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Letter to the Editor

ISO-SWS* spectra of the C-rich AGB star R Scl and dynamical model atmospheres

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Abstract. We have monitored the spectral variations of the carbon rich AGB star R Scl in the $2-45\,\mu$m range using the ISO-SWS instrument. We have also computed hydrostatic and hydrodynamic model atmospheres and corresponding synthetic spectra representative for two phases of R Scl. There is good qualitative agreement between observations and models in the near IR. This demonstrates the theoretical progress and the potential of analysing carbon star spectra with self-consistent dynamical models.

Key words: stars: AGB and post-AGB – stars: atmospheres – hydrodynamics – molecular processes – stars: variables – infrared: stars

1. Introduction

The very successful ISO mission provides for the first time complete and multi-epoch spectroscopic observations of C-rich AGB-variables. The large wavelength coverage of the Short Wavelength Spectrometer (SWS, de Graauw et al. 1996) allows us to simultaneously study the molecular features and the emission from circumstellar dust and their variation with pulsational phase. In view of the strong interplay between gas and dust predicted by models, this aspect is of special importance.

First guaranteed time ISO-SWS observations of several carbon stars have been presented by Yamamura et al. (1998). They mainly compared the observed spectra of stars with different mass loss rates. In this paper we concentrate on the variation of molecular absorption features. We give the first comparison of dynamical model atmospheres for C-rich stars with ISO-SWS observations and hence a first check of the predictions made by these time-dependent models. In forthcoming papers we will discuss in more detail the interaction between absorption band intensities and variations of the dust features.

2. ISO-SWS observations of R Scl

Within our open time ISO observing program the spectral variations of a few representative AGB stars were monitored with the SWS. In this paper we concentrate on the semiregular variable R Scl which has the lowest amount of mass loss among our C-rich target stars. We have selected the two observations closest to visual maximum (JD 2450285.7, $\phi \simeq 0.9$) and minimum (JD 2450452.3, $\phi \simeq 0.4$) light. The phases were estimated from data provided by the AAVSO (visual, Mattei 1995–1997) and by P. Whitelock (JHKL-photometry, partly published in Whitelock et al. 1997 where the near IR light curve of this star is discussed). The spectra were obtained with SWS01, speed 2, so the typical resolution is about 600. The data were reduced with the ISO Spectral Analysis Package. The AOT-bands were combined with band 1A as a flux reference. The resulting SWS L-band flux agreed within $0\overset{\mathrm{m}}{.}15$ with the above mentioned JHKL-photometry. The spectra were then rebinned to a resolution of 100 to make them comparable with our synthetic spectra.

In Fig. 1 we show two observations of R Scl together with the identification of the main features. The arrows indicate the extension of several molecular features beyond $4\,\mu$m as estimated from opacity sampling spectra (see below). The narrow features at 9.3 μm and 11.1μm are artefacts. It is interesting to note that in spite of a change in the bolometric magnitude by about $0\overset{\mathrm{m}}{.}5$, there is no large change in the overall flux level in the SWS range.

An emission band around 8.6 μm has been reported in the IRAS-LRS spectra of carbon stars (Willems 1988), however its identification was not clear. A look at the ISO and the synthetic spectra shows that the emission is much more likely the red wing of an absorption due to strong combination bands of HCN and C_2H_2. In the ISO data only the 8.5–10 μm region shows a noticable change from maximum to minimum but in the opposite sense to the molecular features. One interpretation would be that of a constant molecular absorption feature between 6 μm and about 8.6 μm. At the same time there would be an enhanced emission in the blue wing of the SiC feature near minimum light but the 11 μm SiC peak stays constant. The reason for the enhanced emission could be a contribution from

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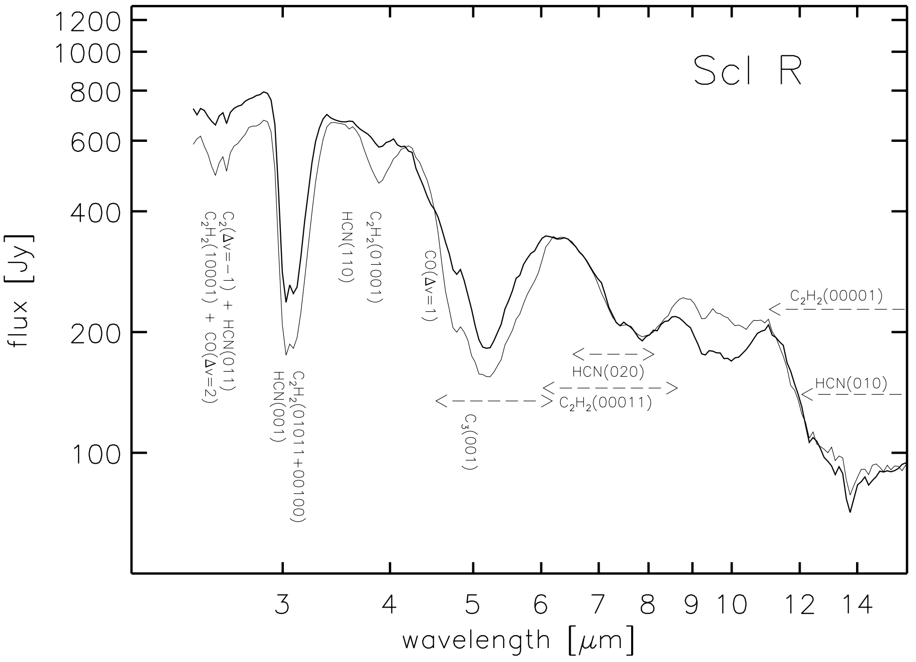

Fig. 1. ISO-SWS spectra of R Scl at visual phases 0.9 and 0.4 (thick and thin lines). The main molecular features are identified, the numbers in brackets are the quantum numbers of the upper vibrational levels for the polyatomic molecules.

β SiC which shows a broad shoulder in its absorption cross section (Borghesi et al. 1985). An alternative explanation would be an increasing 6–8.6 μm molecular absorption towards minimum light accompanied by a weaker SiC feature and a slightly higher continuous dust emission in the 8–10 μm region. Such a rather local dust emission makes the second interpretation less attractive. Since the 6–8.6 μm region is not well reproduced in our synthetic spectra (Sect. 5) a definite identification of the features cannot be given. We also note that PAH's show a broad and strong feature between 7 and 9 μm (e.g. Tielens 1997). The strong interaction between molecular and dust features in the 6–15 μm region of R Scl serves as a warning for the interpretation of ground based mid-IR data.

3. Model atmospheres

To calculate the structure of the atmosphere and circumstellar envelope (density, temperature, degree of condensation, etc.) as a function of time we solve the coupled system of grey radiation hydrodynamics and time-dependent dust formation. Details about physical and numerical aspects of the modelling method can be found in previous papers (Höfner & Dorfi 1997 and references therein). The stellar pulsation of the LPV is simulated by a variable inner boundary (piston) located beneath the photosphere.

The models presented here have been improved compared to those of Höfner & Dorfi (1997) by introducing a more realistic treatment of the gas opacity. Most time-dependent dynamical models use a constant value for the absorption coefficient of the gas. Our present models are calculated using Planck mean absorption coefficients based on the SCAN molecular line data (Jørgensen 1997). As discussed by Höfner et al. (1998) the gas opacity plays a crucial role with regard to the atmospheric structure and, consequently, the near-IR properties of the models.

We selected one particular model with the following parameters: $T_* = 2880$ K and $L_* = 7000 L_\odot$ (for the hydrostatic initial model) and $M_* = 1 M_\odot$ (corresponding to $\log(g) = -0.6$), $\varepsilon_{\rm C}/\varepsilon_{\rm O}$ = 1.4, a pulsation period of 390$^{\rm d}$ and a piston velocity amplitude of 4 km/s. With regard to period, bolometric luminosity and amplitude and mass loss rate, the selected model is quite comparable to R Scl. R Scl's corresponding parameters are 370$^{\rm d}$, 5700 $L_\odot$ (Whitelock et al. 1997), approximately $0\overset{\rm m}{.}5$ (from the VJHKL data) and $\dot{M} \lesssim 10^{-6}\ M_\odot$/yr (from the IRAS colours using Ivezić & Elitzur 1995). The C/O ratio is also close to the values found by Lambert et al. (1986). However, we want to emphasize that it is not our aim to make a specific model for R Scl or to determine its fundamental parameters but rather to compare hydrodynamic and hydrostatic results, and to give a first comparison between the predictions of these models and ISO observations.

For the purpose of comparing synthetic spectra based on hydrostatic and hydrodynamical models, we also computed two hydrostatic models using the MARCS program (Gustafsson et al. 1975) in an updated version (Jørgensen et al. 1992) which includes spherical geometry and opacity sampling treatment of approximately 100 million molecular lines, and which is particularly suitable for carbon stars. The two models computed for the minimum and the maximum luminosity of R Scl have $T_{\rm eff}$ = 2930 K and 2650 K, respectively, C/O=1.40, $\log(g) = -0.5$, and solar metallicity. If one adopts 2930 K as $T_{\rm eff}$ at maximum luminosity (Dyck et al. 1996), the models cover the temperature range expected during a pulsational cycle.

Especially in the upper layers of the atmosphere – which are severely affected by the pulsation-induced shock waves – the dynamical models show a complex structure. This is also reflected by the partial pressures of various molecules (cf. Fig. 2). Such structures give rise to qualitatively new predictions for the spec-

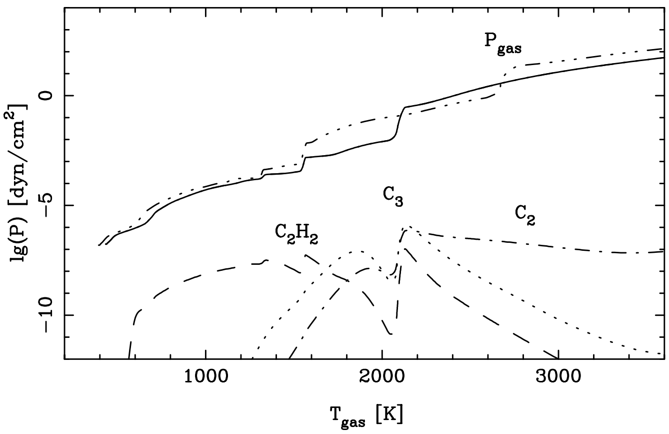

Fig. 2. Gas pressure versus gas temperature for two phases of the hydrodynamical model. The full line corresponds to maximum light ($\phi = 1.0$), the dash-triple-dot line to minimum light ($\phi = 0.5$). The 'steps' in the gas pressure indicate shock waves. Dashed, dotted, and dashed-dotted lines show the partial pressures of C_2H_2, C_3 and C_2, respectively, in the maximum-light model. Note two distinct maxima in the partial pressure of C_2H_2 at T=1500 K and T=2100 K, caused by a shock.

trum and we therefore emphasize the theoretical consistency in contrast to a hydrostatic approach when considering pulsating AGB stars.

4. Partial pressures and synthetic spectra

For the comparison with our ISO observations we calculated synthetic opacity sampling spectra in the wavelength range between 2 and 12 μm for the maximum and minimum light phases of the dynamical model as well as for two MARCS models. The molecules CO, CH, C_2, CN, HCN, C_3, and C_2H_2 were included in the model atmosphere calculation as well as in the spectrum computation.

In Fig. 2 we show the pressure-temperature structure of the main spectrum forming region at the maximum and minimum phase of the dynamical model. Although there is a general decrease in the ratio of polyatomic to diatomic molecules with the increase in temperature inwards a steep increase of the gas pressure as caused by a shock (e.g. at about 2100 K in Fig. 2) can locally invert this trend. For this reason the hydrodynamical models predict for example two distinct peaks in the partial pressure of C_2H_2 (and other polyatomics), as is clearly seen in the figure.

C_2 forms deep in the atmosphere and its partial pressure drops rapidly at $T \lesssim 2000$ K. The bulk of the C_2 band system is in the visual spectral region, but a relatively strong Ballik-Ramsay electronic transition appears around 2.5 μm originating in regions with $T \gtrsim$2500 K. The formation of C_3 requires a combination of high pressure and relatively low temperature and its partial pressure therefore has a rather narrow peak around 2000 K. Its main spectral feature is the fundamental C-C stretching at 5 μm which forms in atmospheric layers with temperatures around 2000 K. On the other hand, the partial pressure of C_2H_2 has a very broad distribution stretching toward much lower temperatures than C_3. The formation of C_2H_2 in a hydrogen dominated atmosphere is less sensitive to the density than C_3 but more sensitive to temperature. The main features of this molecule (at 2.5, 3, 3.8, 7−8 and around 14 μm) originate from layers with temperatures around 2000 K or cooler. HCN is more abundant than C_2H_2 and C_3 in the deeper layers of the atmosphere, but its partial pressure is an order of magnitude lower than the one of C_2H_2 in the upper layers. The strongest HCN bands are at 3 μm, in the 7 μm region, and around 14 μm. The absorption originates at temperatures between about 2000 and 3000 K. The partial pressure of CO follows the structure of the gas pressure at a level of about 3 orders of magnitude below the gas pressure, throughout the region presented in Fig. 2. The CO bands at 5 and 2.5 μm are blended with several other bands, but its trace can be seen in both cases. The CO features form in regions hotter than about 2500 K.

5. Comparison of observed and computed spectra

In Fig. 3 we compare the observed ISO spectra near minimum and maximum light with the model spectra based on two hydrostatic model atmospheres and two phases of the dynamical model. The model spectra are normalized to the theoretical continuum, the ISO spectra by linear interpolation between the fluxes at 2.4, 2.8, 3.6, 4.2, 10.3 and 12.3 μm and scaling this pseudo-continuum to an overall level comparable to the corresponding models. A different mean continuum level or different reference wavelengths change the depths of the various features typically by 10 %. A larger uncertainty exists beyond 6 μm due to the broad molecular features and the dust emission (see also Hron et al. 1997).

In general, the observed molecular features in the 2–6 μm region are qualitatively reproduced by all models. While the spectral differences of the static models result from large-scale differences in the model structure, the spectral variations of a hydrodynamical model are mainly caused by the local shock fronts propagating through the atmosphere. Thus, comparing the variations of features which originate in different atmospheric layers can help to identify dynamical effects and to separate them from global changes of the structure. In this context we note that the ratio of the intensities of the features at 3.8 μm (mainly C_2H_2) and 5 μm (mainly C_3) changes from less than one to greater than one for the static models while the ratio is always less than one for the dynamical model. An explanation could be that the C_3 feature forms at slightly higher temperatures than the C_2H_2 feature where the pressure differences between the hydrostatic models are smaller than for the dynamical models (due to the shocks). On the other hand, the variations of the 3 μm and 3.8 μm features, which both involve mainly C_2H_2, are comparable for the static and dynamical models. This indicates that adjusting only the temperature and gravity in hydrostatic models will probably not be sufficient to explain the observed spectra and their variations. We note however that $T_{\rm eff} = 2930$ K near maximum light, as estimated from angular diameter mea-

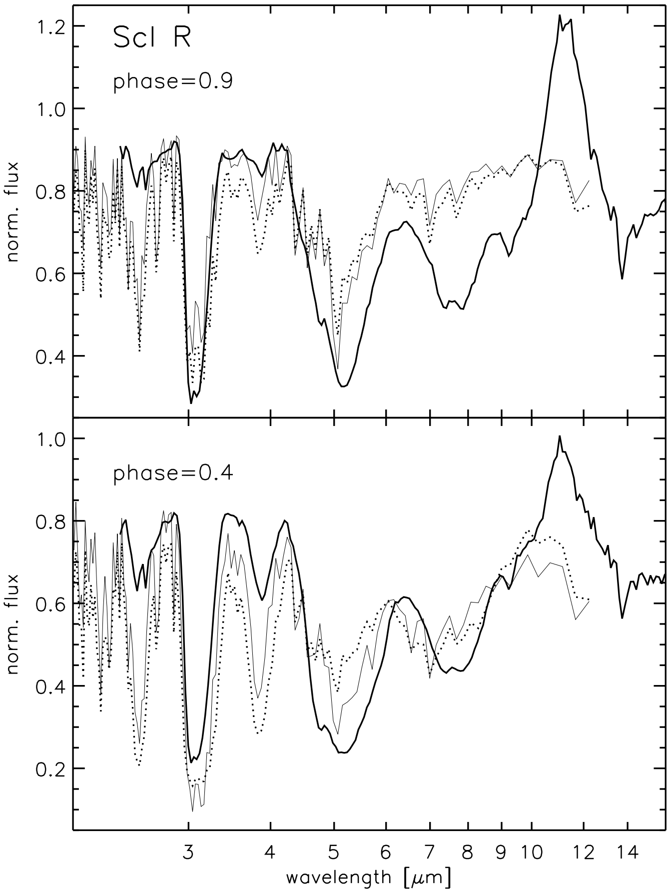

Fig. 3. Comparison of normalized, observed ISO spectra (thick full lines) and model spectra based on hydrostatic atmospheres (dotted lines) and on a dynamical model (thin full lines). The upper panel gives the ISO spectra near phase 0.9, the synthetic spectrum for a similar phase of the dynamical model and a hydrostatic model with $T_{\rm eff}$=2930 K. The lower panel shows phase 0.4 for the SWS data, the dynamical model, and a hydrostatic model with $T_{\rm eff}$=2650 K, respectively.

surements (Dyck et al. 1996) fits the SWS spectrum of R Scl reasonably well.

The observed variations of the features shortward of 5 μm are significantly smaller than predicted by the dynamic (and hydrostatic) models and the observed 2.5 μm and 3.8 μm features are also significantly weaker than in the models. This could point to a smaller change in the C_2H_2 partial pressure, i.e. weaker shocks than in the models. The weaker features could also be caused by a lower mean C_2H_2 abundance, although this would increase the difference in the 3 μm band intensity near maximum light. Since the 3 μm feature contains also a significant contribution from HCN and this molecule also contributes to the 6–8 μm region, the differences between observations and models could also be due to uncertainties in the data (abundance, opacity). The stronger change in the 3.8 μm band intensity compared to the 2.5 μm band intensity variation is qualitatively reproduced by the models and can be understood by the contributions of CO (and to a smaller extent also C_2 and CN) to the 2.5 μm feature. The absorption due to the diatomic molecules originates in deeper layers than the C_2H_2 absorption and hence also shows weaker changes with pulsational phase (Sect. 4).

6. Summary and conclusions

We have presented a first preliminary comparison of ISO-SWS spectra of R Scl with predictions of state-of-the-art dynamical model atmospheres. Considering the uncertainties of some physical input data and the approximations used in the present models we find a good qualitative agreement for molecular features in the near infrared range. We stress the theoretical progress and the potential of analysing the spectra by using self-consistent dynamical models. Only dynamical models open the possibility to include the effects of pulsation, shock waves, dust formation and a circumstellar envelope and to investigate dynamical phenomena like line doubling due to shock waves in the atmosphere. More and better processed data from the ISO mission are becoming available, which will continue to give better constraints for the models.

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