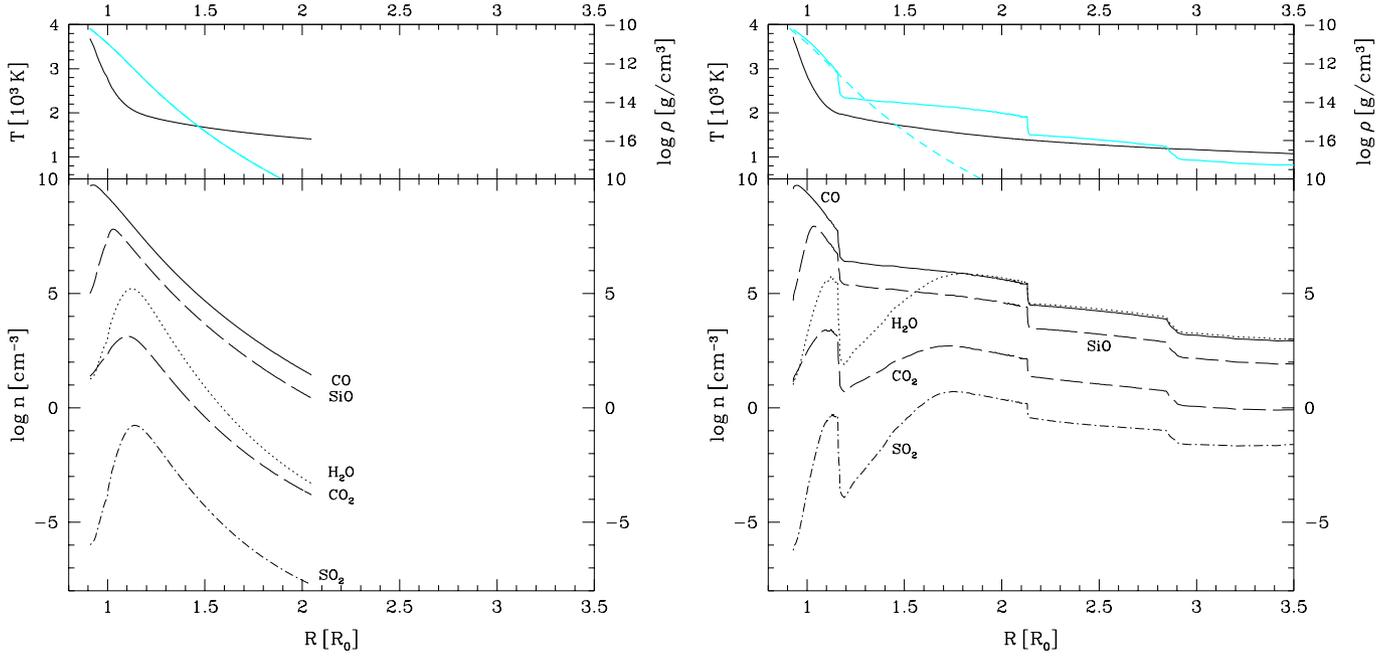


Fig. 2. Molecular number densities in the hydrostatic case (l.h.s.) and in the time-dependent hydrodynamic case (r.h.s.). The upper panel shows the temperature (full black) and the gas density (dashed grey = static, full grey = dynamic). The radial distance is given in units of the stellar radius R_0 of the initial model. The model parameters are the same as in Fig. 1.

value of $\sim 10^{12} \dots 10^{13} \text{ cm}^{-3}$. The rotational temperatures T_{rot} stay longer coupled to T_g , but finally deviate also substantially from T_g below a critical density of $\sim 10^8 \dots 10^{10} \text{ cm}^{-3}$, dependent on the molecule. This behavior is a consequence of the shorter radiative lifetimes of the vibrational levels and of the smaller collisional rates for vibrational de-excitation as compared to the respective rotational quantities.

In order to allow for a quantitative comparison to the results of radiative transfer calculations which adopt a static, uniform layer (see references in Table 1), we have calculated straight means of the calculated excitation temperatures¹ as defined by $\langle T_{\text{exc}}^{\text{mol}} \rangle = (\int_{r_1}^{r_2} n_{\text{mol}} T_{\text{exc}}^{\text{mol}} 4\pi r^2 dr) / (\int_{r_1}^{r_2} n_{\text{mol}} 4\pi r^2 dr)$. The integrations are carried out from the first shock front ($r_1 = 1.2 R_0$) to the outer boundary of the model ($r_2 = 3.5 R_0$). The results are summarized in Table 2. While the column densities of CO and H₂O agree with the observations within a factor of 3, the amounts of CO₂ and SO₂ molecules are too low, by factors of ~ 50 and $\sim 10^5$, respectively. The calculated excitation temperatures of H₂O are consistent with the observations. For CO, the calculated mean rotational temperature is a bit too low, but this value – only in case of CO – depends strongly on r_1 and would increase to 1930 K if $r_1 = 1.1 R_0$ was assumed. The mean rotational temperatures of CO₂ and SO₂ are too high in the model, roughly by a factor of 2.

Table 2 also shows the maximum of the calculated Sobolev optical depths τ_S^{max} of the individual ro-vibrational lines (see Woitke et al. 1996) of some vibrational bands at $1.7 R_*$, taking into account the actual velocity gradient. The individual lines

¹ More sophisticated means based on calculated line-ratios in the optically thin limit case lead to very similar results.

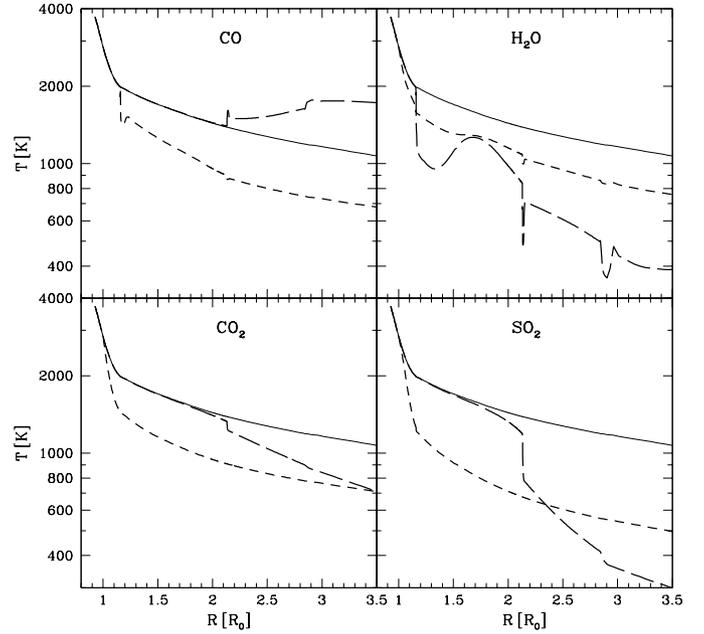


Fig. 3. Rotational (long dashed) and vibrational (short dashed) molecular excitation temperatures as function of radial distance. The full line shows the kinetic gas temperature, which is assumed to equal the grey temperature of the hydrodynamic model.

are mostly found to be optically thin, but some strong lines of CO and H₂O can exceed $\tau_S = 1$. If the molecular concentrations of CO₂ and SO₂ were multiplied by 50 and 10^5 (see above), the same would be found for these molecules.

Table 2. Calculated molecular properties (see text).

	$\langle T_{\text{rot}} \rangle$ [K]	$\langle T_{\text{vib}} \rangle$ [K]	col. density [10^{17}cm^{-2}]	tot. no. [10^{44}]	$\tau_{\text{S}}^{\text{max}}$ [band @ μm]
CO	1660	1200	310	8200	150 [4.6]
H ₂ O	1060	1190	94	3700	10 [2.7]
CO ₂	1480	1010	0.069	2.5	0.1 [4.2] 0.03 [15.0]
SO ₂	1290	740	0.00061	0.024	$5 \cdot 10^{-5}$ [7.3]

4. Discussion

The dynamical model presented here in fact exhibits a molecular “layer” at $r/R_* \approx 1.6 \dots 2.1$ with a total hydrogen particle density of $n_{\langle \text{H} \rangle} \approx 10^{10} \text{cm}^{-3}$. This total amount of levitated gas due to pulsations (also the calculated CO and H₂O column densities) agree reasonably well with the lower limits inferred from the observations (Table 1). In contrast, the *concentrations* of the CO₂ and SO₂ molecules (i. e. $n_{\text{SO}_2}/n_{\langle \text{H} \rangle}$) are not sufficient to explain the strength of the observed molecular bands. This different degree of agreement for different molecules provides a strong argument for chemical non-equilibrium effects. Especially for SO₂, the discrepancy is out of reach in the framework of equilibrium chemistry. Recently, Duari et al. (1999) have reported on higher CO₂ concentrations, if time-dependent shock-chemistry is considered.

A better agreement between theory and observations might be achieved if a lower kinetic gas temperatures close to the star was assumed. A gas temperature being 500 K lower than the grey equilibrium temperature of our model increases the column densities of CO, H₂O, CO₂ and SO₂ by factors of 1.03, 3.9, 4.2 and 2.5, respectively, and also lowers the rotational excitation temperatures, since they remain coupled to T_{g} in the relevant density range. Support for this idea comes from frequency-dependent radiative transfer calculations, which in fact show that the temperature in the outer parts of stellar atmospheres can be much lower than expected from the grey solution. A balancing of radiative heating and cooling in C-star envelopes leads to similar conclusions (Woitke & Sedlmayr 1999).

The stellar parameters (e. g. the surface gravity) have probably an important effect on the resultant total amount of levitated gas and their influence should be investigated more thoroughly. Furthermore, a larger pulsation amplitude should amplify the effect demonstrated in this letter, although the formation of molecular layers also occurs in case of very weak pulsations, since even small-amplitude waves steepen into strong shocks when they propagate through the exponential photospheric density gradient. Furthermore, dust formation will very likely increase the total amount of levitated gas (see e. g. Fleischer et al. 1992, Feuchtinger et al. 1993). A simultaneous occurrence of dust and molecular layers is suggested from an observed correlation between the CO₂ 15 μm band and the 13 μm dust feature

(Justtanont et al. 1998). The role of dust formation and the influence of the stellar parameters will be investigated in a forthcoming paper.

5. Conclusions

Dynamical models for the outer atmospheres for oxygen-rich AGB stars reveal a layered structure of the molecules and much higher column densities than predicted by hydrostatic models. This is a natural consequence of the shock waves occurring in these models, even in case of a low pulsational activity. The overall amount of levitated gas found in the model exceeds the lower limits inferred from observations. Therefore, the levitation by shock waves seems to provide a physical explanation for the generation of “warm molecular layers” as suggested by recent ISO observations, though it is not yet clear, whether this effect alone can explain the very large amounts of observed molecules. Other effects like dust formation and chemical non-equilibrium (in particular concerning SO₂ and CO₂) are probably involved.

The rotational excitation temperatures of CO, CO₂, and SO₂ are found to remain close to the kinetic gas temperature down to densities of $\sim 10^8 \text{cm}^{-3}$. Therefore, the observed rotational fine-structures of the vibrational bands of these molecules provide a reliable and easy-to-access probe for the kinetic gas temperature in the outer atmospheres of AGB stars. However, optical depths effects, velocity gradients, and vibrational non-LTE effects should be taken into account.

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