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ASTRONOMY AND ASTROPHYSICS

LETTER

Letter to the Editor

Detection of warm SO_2 gas in oxygen-rich AGB stars*

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Abstract. We report the discovery of the ν_3 band of SO_2 at 7.3 μm in the ISO/SWS spectra of oxygen-rich AGB stars. The band is clearly detected in three stars, UX Cyg, *o* Cet and T Cep, and marginally detected in at least four other stars. The band is seen in absorption in UX Cyg, while it is in emission in *o* Cet. Seven spectra of T Cep taken at different phases show that the feature changes from emission to absorption on a time scale of twice the pulsation period. Using an LTE model, we find that the excitation temperature of SO_2 is typically 600 K, and that in T Cep the molecule occupies a region with dimensions of several stellar radii. The total number of molecules contained in this region is of order 10^{47}, which requires a local gas density of at least 10^9 H_2 cm^{-3}, and possibly up to 10^{11} H_2 cm^{-3} depending on the SO_2 abundance. The variation with phase of the T Cep spectra can be explained by photodissociation of SO_2 molecules by soft UV photons.

Key words: stars: AGB and post-AGB – stars: atmospheres – stars: circumstellar matter – stars: late-type – stars: mass-loss – infrared: stars

1. Introduction

Recent observations with the Infrared Space Observatory (ISO; Kessler et al. 1996) have greatly enhanced our knowledge of the atmospheres and circumstellar envelopes of late-type giant stars (see Justtanont et al. 1996, Barlow et al. 1996, Cernicharo et al. 1996). One of the most remarkable discoveries made with the ISO Short Wavelength Spectrometer (de Graauw et al. 1996) are the CO_2 emission bands detected in the 13–17 μm wavelength region of oxygen-rich AGB stars (Cami et al. 1997, Justtanont et al. 1998, Ryde et al. 1998). These bands are commonly detected in Miras and semi-regular variables with relatively small mass-loss rates ($\leq 10^{-7}$ $M_\odot$ yr^{-1}), exhibiting the 13 μm dust feature. Preliminary modeling indicates that the CO_2 bands are formed in a dense warm molecular gas layer, probably located at a few stellar radii in between the stellar photosphere and the circumstellar envelope. The existence of such a layer has been postulated by Tsuji et al. (1997) and could be generated by pulsation shocks just above the stellar photosphere (see Bowen 1988, Bessel et al. 1996).

In this letter, we report the detection of another dioxide molecule, SO_2, in the ISO/SWS spectra of oxygen-rich AGB stars. SO_2 has been detected before in the circumstellar envelopes of some oxygen-rich stars by mm and sub-mm observations of its pure rotational transitions (Lucas et al. 1986, Guilloteau et al. 1986, Omont et al. 1992). However, this is the first detection ever of ro-vibrational bands of SO_2 in the spectra of cool giants stars.

2. Observational result

The data were obtained using the SWS/AOT01 observing mode which provides full-grating spectra from 2.38 to 45.2 μm with a resolution of 300–1000 (depending on scan speed and wavelength). The data were reduced with the SWS Interactive Analysis package developed by the SWS Instrument Dedicated Team using the most recent set of calibration parameters (as of April 1998).

In the guaranteed time program AGBSTARS (P.I. T. de Jong) we observed a sample of 35 AGB stars with a wide range of mass-loss rates and chemical compositions (Justtanont et al. 1996, Yamamura et al. 1998). Only recently we found a remarkably strong absorption band of SO_2 at 7.3 μm in the spectrum of one of the O-rich Mira variables, UX Cyg (M5, period 560 d). A successive careful search for this band in the other stars resulted in a definite detection in *o* Cet (M7IIIe, period 325 d) and at least four additional marginal detections (R Cen, RX Boo, Z Cas, π^1 Gru) out of 10 O-rich Mira/semi-regular variables and 4 S-type stars. The spectra of UX Cyg and *o* Cet between 6.5 and 8.5 μm are shown in Fig. 1. The band is seen as a deep absorption in UX Cyg, while it is in emission in *o* Cet.

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The 7.3 μm SO_2 band is also detected in the Mira variable T Cep (M7IIIe, period 393 d). This star has been monitored over 16 months with the ISO/SWS in the open time program TIMVAR (P.I. T. Onaka) using the AOT01 observing mode (Onaka et al. 1997). Seven observations were carried out with a phase interval of about 0.2 (Table 1). In T Cep, the SO_2 band is seen in emission at the first minimum, then decreases in intensity around maximum and turns to absorption at the next minimum.

SO_2 has several ro-vibrational bands in the wavelength region covered by the SWS. The $\nu_3 + \nu_1$ band at 4.0 μm is also detected in UX Cyg, but all bands other than the ν_3 one are contaminated by other spectral features such as the SiO first overtone band at 4.1 μm and the 10 and 18 μm silicate dust features, and are not suitable for detailed analysis.

3. Spectral modeling

A simple plane-parallel LTE model has been developed to derive physical parameters for the SO_2 layer. The geometry adopted is illustrated in Fig 2. The star is assumed to radiate like a blackbody. Molecular layers with uniform excitation temperatures and densities are placed in front of the star and radiative transfer is calculated through these layers one by one. The layer can be extended beyond the star in order to reproduce the emission feature. The molecular layer is thus characterized by a set of four parameters: the excitation temperature (T), the column density (N), the turbulent velocity ($v_{\rm turb}$) and the radius of the layer (R). In the present calculation a constant turbulent velocity, $v_{turb} = 3$ km s^{-1}, is assumed for all molecular layers. The resulting spectrum is not much affected by v_{turb} as long as it is within a factor two from the value adopted. The infrared line data for SO_2 are taken from the HITRAN database (Rothman et al. 1996). The list contains 3818 lines in the ν_3 band of $^{32}S^{16}O_2$ with energies of the lower levels up to about 1745 cm^{-1}. We have also included the molecules H_2O and SiO in the modeling because they affect the shape of the baseline spectrum. Since these molecules are assumed to be in or just above the photosphere we adopt $R_{\rm H_2O} = R_{\rm SiO} = R_\star$.

In the modeling we first adjust the blackbody temperature of the star and the H_2O and SiO parameters to reproduce the background spectrum. A relatively high temperature of 3000 K is necessary to reproduce the T Cep spectra. Somewhat lower temperatures of 1500 K and 2000 K are used for UX Cyg and *o* Cet, respectively. The three independent parameters for the SO_2 layer ($T_{\rm SO_2}$, $N_{\rm SO_2}$, $R_{\rm SO_2}$) can be determined separately. $R_{\rm SO_2}$ determines whether the feature is seen in emission or absorption. A higher excitation temperature broadens the band shape. The column density affects the strength of the feature as well as the shape of the band. This is because part of the SO_2 lines are optically thick and saturated. Larger column densities increase the number of saturated lines while the relative contributions of the saturated and the unsaturated lines in the band affect the global shape of the feature. Model spectra are calculated with various sets of parameters exploring a reasonable fraction of parameter space and the results are evaluated by a χ^2 test of the residual as well as by eye-fitting. The best fit model spectra are shown in Fig. 1 by dotted lines overlaying the observations. The estimated error of the parameters are ± 100 K for $T_{\rm SO_2}$, a factor of two for $N_{\rm SO_2}$, and about 5% in $R_{\rm SO_2}$.

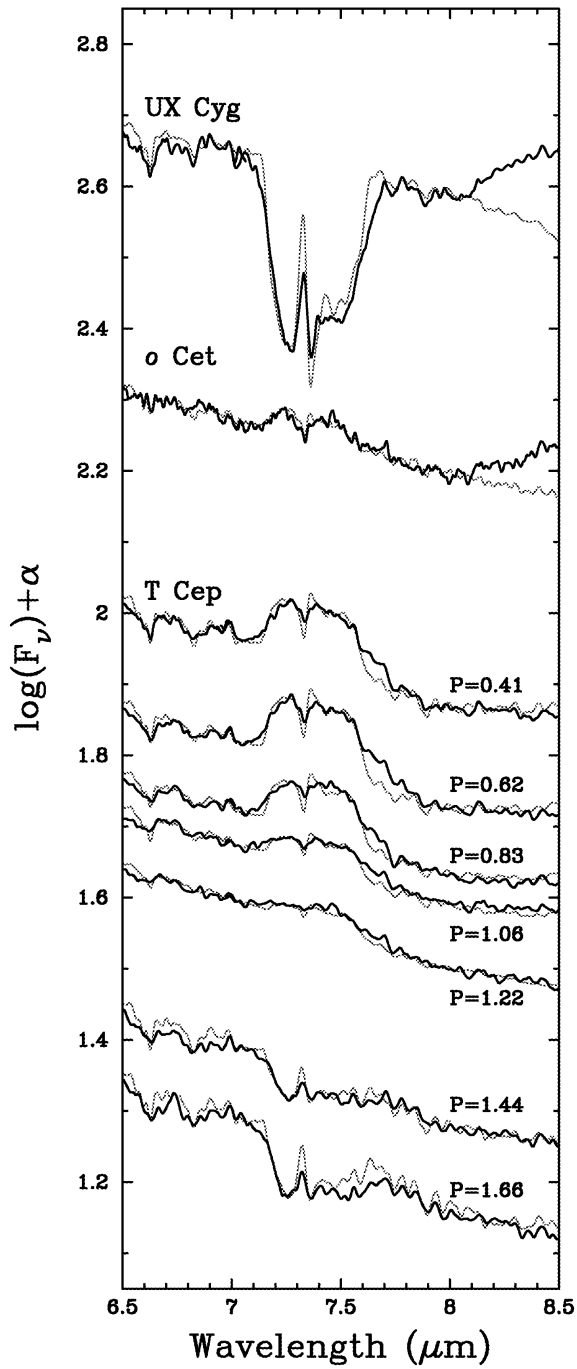

Fig. 1. ISO/SWS spectra (*thick solid line*) and the best fit models (*thin dotted line*) of the SO_2 ν_3 band in three oxygen-rich Miras. The spectral resolution is about 500 for *o* Cet and 300 for the other stars. The phase of the observations is indicated for T Cep. The discrepancy between the models and the observations in the wings of the band is due to lack of line data at high energy levels.

We find that an excitation temperature of 600 K gives the best results for all spectra fitted. The column density can be

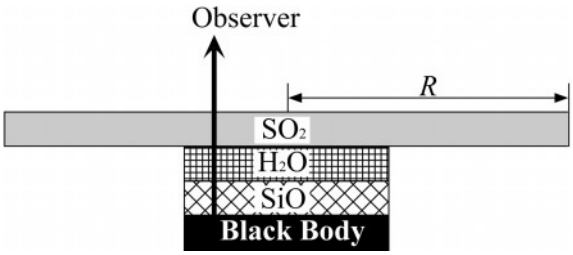

Fig. 2. Geometry adopted in the model calculation.

translated into the total number of SO_2 molecules by $\mathcal{N}_{SO_2} = N_{SO_2}\,\pi\,(R_{SO_2})^2$, and the average density of SO_2 molecules in the shell between the stellar surface and R_{SO_2} equals $n_{SO_2} = \mathcal{N}_{SO_2}/(4/3\pi\,\{(R_{SO_2})^3 - (R_\star)^3\})$.

The numbers derived are listed in Table 1. We have assumed the same stellar radius $R_\star = 3.0 \times 10^{13}$ cm for all stars.

4. Discussion

The results of our simple model analysis suggest that the SO_2 molecules are located in a region just above the stellar atmosphere within a few stellar radii from the surface of the star, where the temperature is typically 600 K. A crude estimate of the gas density in this region can be made based on the derived value of the SO_2 density, n_{SO_2}. Although the abundance of the SO_2 molecule is not known, the high number density found from the model fitting suggests that a large fraction of the sulfur atoms is in the form of SO_2. Assuming that all sulfur is in SO_2 and that the sulfur abundance is little affected by dredge-up processes in low- and intermediate-mass stars, we may adopt the cosmic abundance, $\mathrm{S/H} = 1.5 \times 10^{-5}$, as an upper limit for the SO_2 abundance. We then find lower limits to the hydrogen gas density of $n_{H_2} = 4.4 \times 10^9$ cm^{-3} (UX Cyg), 1.0×10^8 cm^{-3} (o Cet), and 8.5×10^8 cm^{-3} (T Cep, average), respectively. In a more realistic model calculation Beck et al. (1992) find a SO_2 peak abundance of a few times 10^{-6} which would raise the gas densities by about one order of magnitude. Also, if the SO_2 molecules are concentrated in a thin shell at R_{SO_2} or in clumps, rather than uniformly distributed above the photosphere, this would further increase the estimated gas density. We therefore conclude that the local gas density in the SO_2 layer is very likely in the range $10^{11} - 10^{12}$ cm^{-3}.

We note that the detailed model analysis of five CO_2 emission bands in the high-resolution (AOT06) ISO/SWS spectrum of the O-rich AGB star EP Aqr by Cami et al. (1997) indicate the existence of an extended molecular layer with temperatures and densities similar to those derived here for the SO_2 layer. Recently, Reid and Menten (1997) reported the detection of radio continuum emission from Mira. They explained this as due to a "radio photosphere" at 5–6 stellar radii with a Hydrogen gas density of about 10^{12} cm^{-3}, in quite good agreement with the picture that results from our analysis.

In Fig. 3 we plot values of $\mathcal{N}_{SO_2}$ and of R_{SO_2} for T Cep as a function of the optical phase. The plot shows that the total number of SO_2 molecules around T Cep decreases to about 20% of the maximum value in one year, and that simultaneously R_{SO_2} shrinks by about 30%. We note that the CO_2 emission features in T Cep increase in strength with time (see also Onaka et al. 1997). Modeling the CO_2 emission features using a model similar to that used for SO_2 indicates that the total number of CO_2 molecules is one order of magnitude smaller than the number of SO_2 molecules, and probably increases while SO_2 decreases. The process which destroys SO_2 apparently does not affect the CO_2 molecules. It is even conceivable that the oxygen atoms released from SO_2 are used to form additional CO_2 molecules.

One possible destruction process of SO_2 is photodissociation by UV photons. The photodissociation cross section of CO_2 rapidly decreases with increasing wavelength and drops off to about 10^{-3} of the maximum value at 160 nm, while that of SO_2 is still 10^{-1} of the maximum value at 180 nm (van Dishoeck, private communication; see also van Dishoeck and Dalgarno 1984 and Lee 1984). This difference could have a large effect in a low-temperature radiation field. We note that the SO_2 gas observed in our stars is optically thick in the UV so that all stellar photons are available for destruction of SO_2.

To dissociate the number of SO_2 molecules observed to disappear in T Cep in one year we need a radiation field with a

Table 1. Optical phases and best fit model parameters

Name	Obs.Date D/M/Y	Phase[1]	R_{SO_2} $\times R_\star$	$\mathcal{N}_{SO_2}$ $\times 10^{47}$	n_{SO_2} $\times 10^4$cm^{-3}
UX Cyg	08/11/96	0.53	1.82	0.75	13.2
o Cet	09/02/97	0.99	4.58	0.30	0.28
T Cep 1	05/08/96	0.38	5.74	4.67	2.19
T Cep 2	27/10/96	0.58	5.87	6.83	2.99
T Cep 3	15/01/97	0.79	5.74	7.46	3.50
T Cep 4	13/04/97	1.02	5.47	6.76	3.68
T Cep 5	13/06/97	1.17	5.40	3.30	1.86
T Cep 6	07/09/97	1.39	4.44	1.67	1.71
T Cep 7	01/12/97	1.61	4.01	1.37	1.90

[1] Phases are determined based on AAVSO data.

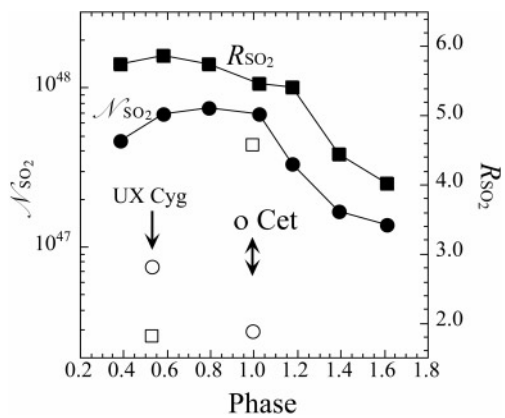

Fig. 3. Derived total number of SO_2 molecules (*circles*) and the size of the SO_2 layer (in units of the stellar radius, *squares*) plotted against variable phase. Filled symbols connected by lines are for T Cep, and open symbols are for UX Cyg and o Cet.

luminosity of $\sim 10^{-4}$ $L_\odot$ in the 150–200 nm window. This luminosity happens to be exactly emitted by a star with the parameters that we have adopted for T Cep in our model calculations. In this radiation field SO_2 is about 800 times more easily dissociated than CO_2. The temperature of the radiation field should not exceed 9500 K because then the CO_2 photodissociation rate reaches a value of about 0.1 of SO_2 so that the CO_2 molecules would be dissociated at the same rate as SO_2. This is inconsistent with the observed increase in CO_2 unless the formation rate of CO_2 would be much higher than that of SO_2.

Using a crude energy balance argument we estimate that the soft UV photons required for the destruction of SO_2 might also be generated as cooling line radiation in the gas behind pulsation shocks.

According to a similar estimate as given above for T Cep the SO_2 molecules in *o* Cet could also be destroyed by the UV radiation field of its B-type companion star (cf. Karovska et al. 1997).

The formation process of SO_2 is not clear. The major sulfur containing molecules under LTE condition are H_2S, SiS, and HS (Tsuji 1973). Based on their non-equilibrium chemical calculations Beck et al. (1992) found SO_2 abundances up to a few times 10^{-6}. It is also known that slow shocks with velocities below 15 km s^{-1} can change the chemical composition in molecular clouds, and enhance the abundances of sulfur containing molecules (Mitchell 1984).

Our results suggest the existence of a close relation between the physical and chemical conditions in the extended atmosphere and the presence of shocks due to stellar pulsation. The warm gas detected in SO_2 and CO_2 molecules could be the site of dust formation.

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