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LETTER TO THE EDITOR

Discovery of a TiO emission band in the infrared spectrum of the S star NP Aurigae

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ABSTRACT

We report on the discovery of an infrared emission band in the *Spitzer* spectrum of the S-type AGB star NP Aurigae that is caused by TiO molecules in the circumstellar environment. We modeled the observed emission to derive the temperature of the TiO molecules (≈ 600 K), an upper limit on the column density ($\approx 10^{17.25}$ cm^{-2}) and a lower limit on the spatial extent of the layer that contains these molecules. ($\approx 4.6 R_\star$). This is the first time that this TiO emission band is observed. A search for similar emission features in the sample of S-type stars yielded two additional candidates. However, owing to the additional dust emission, the identification is less stringent. By comparing the stellar characteristics of NP Aur to those of the other stars in our sample, we find that all stars with TiO emission show large-amplitude pulsations, s-process enrichment, and a low C/O ratio. These characteristics might be necessary requirements for a star to show TiO in emission, but they are not sufficient.

Key words. stars: AGB and post-AGB – circumstellar matter – infrared: stars – techniques: spectroscopic

1. Introduction

The spectral class of S stars contains objects that show absorption bands from oxides such as ZrO, LaO and YO in addition to the absorption bands of TiO that characterize M stars (Merrill 1922; Keenan 1954). It is often said that S-type stars have C/O ratios close to one. Although the ZrO bands become more pronounced when the C/O ratio is closer to unity, a star can show ZrO absorption bands while the C/O ratio is as low as 0.5 (Van Eck et al. 2011a). This is only possible if the stars have enhanced abundances of s-process elements such as Zr, La and Y. If this s-process enrichment is caused by nucleosynthesis and dredge-up on the thermally-pulsing AGB, these stars are *intrinsic* S stars. *Extrinsic* S stars are enriched through pollution by a binary companion (Groenewegen 1993; Van Eck & Jorissen 1999).

The infrared spectra of S stars are diverse and show a mix of dust species typical for either oxygen-rich or carbon-rich circumstellar environments, molecular emission bands, or no excess emission at all (Chen & Kwok 1993; Hony et al. 2009; Smolders et al. 2010, 2012). This heterogeneity of the infrared appearance within one spectral class is caused by the peculiar chemical composition of the stellar atmosphere of S stars. In

oxygen-rich stars, the stable CO molecule forms at high temperatures in the stellar outflows until almost all free carbon is consumed, leaving only the free oxygen atoms to produce molecules and dust. For carbon-rich stars, the oxygen is depleted and only carbon is left to form molecules or dust grains. This CO dichotomy explains the differences in spectral appearance (Millar et al. 2000; Willacy & Millar 1997; Treffers & Cohen 1974). Because S-type stars span a range of C/O ratios from near solar values to near unity, and since the composition of the molecular shell and dusty wind is highly sensitive to the actual C/O ratio, a rich diversity in gas and solid-state species can be expected (Smolders et al. 2012).

The results discussed in this Letter are part of a program to study a large sample of S-type AGB stars (Program ID 30737, P.I. S. Hony), observed with the Infrared Spectrograph (IRS, Houck et al. 2004) onboard the *Spitzer* Space Telescope (Werner et al. 2004). The sample was selected from the Stephenson S star catalog (Stephenson 1994), limited to those targets that are observable with *Spitzer* based on the 2MASS and IRAS data. The extrinsic S stars were excluded from the sample based on the amplitude of variability (Smolders et al. 2012). The final sample consists of 87 S-type stars in total, containing 32 stars with dust emission features, 3 stars with only molecular emission features, 4 stars with hydrocarbon emission, and 47 stars without significant emission features. In addition to the infrared spectra, we acquired high-resolution optical spectroscopy using
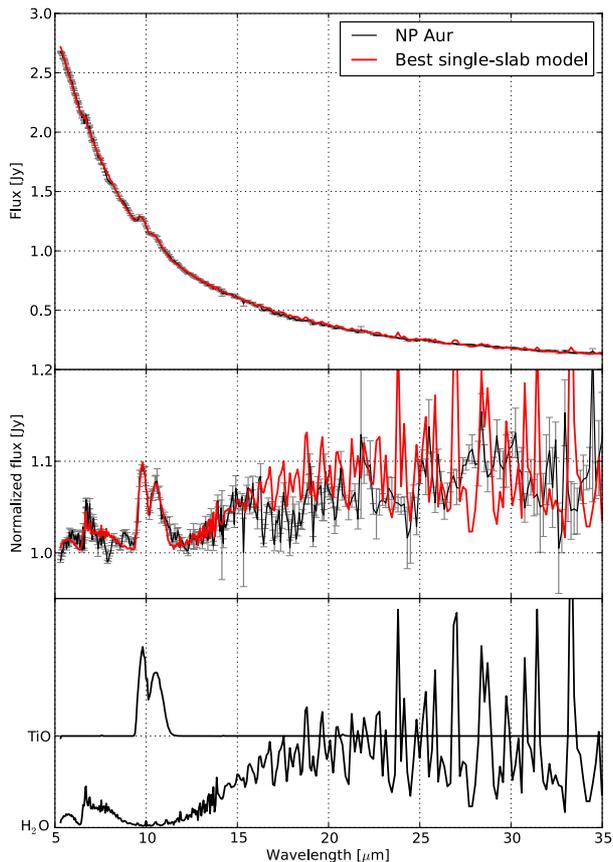

Fig. 1. *Top panel*: the infrared spectrum of NP Aur shown in black and the slab model, shown in red; *middle panel*: spectrum and model, divided by the blackbody radiation of the stellar disk; *bottom panel*: the contribution of TiO and H_2O separately.

Fig. 2. Normalized *Spitzer* spectrum of NP Aur, the opacities of candidate dust species and the normalized absorption of TiO and H_2O. The gray area and lines indicate the position of the TiO emission features.

the HERMES échelle spectrograph at the Mercator telescope in La Palma (Raskin et al. 2011), covering 3770–9000 Å with a resolving power of $R \approx 85\,000$. Smolders et al. (2012) provide more details on the data and the sample selection.

Previous studies of this sample have already led to the identification of the fundamental ro-vibrational band of SiS at 13 μm and its first overtone at 6.7 μm in absorption (Cami et al. 2009) and in emission (Sloan et al. 2011). Furthermore, four stars in this sample show the typical hydrocarbon emission features on top of an oxygen-rich photosphere (Smolders et al. 2010). In this letter we focus on NP Aurigae, which shows a double peaked emission feature in the 9.8–10.5 μm region, which we identify as the fundamental vibrational band of TiO. In Sects. 2 and 3 we present the identification and modeling of the emission feature. In Sect. 4, we discuss the search for TiO and TiO_2 in circumstellar environments and we show the tentative detection of TiO in two other S-type stars. Finally, we conclude in Sect. 5 with the implications of this finding.

2. Identification of the TiO emission

As can be seen from the full infrared *Spitzer* spectrum in Fig. 1, the infrared continuum can be well reproduced by a single, 1900 K black body. Figure 2 shows the observed spectrum, normalized to a black-body emission spectrum with a temperature of 1900 K and an angular radius of 1.17 mas. Above the normalized spectrum, we show the opacities of a selection of common dust species with emission features in the 10 μm region (the
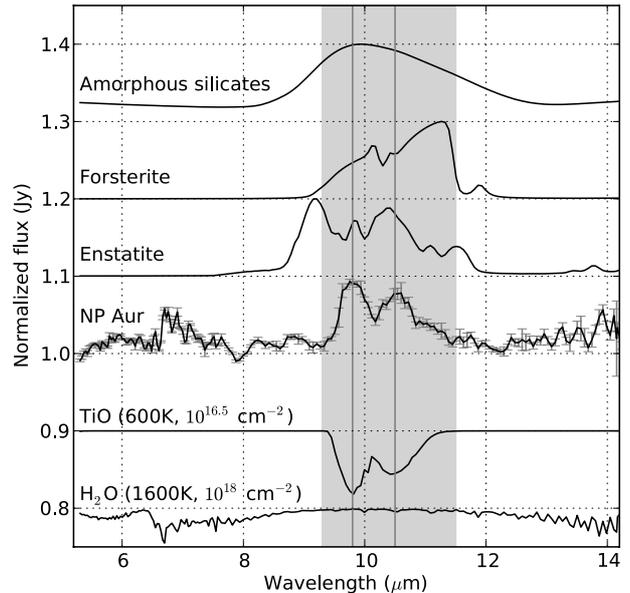
dust opacities were computed as a distribution of hollow spheres (DHS) as presented by Min et al. 2008). Below the spectrum, we show the normalized absorption of TiO and H_2O molecules, calculated from the linelist of Schwenke (1998) and Partridge & Schwenke (1997). The region of interest in this paper is indicated by a gray band. The complex of emission lines in the 5−8 μm range can be attributed to the emission by H_2O molecules, presumably in a molecular shell close above the stellar photosphere.

This figure already suggests that TiO is the only valid candidate to explain the new feature(s). The crystalline dust grains show emission features at similar wavelengths, but are always accompanied by other strong emission features that are not observed. The emission feature caused by amorphous silicates is too broad to explain the observed spectrum. Furthermore, if the 10 μm emission were due to silicates, the spectrum should show more structure in the 18–20 μm range.

Figure 3 shows the emission feature of TiO for different column densities and different temperatures. The column densities for the models in the upper left panel correspond to optically thin emission, where the P and R branches are clearly visible as two emission features centered at 9.8 and 10.3 μm, respectively. For higher column densities, this difference becomes less pronounced as we move toward the optically thick regime. The lower right panel shows the optically thick TiO emission, where the P and R branches have blended into a single broad emission feature. It is clear from this figure that an increase in temperature results in a broader emission band for all column densities, while the peak of the R branch shifts from 10.3 to 10.6 μm. An increase in temperature enhances the relative difference in peak flux between both branches.

3. Modeling the TiO emission

To reproduce the infrared spectrum of NP Aur, we adopted a plane-parallel geometry and constructed a model by superimposing two extended molecular slabs above a stellar disk that provided blackbody continuum radiation. The first molecular slab contains H_2O, the second contains TiO. Both slabs are assumed
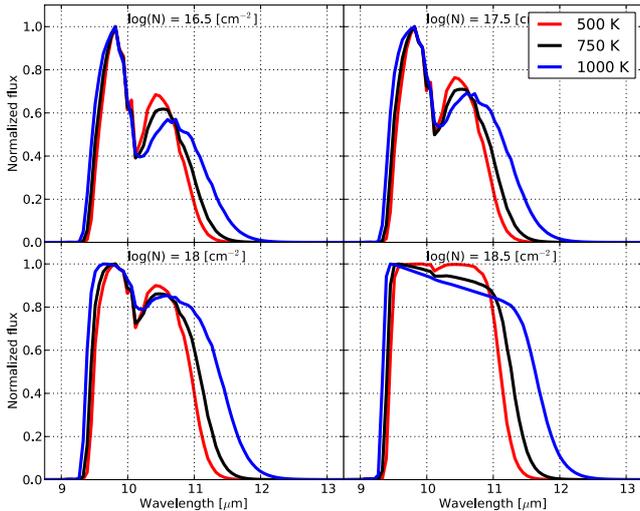
Fig. 3. Shape of the TiO emission, with the separate P and R branches visible at 9.8 and 10.3 μm. The figures are arranged by increasing column density. The color indicates the temperature of the molecular slab.

to be isothermal, in LTE, and can be geometrically extended with regard to the stellar disk, as expected for extra-photospheric molecular layers.

As was shown in Fig. 3, it is possible to constrain the temperature of the TiO molecules based on the characteristics of the emission features. However, because the column densities of TiO are close to the optically thin regime, increasing the density or the radius has approximately the same effect on the emission feature. Therefore, we cannot constrain the radius and the column density based on this TiO emission band alone. However, we can derive an upper limit on the column density of $10^{17.25}\,\mathrm{cm}^{-2}$. For this upper limit, the TiO emission is optically thick. Increasing the column density above this value changes the width and shape of the emission feature significantly. This upper limit on the column density corresponds to a lower limit on the radius of the molecular layer of $4.6\,R_*$. For these limit values, the molecular layer is situated in the so-called *inner wind* or extended atmosphere (Cherchneff 2006).

Figure 1 shows the infrared spectrum of NP Aur in black and the model spectrum in red. The stellar disk has a temperature of 1900 K and a radius of 1.17 mas. This temperature is noticeably lower than the stellar temperature, but could be explained by an optically thick layer of water that contributes to the continuum emission of the stellar disk (Tsuji 2000). The H_2O slab has a temperature of 1600 K, a radius of $1.5\,R_\star$ and a column density of $10^{19.25}\,\mathrm{cm}^{-2}$. For the TiO slab, we used a temperature of 600 K and the limit values for the radius and the column density of $4.6\,R_\star$ and $10^{17.25}\,\mathrm{cm}^{-2}$, respectively. From this figure we can see that the model assuming isothermal, molecular slabs can already explain the observed emission features quite well. Adding more slabs to the model and/or adding SiO molecules did not significantly improve the goodness-of-fit.

4. Discussion

4.1. The search for TiO and TiO₂ emission lines

The absorption bands of TiO are one of the most prominent features in the optical spectra of cool oxygen-rich stars, for which they are often used as a temperature indicator (Alvarez & Mennessier 1997). The rotational spectrum of TiO molecules

has also been extensively studied in the laboratory at millimeter and radio wavelengths (Steimle et al. 1990; Namiki et al. 1998). But until now, the search for infrared, millimeter or radio emission of TiO molecules in the AGB wind or in molecular clouds has not yielded significant detections (Churchwell et al. 1980; Millar et al. 1987; Brünken et al. 2008). This lack of observed TiO emission may indicate that in most stars, TiO has been depleted into molecular or solid-state TiO_2 as soon as it was lifted above the stellar photosphere.

Assuming chemical equilibrium, Gail & Sedlmayr (1998) showed that TiO_2 gas forms efficiently from a reaction of H_2O and TiO once the temperature drops below 1200 K. Furthermore, they showed that for temperatures below 1000 K, this reaction converts almost all TiO into TiO_2 gas. This TiO_2 gas can then be used to form solid titanium oxides, which are considered to be the primary seed grains onto which different oxides and silicates can condense (Onaka et al. 1989; Tielens 1990; Jeong et al. 1999).

From our analysis, we conclude that the circumstellar environment of NP Aur contains both H_2O and TiO. Under these conditions all TiO should be converted to TiO_2 or to solid titanium oxides (Gail & Sedlmayr 1998). However, the presence of molecular TiO in the circumstellar environment of this star indicates that these reactions did not or do only partially take place. The reason for this might be the high temperatures in the shocked gas near the star. Furthermore, we compared the *Spitzer* spectrum to the theoretical emission spectra of TiO_2 grains and other titanium oxides (optical constants and opacities taken from Posch et al. 2003). Although all synthetic spectra show clear emission features in the 14–20 μm range, we did not detect any significant emission because of these dust species.

4.2. TiO emission from oxygen-rich Mira-type S stars

Out of a sample of 87 S-type AGB stars, 49 sources do not show significant dust emission features, and of these NP Aur is the only star that shows a clear detection of TiO. A search of the entire sample indicates that two other stars, V899 Aql and RX Psc, show similar double peaked emission, shown in Fig. 4. This can be explained by a superposition of TiO molecular emission on top of dust emission from silicates and alumina.

The HERMES high-resolution spectra of NP Aur show the Tc absorption at 4238, 4262, 4296, and 5924 Å. Because the half-life time of Tc is approximately 2×10^5 years, we can conclude that this Tc has recently been produced during a third dredge-up event. Furthermore, by comparing optical photometric and spectroscopic data to the MARCS model atmospheres calculated specifically for S-type AGB stars, it is possible to derive the stellar parameters (Van Eck et al. 2011b). For NP Aur we find an effective temperature of 3200 ± 300 K and a C/O ratio of 0.5 ± 0.1. Although the C/O ratio is one of the lowest for the stars in our sample, this is not an unusual value for MS- and S-type stars and the C/O ratio is consistent with the classification of NP Aur as a M5:S star by Stephenson (1994). Furthermore, the star shows large-amplitude variations in the *V*-band and is classified in the General Catalog of Variable Stars as a Mira with a 334-day period (Samus et al. 2009).

A comparison of the stellar properties of NP Aur and the other stars with a tentative detection of TiO emission shows some similarities. First of all, they show only weak (or even no) dust emission, which is necessary because the contrast of the TiO emission decreases with stronger dust emission. Furthermore, all three stars are large-amplitude Mira-type pulsators, with a period
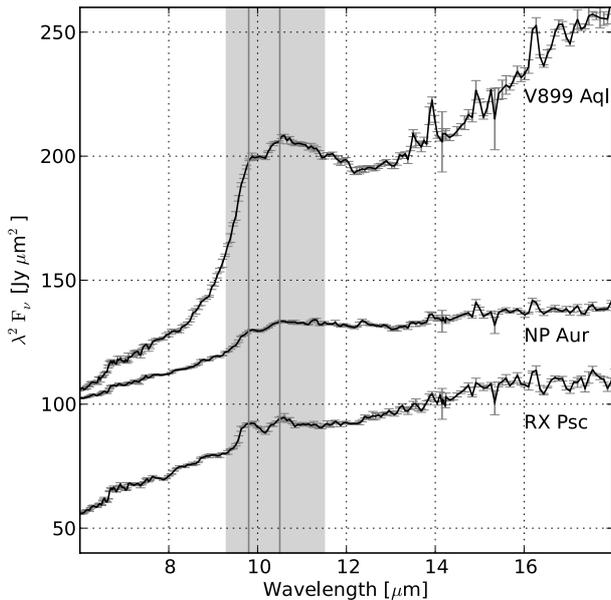
Fig. 4. Three stars in our sample with possible TiO emission features, shown in Rayleigh-Jeans units. From top to bottom: V899 Aql, NP Aur, RX Psc. The gray area and lines indicate the position of the TiO emission features.

of 281 days for RX Psc and 347 days for AU Car (Smolders et al. 2012). This is consistent with the idea that large-scale pulsations are necessary to lift the molecular layer of TiO far enough above the stellar atmosphere. Finally, both NP Aur and RX Psc have been classified as MS stars and are thus oxygen-rich S stars. For V899 Aql, we found no spectral classification.

However, these pulsations and stellar characteristics resemble those of many other stars (for example AU Car, shown in Fig. 4) in our sample and we conclude that apart from the TiO emission features, these targets, and NP Aur in particular, are typical oxygen-rich S-type AGB stars. Although large-amplitude pulsations, s-process enrichment and/or a low C/O ratio could be strict requirements to observe TiO in emission, they are not sufficient. A possible explanation for this might be that TiO is only visible during a short timespan, for example at a certain phase of a pulsation cycle or a short evolutionary phase.

5. Conclusion

We presented the detection of a new, unusual emission feature in the 9–11 μm region. We identified this feature as the fundamental vibrational band of gaseous TiO. We showed that it is possible to reproduce this emission band using a simple isothermal, single molecular slab. This model can constrain the temperature of the TiO molecules, but because the emission comes from an approximately optically thin region, we cannot put strict constraints on the column density or outer radius of the emitting region. We discussed that this is the first time that TiO molecules are observed in the circumstellar environment of an AGB star. Based on the stellar properties of NP Aur, the two stars with a tentative detection of this TiO emission band, and the other S stars in our

sample, we argue that (i) large-amplitude pulsations; (ii) a low C/O ratio; and (iii) weak dust emission in the 9–11 μm region might be necessary, but not sufficient requirements for the infrared spectrum to show TiO emission.

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