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LETTER

Letter to the Editor

On the formation of *warm molecular layers*

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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, H_2O, CO_2 and SO_2 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 $2 \ldots 16\,\mu$m) 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 CO_2, SO_2 and H_2O 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 $500 \ldots 2000$ 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.

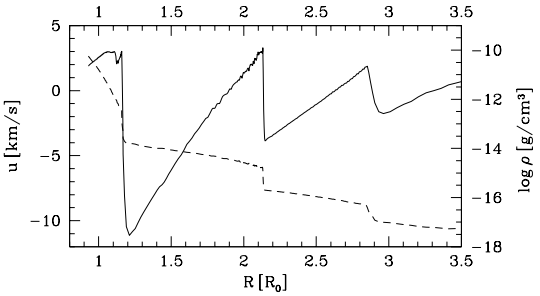

Fig. 1. Radial structure of an oxygen-rich time-dependent model at one instant of time (full line: velocity u, dashed line: gas density ρ). Model parameters: $T_* = 2800$ K, $L_* = 10^4\,L_\odot$, $M_* = 1\,M_\odot$, $C/O = 0.43$, piston amplitude $\Delta u = 2\,\mathrm{km\,s^{-1}}$, pulsation period $P = 650$ 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, H_2O 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 ($a_{\rm rad}/g < 0.3$), 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 $T_{\rm exc}$ are deduced from the shape (i. e. the rotational fine-structure) of the bands. Consequently, $T_{\rm exc}$ 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	$T_{\rm exc}$ [K]	col. density [10^{17} cm^{-2}]	total number [10^{44}]	R [R_*]	$n_{\rm H_2}$ [cm^{-3}]	ref.
CO	4.6	SW Vir	em.	2160	1000	–	2	10^{11}	(1)
H_2O	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	$>4.4\cdot10^9$	(4)
	7.3	o Cet	em.	600	–	300	4.6	$>1.0\cdot10^8$	(4)
	7.3	T Cep	abs./em.	600	–	$1400-6800$	$4-5.8$	$>8.5\cdot10^8$	(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 stepwise 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 ($1 \ldots 1.2\,R_0$) and a region further out ($1.6 \ldots 2.1\,R_0$, 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 CO_2, H_2O, and SO_2, 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 $5000 \ldots 10\,000$ ro-vibrational levels and $\sim 30\,000$ lines for H_2O, CO_2 and SO_2 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 H_2O. The code calculates two excitation temperatures ($T_{\rm rot}$ and $T_{\rm vib}$) 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, H_2O, CO_2 and SO_2. The figure indicates that LTE ($T_{\rm g} = T_{\rm vib} = T_{\rm rot}$) only holds very close to the star. As the gas density decreases with increasing distance from the star, first the vibrational temperatures $T_{\rm vib}$ decouple from $T_{\rm g}$ as soon as the gas density approaches a critical

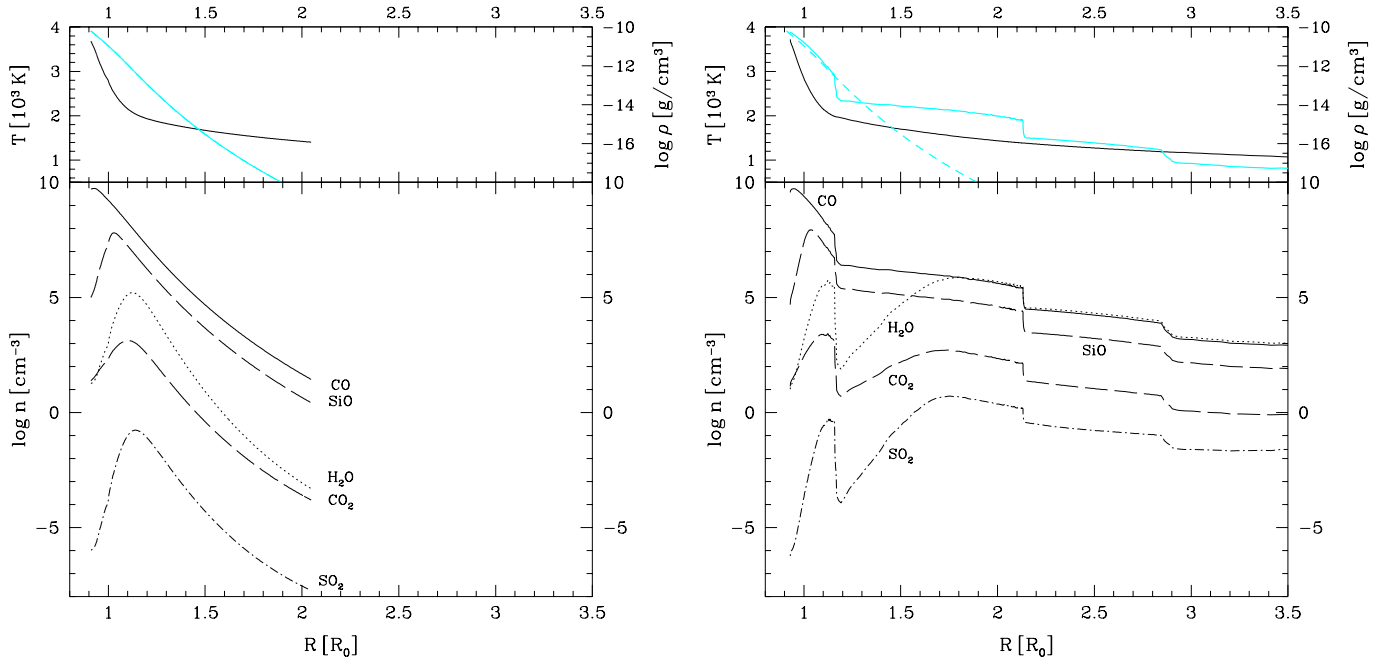

Fig. 2. Molecular number densities in the hydrostatic case (l.h.s.) and in the time-dependent hydrodynamic case (r.h.s.). The upper panel shows the temperature (full black) and the gas density (dashed grey = static, full grey = dynamic). The radial distance is given in units of the stellar radius R_0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

value of $\sim 10^{12}...10^{13}\,\mathrm{cm}^{-3}$. The rotational temperatures $T_{\rm rot}$ stay longer coupled to $T_{\rm g}$, but finally deviate also substantially from $T_{\rm g}$ below a critical density of $\sim 10^{8}...10^{10}\,\mathrm{cm}^{-3}$, 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 temperatures[1] as defined by $\langle T_{\rm exc}^{\rm mol}\rangle = (\int_{r_1}^{r_2} n_{\rm mol}\, T_{\rm exc}^{\rm mol}\, 4\pi r^2\, dr)/(\int_{r_1}^{r_2} n_{\rm mol}\, 4\pi r^2\, dr)$. 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 H_2O agree with the observations within a factor of 3, the amounts of CO_2 and SO_2 molecules are too low, by factors of ~ 50 and $\sim 10^5$, respectively. The calculated excitation temperatures of H_2O 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 CO_2 and SO_2 are too high in the model, roughly by a factor of 2.

Table 2 also shows the maximum of the calculated Sobolev optical depths $\tau_{\rm S}^{\rm max}$ 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 are mostly found to be optically thin, but some strong lines of CO and H_2O can exceed $\tau_{\rm S} = 1$. If the molecular concentrations of CO_2 and SO_2 were multiplied by 50 and 10^5 (see above), the same would be found for these molecules.

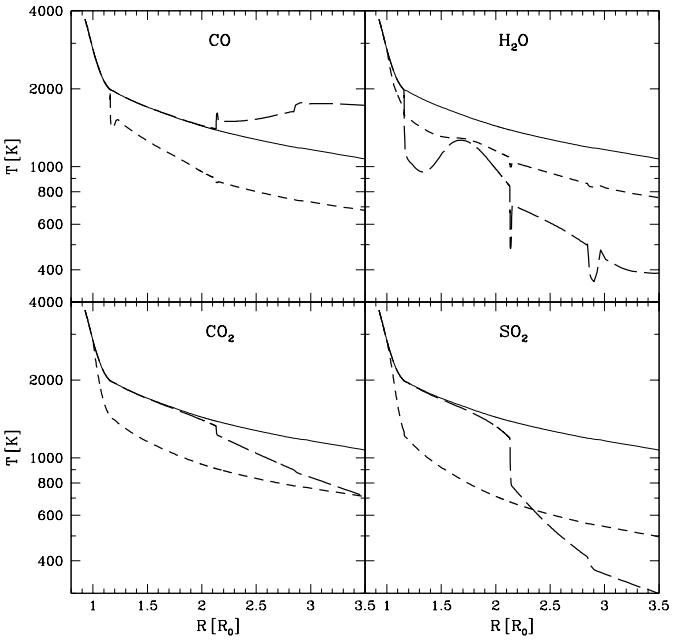

Fig. 3. Rotational (long dashed) and vibrational (short dashed) molecular excitation temperatures as function of radial distance. The full line shows the kinetic gas temperature, which is assumed to equal the grey temperature of the hydrodynamic model.

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

Table 2. Calculated molecular properties (see text).

	$\langle T_{\rm rot}\rangle$ [K]	$\langle T_{\rm vib}\rangle$ [K]	col. density $[10^{17}{\rm cm}^{-2}]$	tot. no. $[10^{44}]$	$\tau_{\rm S}^{\rm max}$ [band @ μm]
CO	1660	1200	310	8200	150 [4.6]
H_2O	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	$5\cdot10^{-5}$ [7.3]

4. Discussion

The dynamical model presented here in fact exhibits a molecular "layer" at $r/R_* \approx 1.6 \ldots 2.1$ with a total hydrogen particle density of $n_{<\rm H>} \approx 10^{10}{\rm cm}^{-3}$. This total amout of levitated gas due to pulsations (also the calculated CO and H_2O column densities) agree reasonably well with the lower limits inferred from the observations (Table 1). In contrast, the *concentrations* of the CO_2 and SO_2 molecules (i. e. $n_{\rm SO_2}/n_{<\rm H>}$) 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 SO_2, the discrepancy is out of reach in the framework of equilibrium chemistry. Recently, Duari et al. (1999) have reported on higher CO_2 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, H_2O, CO_2 and SO_2 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 $T_{\rm g}$ 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 occurence of dust and molecular layers is suggested from an observed correlation between the CO_2 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 SO_2 and CO_2) are probably involved.

The rotational excitation temperatures of CO, CO_2, and SO_2 are found to remain close to the kinetic gas temperature down to densities of $\sim 10^8{\rm cm}^{-3}$. 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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References

Cami J., Justtanont K., de Jong T., et al. 1997, 1st *ISO Workshop on Anal. Spectr.*, ed. A.M. Heras et al. , ESA SP-419, 159
Duari D., Cherchneff I., Willacy K., 1999, A&A 341, L47
Feuchtinger M.U., Dorfi E., Höfner S., 1993, A&A 273, 513
Fleischer A.J., Gauger A., Sedlmayr E., 1992, A&A 266, 321
Hollenbach D., McKee F., 1979, ApJS 41, 555
Höfner S., Jørgensen U.G., Loidl R., et al. 1998, A&A 340, 497
de Jong T., 1999, 2nd *Austr. ISO Workshop*, ed. J. Hron, S. Höfner, pp. 53
Justtanont K., Feuchtgruber H., de Jong T., et al. 1998, A&A 330, L17
Millikan R.C., White D.R., 1964, J. Chem. Phys. 39(4), 3209
Rothman L.S., Gamache R.R., Goldman A., et al. 1987, Applied Optics 26(19), 4058
Ryde N., Eriksson K., Gustafsson, B., 1999, A&A 341, 579
Tsuji T., Ohnaka K., Aoki W., et al. 1997, A&A 320, L1
Woitke P., Sedlmayr E., 1999, *IAU Symp. 191*, P. 3–17, (see http://export.physik.tu-berlin.de/∼woitke/arbeiten.html)
Woitke P., Krüger D., Sedlmayr E., 1996, A&A 311, 927
Yamamura I., de Jong T., Onaka T., et al. 1999, A&A 341, L9