Letter to the Editor

Infrared emission of hot water in the atmosphere of Mira[⋆]

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Abstract. The ISO/SWS spectrum of o Cet taken at its maximum exhibits an absorption-like feature between 3.5 and 4.0 μm. We present evidence that the feature is due to emission of H_2O and SiO molecules, in a layer extended to about two stellar radii with an excitation temperature of 2000 K. These hot molecules are also observed in a spectrum of Z Cas near minimum, but this time in absorption. A simple plane-parallel model is used to fit the spectra of these two stars. The H_2O column densities and excitation temperatures in the layers are found to be similar in both stars. The difference of the H_2O band is thus primarily due to the layer size. The H_2O layers seem to be more extended at visual maximum, probably related to the stellar pulsation. The estimated lower limit to the local gas density in the layers of $\sim 10^{11}$ cm^{-3} is in good agreement with theoretical predictions from dynamical model atmospheres.

Key words: stars: AGB and post-AGB – stars: atmospheres – stars: late-type – infrared: stars

1. Introduction

Model calculations of the atmospheres of pulsating AGB stars suggest that these atmospheres are quite extended (e.g., Höfner et al. 1998). Matter lifted by pulsation shocks slowly propagates through this extended atmosphere, and is eventually ejected in the circumstellar envelope. Recent space-borne infrared observations have revealed the complicated nature of this region. Based on observations by the Short-Wavelength Spectrometer (SWS; de Graauw et al. 1996) onboard the Infrared Space Observatory (Kessler et al. 1996), Tsuji et al. (1997) confirmed the presence of the "warm molecule forming region" (T_{ex} = 750–1250 K) located above the photosphere in M-type giants, including the M2 irregular variable β Peg. Matsuura et al. (1999) also

detected the water absorption in six stars earlier than M6, using two spectrometers onboard the Infrared Telescope in Space (IRTS; Murakami et al. 1996). Detections of SO_2 (Yamamura et al. 1999) by ISO/SWS have provided further insight into the extended atmosphere. According to Yamamura et al. (1999) the SO_2 molecules are located typically at 5 R$_\star$ with an excitation temperature of ~ 600 K. The variation of the SO_2 band in T Cep does not correlate with the optical variability of the star, indicating that complicated dynamical processes and/or non-equilibrium chemistry are taking place in the extended atmosphere. In addition, the estimated gas density of the SO_2 layer is about 2 orders of magnitude higher than that expected from theoretical models (Bessell et al. 1996; Höfner et al. 1998). Similar conclusions are drawn from the analyses of CO_2 bands (Cami et al. 1997; Ryde et al. 1999).

H_2O is one of the most abundant molecules in the atmospheres of O-rich red giants. However, because of the large opacity of the terrestrial atmosphere, observations of H_2O bands from the ground have been quite difficult. In this paper, we study the near-infrared H_2O band as a probe of the extended atmosphere of Mira variables, based on the data obtained by the ISO/SWS.

2. Observational result

Data are taken from the ISO guaranteed time program AGB-STARS (P.I. T. de Jong), using the SWS full-grating scan mode (AOT 01, speed 1–3), which covers the wavelength range between 2.38–45.2 μm with a resolution of $\Delta\lambda/\lambda = 300$–$1000$ (depending on the wavelength and scanning speed). Data are reduced using the SWS Interactive Analysis package developed by the SWS Instrument Dedicated Team. The calibration parameters as of April 1998 are used for wavelength, detector responsivity, and absolute flux calibration. Small residuals in flux level between different instrumental bands are corrected by scaling the bands with respect to band 1B (2.6–3.0 μm). The correction factor is always within a few% in band 1 ($< 4\,\mu$m) and up to 15% in band 2 ($> 4\,\mu$m).

In Fig. 1 we show the spectra of two O-rich Mira variables, o Cet and Z Cas, between 2.4 and 5.3 μm. The molecules H_2O,
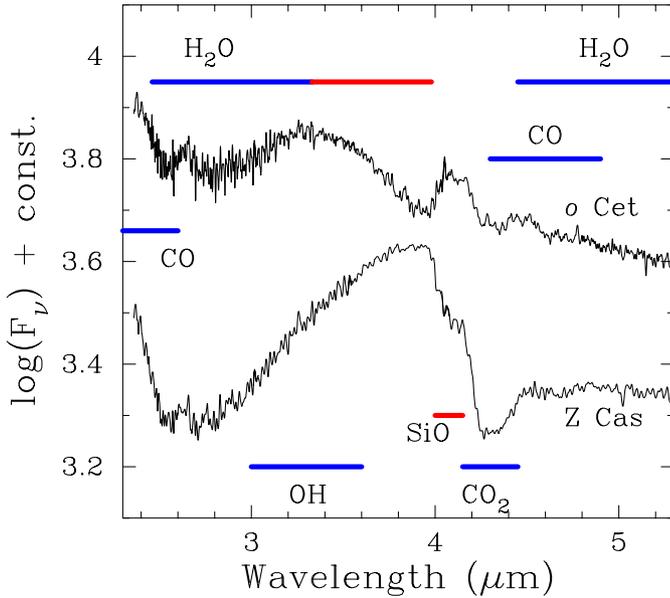
Fig. 1. ISO/SWS spectra of two oxygen-rich Miras between 2.4–5.3 μm. The spectral resolution is about 600 for o Cet and 300 for Z Cas. Identifications for the major spectral features are indicated.

Fig. 2. Synthesized spectra of H$_2$O for different layer sizes R (in units of R$_\star$), placed on top of a 3000 K blackbody. We adopted $N = 3.0 \times 10^{21}$ cm^{-1} and $v = 5$ km s^{-1} for all cases. The background blackbody is indicated by the grey line. Spectra are smoothed to a resolution of 600. The relative flux levels of the three spectra for $T = 2000$ K and the blackbody are correct. The spectrum for $T = 1200$ K is lowered by 0.4 dex.

SiO, CO, OH, and CO$_2$ provide the major opacity sources in this wavelength region. o Cet and Z Cas were observed at maximum ($\phi = 0.99$) and near minimum ($\phi = 0.50$) of their visual magnitude, respectively. It is striking that o Cet shows a distinct absorption-like feature around 3.8 μm, while Z Cas shows a rather smooth rise in the wing of a deep H$_2$O absorption. There are not many molecules which have transitions in this wavelength range. Sulfur-bearing molecules such as H$_2$S, SH, or CS are potential candidates in view of the presence of the SO$_2$ band in o Cet (Yamamura et al. 1999). However, none of these molecules can explain the observed absorption in o Cet. Although we cannot rule out the possible presence of these species in the star, it is unlikely that these molecules are responsible for this "3.8 μm feature".

Instead, we found that the profile between 3.5 and 4.0 μm in o Cet is explained by emission of hot H$_2$O. If the molecular layer is extended well beyond the star, and the excitation temperature is high enough, the bands can be seen in emission, as is the case for SO$_2$ (Yamamura et al. 1999). The observed spectrum of o Cet in the 3.5–4.0 μm region is in good agreement with the emission spectrum of H$_2$O at 2000 K, while that of Z Cas is consistent with the absorption spectrum at the same temperature (see Fig. 2). In addition, we also identified the SiO first-overtone band at 4 μm in emission in o Cet, while it is in absorption in Z Cas. These observational results suggest that a molecular layer as hot as 2000 K is present in the extended atmosphere of o Cet, while it is located close to the photosphere in Z Cas.

3. Modeling

We have modeled the spectra of o Cet and Z Cas in a very simple manner. The model is basically the same as that used by
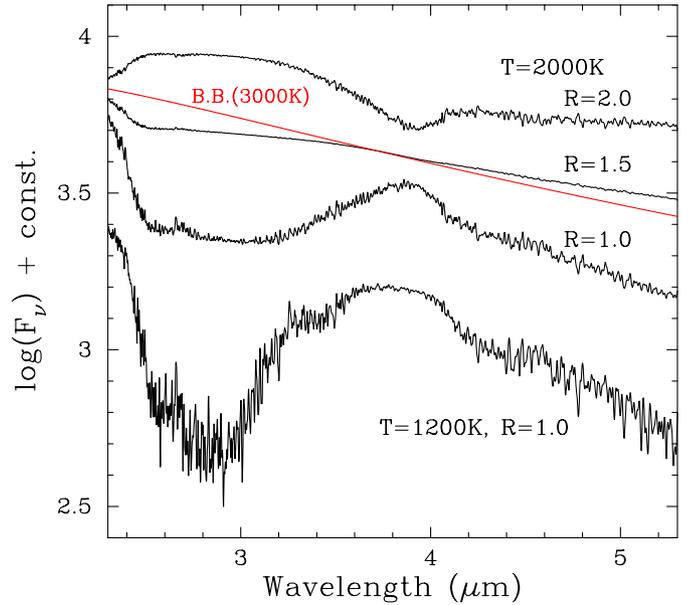
Yamamura et al. (1999) to model the SO$_2$ band. Plane-parallel, uniform molecular layers are laid one over the other, and radiative transfer through the layers is calculated. Energy level populations of molecules are calculated by assuming LTE (local thermodynamic equilibrium). Each layer is described by four parameters, T: the excitation temperature, N: the column density, v: the Gaussian line width, and R: the radius of the layer (in units of the stellar radius). If one layer is larger than the layers below, it causes extra emission. Fig. 2 demonstrates how the size parameter R affects the spectrum. In this example, three synthesized spectra of H$_2$O at 2000 K and $N = 3 \times 10^{21}$ cm^{-2}, placed on top of a 3000 K blackbody star are presented. In this particular case, the additional emission compensates the absorption when $R = 1.5$ R$_\star$ so that an almost flat spectrum results. The spectrum turns to emission for larger values of R. A spectrum of cooler H$_2$O at $T = 1200$ K is also shown in Fig. 2. Such a cool H$_2$O layer is necessary to reproduce the absorption at the band center, and does not contribute to the 3.5–4.0 μm region. The very highly-excited lines that appear in this wavelength range are only included in a few, recently calculated line lists, one of which by Partridge & Schwenke (1997) is used in the present calculations.

In the model, two (hot and cool) H$_2$O layers are considered. It is reasonable to assume that the temperature decreases with distance from the star. Therefore, we place the cool layer on top of the hot layer, and hence it is more extended than the hot layer. We do not take the molecules behind the star into account, since the hot H$_2$O layer is so optically thick and masks

the components behind it. The cool layer mainly contributes as an absorber against this hot layer. Our preliminary calculations with spherical geometry confirm that the results by the plane-parallel model do not differ from spherical model by more than the uncertainties of the parameters.

We applied a constant line width of $v = 5\,\mathrm{km\,s^{-1}}$ for all layers. This is a rather arbitrary assumption, but the value adopted is consistent with the result of Hinkle & Barnes (1979). The blackbody temperature of the star is fixed at 3000 K. The model spectra are hardly affected by the stellar temperature, because of the high opacity of the hot H_2O layer.

The parameters of each layer can be determined uniquely. The hot H_2O contributes to the spectrum exclusively between 3.5–4.0 μm. Column density and layer size are constrained by the slope and amplitude of the small features of the spectrum. The parameters for the cool H_2O layer are constrained from the band center region. The fits are evaluated by eye-fitting and a χ^2-test. The parameters were searched in a rather rough grid spacing (steps of 200 K in T, factors of 2 for N, and steps of 0.1 $\mathrm{R_\star}$ in R). The results are thus uncertain by these step sizes.

Besides H_2O, we consider SiO (Glenar et al. 1985; Langhoff & Bauschlicher 1993), and CO_2 (Rothman et al. in preparation) to improve the spectrum between 4.0–4.5 μm. The parameters for these molecules are less constrained. We assume that SiO co-exists with hot H_2O, and thus apply the same T and R. Only N is adjusted. CO_2 is placed on top of the cool H_2O layer. Since the radius of the CO_2 layer is poorly constrained by our model fitting procedure, we assumed the same R as for the cool H_2O layer. With this assumption, T and N are well determined, although the N obtained should be regarded as a lower limit. Other molecules, namely CO and OH, are not included, since their parameters are not constrained in the present model fits. CO at 2000 K only contributes in the wavelength range shortward of $\sim 2.6\,\mu$m and longward of 4.3 μm, which we ignored in the fitting. OH exhibits sharp lines between 2.5–4.0 μm, but it does not affect the shape of the spectrum.

The obtained parameters are summarized in Table 1, and the synthesized spectra are presented in Fig. 3 together with the contributions of the individual layers.

4. Discussion

The results of the present model analysis show that the differences of the H_2O bands in the spectra of two stars are primarily caused by differences in their layer sizes, and that the temperatures and the column densities are similar in two stars. Although these are the results of two different stars, we suspect that the H_2O layers in Mira variables are generally more extended at maximum than at minimum. Indeed, time variations of the SWS spectra of Z Cyg (Onaka et al. 1998) show that the H_2O absorption bands are deeper at minimum.

It is interesting to compare the present results with the previous study by Hinkle & Barnes (1979), based on high-resolution spectroscopy of the 1.9 μm H_2O band in R Leo. They detected two distinct components with excitation temperatures of 1700 and 1150 K, similar to the temperatures in our two layers. How-
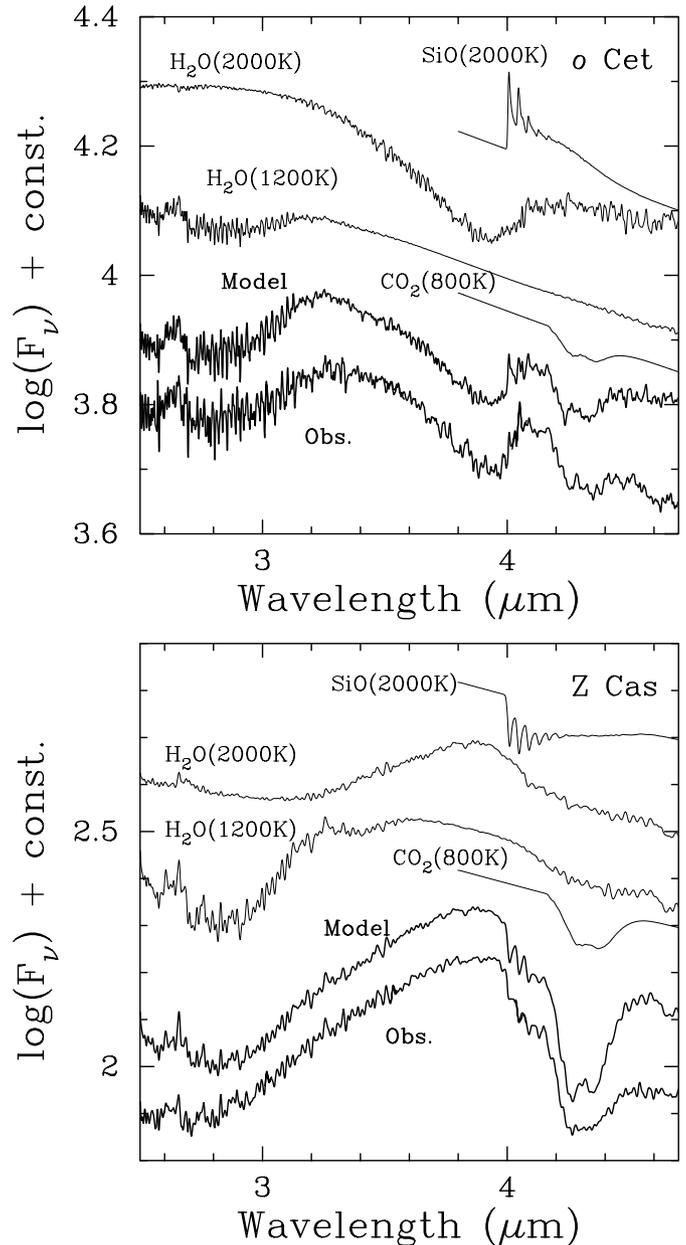

Fig. 3. The SWS spectra of o Cet (*upper-panel*) and Z Cas (*lower-panel*) in 2.5–4.5 μm region are compared with the model spectra. The individual contributions of hot H_2O and SiO, cool H_2O, and CO_2 are also shown. Since the model spectrum is the result of radiative transfer through the layers from top (2000 K SiO and H_2O) to bottom (CO_2), it is not the simple sum of these components. Discrepancies between models and observations at both end of the plots are due to lack of CO in the model.

ever, the column density of their warm component (1700 K) of $3 \times 10^{20}\,\mathrm{cm^{-2}}$ is a factor of 10 smaller than our result. Furthermore, they found that the warm component disappears when the star is at maximum, which they explained by strong pulsation shocks dissociating H_2O molecules in the layer. The present study shows that o Cet holds large amounts of H_2O in its hot layer even at maximum.

Table 1. Properties of the stars and results of modeling.

Object	o Cet			Z Cas		
Sp. Type[1]	M5e–M9e			M7e		
Period[1]	331.96d			495.71d		
	$N(\mathrm{cm}^{-2})$	$T(\mathrm{K})$	$R(\mathrm{R}_\star)$	$N(\mathrm{cm}^{-2})$	$T(\mathrm{K})$	$R(\mathrm{R}_\star)$
H$_2$O (hot)	$3.0\,10^{21}$	2000	2.0	$3.0\,10^{21}$	2000	1.1
SiO	$1.0\,10^{21}$	2000†	2.0†	$1.0\,10^{22}$	2000†	1.1†
H$_2$O (cool)	$3.0\,10^{20}$	1400	2.3	$1.0\,10^{21}$	1200	1.7
CO$_2$	$2.0\,10^{17}$	800	2.3†	$1.5\,10^{18}$	800	1.7†
$\mathcal{N}_{\mathrm{H_2O}}$ (hot)	$2.7\,10^{49}$			$8.3\,10^{48}$		
$\mathcal{N}_{\mathrm{H_2O}}$ (cool)	$3.6\,10^{48}$			$6.6\,10^{48}$		
$n_{\mathrm{H_2O}}$ (hot)	$4.8\,10^7$ cm^{-3}			$3.0\,10^8$ cm^{-3}		
$n_{\mathrm{H_2O}}$ (cool)	$1.1\,10^7$ cm^{-3}			$2.2\,10^7$ cm^{-3}		
Phase[2]	0.99			0.50		

[1] Taken from General Catalogue of Variable Stars (Kholopov et al. 1988).
[2] Based on AAVSO light curves.
† Assumed (see text).

Hinkle & Barnes also observed that the velocity variation of their warm H$_2$O component is similar to that of the photosphere, traced by hot CO and OH (Hinkle 1978). These velocity variations imply that the photosphere is most extended around minimum, and shrinks toward maximum, with gas falling-back velocities up to $20\,\mathrm{km\,s^{-1}}$. This is in the opposite sense from our result.

Unfortunately, R Leo was never visible for ISO and a direct comparison is not possible. This inconsistency between the two studies, at least partly, arises from the fact that we are comparing different stars. In addition to this, however, we suggest that the high-resolution measurements at short wavelengths by Hinkle & Barnes (1979) actually probe the inner region of the atmosphere, and that our hot component is located further out in the region, where matter behaves differently. Theoretical calculations of dynamical atmospheres by Bessell et al. (1996) and Höfner et al. (1998) show that there is a significant phase lag between the motions at inner and outer parts of the atmosphere.

The total numbers of H$_2$O molecules in the hot and cool layers of o Cet are estimated as $\mathcal{N} = N \cdot \pi R^2 = 2.8 \times 10^{49}$ and 3.6×10^{48}, respectively. Assuming that the molecules are uniformly distributed in shells between $R = 1.0$ and 2.0, and $R = 2.0$ and 2.3, we obtain average H$_2$O densities of $n = 4.8 \times 10^7$ and $1.1 \times 10^7\,\mathrm{cm^{-3}}$, which can be further converted to lower limits to the local gas density of $n_{\mathrm{H_2}} \sim 1.6 \times 10^{11}$ and $3.7 \times 10^{10}\,\mathrm{cm^{-3}}$, by assuming an abundance of H$_2$O of $\sim 3 \times 10^{-4}$. These numbers are comparable with the value expected from dynamic model atmospheres (Bessell et al. 1996; Höfner et al. 1998).

In summary, our analysis indicates that the hot molecular layer of $\sim 2000\,\mathrm{K}$ extends out to two stellar radii in o Cet. It is suggested that the near-infrared H$_2$O band is useful probe of the inner region of the extended atmosphere. For better understanding of the physics and chemistry taking place in the region (see resent theoretical approach by Woitke et al. 1999), further investigations based on larger samples, especially time variation data, are needed.

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