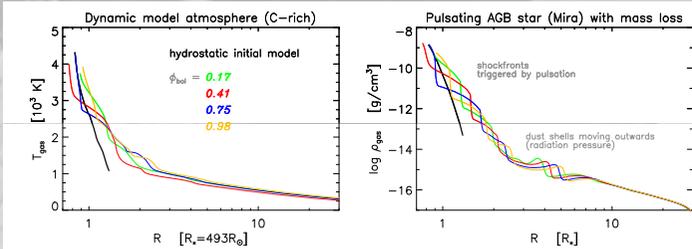


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## Motivation

The concept of warm molecular layers (**MOLspheres**) has been introduced in the late 1990s in order to explain excess absorption/emission features seen in infrared spectra of cool giants and supergiants (e.g. Tsuji et al. 1997). Now they are also used to interpret interferometric observations (e.g. Ohnaka 2004). The properties of such extra atmospheric layers are usually derived for individual molecular species independently. In this poster we discuss the spectroscopic and interferometric implications of such a layer for the TiO molecule when equilibrium chemistry is assumed.



**Figure 1:** Temperature and density structure of a representative, C-rich dynamic atmosphere (Höfner et al. 2003, Nowotny et al. 2005). The different colors denote different phases of the pulsation, the black line is a corresponding hydrostatic model. Note the large extension and the local maxima, which (between 1 and 2R<sub>\*</sub>) are the equivalent to a MOLsphere.

## MOLspheres and stellar pulsation

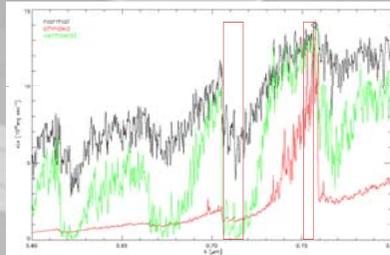
As has been convincingly already argued by Woitke et al. (1999), the levitation of the outer atmospheres of AGB stars by pulsation provides a physical explanation for the formation of a MOLsphere. This applies both to M-type and C-rich stars. The density and temperature structure of such a strongly pulsating atmosphere is illustrated in Fig. 1. Applying dynamic model atmospheres to interpret observations (see e.g. talks by Sacuto and Höfner) of Mira(like) stars thus allows a physically consistent treatment and limits the number of free parameters involved. For stars with much weaker pulsations, the (ad-hoc) addition of atmospheric layers can however provide first important clues on the properties of the upper atmosphere.

## MOLspheres and TiO

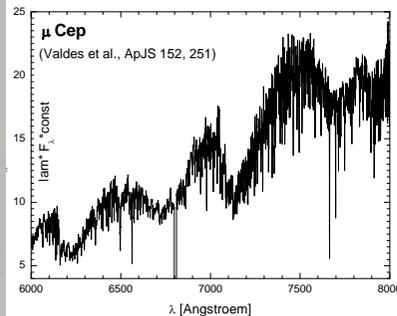
TiO is an especially interesting molecule for testing chemical equilibrium as it has a lot of opacity in the visual and is abundant in temperature/density regimes relevant for MOLspheres. Unfortunately, no star having (a) published parameters of a MOLsphere and (b) spectroscopy AND interferometry in strong TiO bands could be found. Thus we combined information for  $\alpha$  Ori and its „relative“  $\mu$  Cep (Ryde et al. 2006) to construct two test cases:

- (1) Ohnaka (2004) found that MIR diameters and spectra of  $\alpha$  Ori were best reproduced by a MOLsphere with  $T=2050K, R=1.45R_*$ , and  $n(H_2O)=2 \times 10^{20} \text{ cm}^{-2}$
- (2) Verhoelst et al. (2006) could model ISO-SWS spectra of  $\alpha$  Ori using a MOLsphere having  $T=1750K, R=1.45R_*, n(H_2O)=2 \times 10^{19} \text{ cm}^{-2}$

These two versions of a MOLsphere were then added to a hydrostatic model with  $T=3600K, M=15M_{\text{sun}}, \log g=0.0$ . Using *chemical equilibrium*, spectra (Fig. 2) and intensity profiles (Fig. 4) were calculated around strong TiO bands.



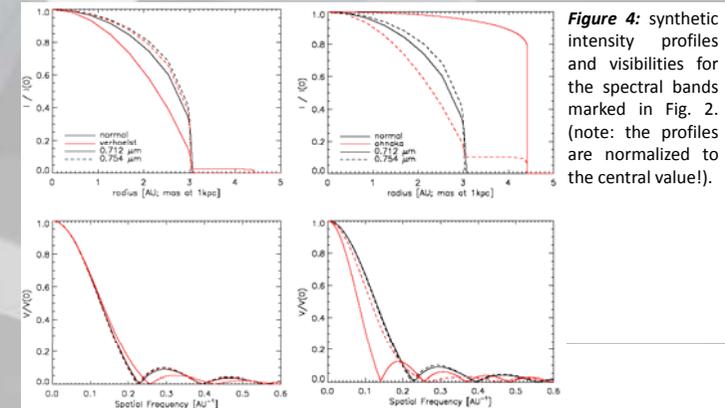
**Figure 2:** synthetic spectra for the hydrostatic model (black) alone and for the two versions with a MOLsphere added (red and green). Note the prominent TiO bands. The two rectangles mark the spectral ranges of the interferometric measurements by Quirrenbach et al. (1993).



**Figure 3:** observed spectrum of  $\mu$  Cep, the  $\alpha$  Ori analogon. Obviously, the **models with a MOLsphere show much too deep TiO bands** while the observed spectrum agrees quite well with a pure hydrostatic model.

## TiO Diameters

Quirrenbach et al. (1993) derived uniform disk radii for  $\mu$  Cep in a TiO band (712nm) and a nearby “continuum” region (754nm):  
 $R_{UD}(712\text{nm}) / R_{UD}(754\text{nm}) = 1.17 \pm 0.02$   
Using our models gives the following results:  
*No MOLsphere:* 1.01 *Verhoelst:* 0.95–0.97 *Ohnaka:* 1.40– 1.47 (range of results for UD-fits at  $V=0.3, 0.1$  &  $0.4$  and  $V>0.1$ )  
Thus **none of the models fits within the error bars**, although a MOLsphere with a density intermediate between our two adopted values might give compatible radii.



**Figure 4:** synthetic intensity profiles and visibilities for the spectral bands marked in Fig. 2. (note: the profiles are normalized to the central value!).

## Conclusions

Assuming chemical equilibrium, the MOLspheres of our test cases are incompatible with observed spectra and probably also diameters. Possible solutions are:

- Adopting frozen chemistry (i.e.  $n(\text{TiO})/n(\text{H}_2\text{O})$  of the MOLsphere and of the outermost atmospheric layer are the same) makes the situation even worse. As TiO is a very stable molecule a strong depletion in the MOLsphere seems unlikely, though detailed non-equilibrium calculations are needed.
- Spots instead of a full MOLsphere might be reconciled with the observations, provided the spot filling factor is low enough. In this case variability with time/position angle is to be expected.
- Finally, the approximation of a constant temperature and density in the MOLsphere might be too crude and more elaborate scenarios should be used.