

Probing chemical processes in AGB stars

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Abstract. We are conducting multi-transition observations of circumstellar line emission from common molecules such as HCN, SiO, CS, SiS and CN for a large sample of AGB stars with varying photospheric C/O-ratios and mass-loss characteristics. Our recently published results for SiO and SiS clearly show that major constraints on the relative roles of non-equilibrium chemistry, dust condensation, and photodissociation can be obtained from the study of circumstellar molecular line emission. Presented here are also preliminary results based on detailed radiative transfer modelling of HCN line emission.

Keywords. Stars: AGB and post-AGB, circumstellar matter, mass loss

1. Introduction

Stellar winds from evolved stars carry the products of internal nuclear processes, activated during the evolution along the asymptotic giant branch (AGB), and thus contributes to the enrichment of heavy elements in the ISM and the chemical evolution of galaxies (e.g., Gustafsson 2004). Of paramount importance is gaining knowledge of the fraction of these products that are accreted onto dust grains and the fraction that remains in the gas phase. Moreover, the mass loss will also have a profound effect on the future evolution of the star, and eventually terminate its life as a star, as well as their descendents, the planetary nebulae. The study of the circumstellar envelopes (CSEs) produced by the stellar winds is crucial to our understanding of the late stages of stellar evolution and its implications on the cosmic gas cycle.

Molecules can easily form in large abundance in the cool atmospheres of AGB stars and initiate a relatively complex chemistry that is further enhanced by photodissociation in the CSEs. The molecular and grain type setups in the CSEs are to a large extent determined by the C/O-ratio of the central star but also the thickness of the envelope and the ambient ultraviolet field are of importance. AGB stars divide in two chemically distinct groups; carbon stars ($C/O > 1$) which show a more rich chemistry than the M-type AGB stars ($C/O < 1$). There is also a class of putative transition objects, the S-stars, where the photospheric C/O-ratio is ≈ 1 . For objects with high mass-loss rates where the photosphere can not be directly observed the study of the CSE is the only way to follow the future evolution of the star.

We have already obtained multi-transition CO observations for a large sample of some 150 AGB stars with varying C/O-ratios. The characteristics of their stellar winds such as mass-loss rate, expansion velocity, and kinetic temperature structure has been determined through detailed non-LTE, and non-local, radiative transfer modelling of the CO data (Schöier & Olofsson 2001, Olofsson *et al.* 2002, Gonzalez Delgado *et al.* 2003, Ramstedt *et al.* 2006). These models form the basis for the excitation analysis of other molecular species.

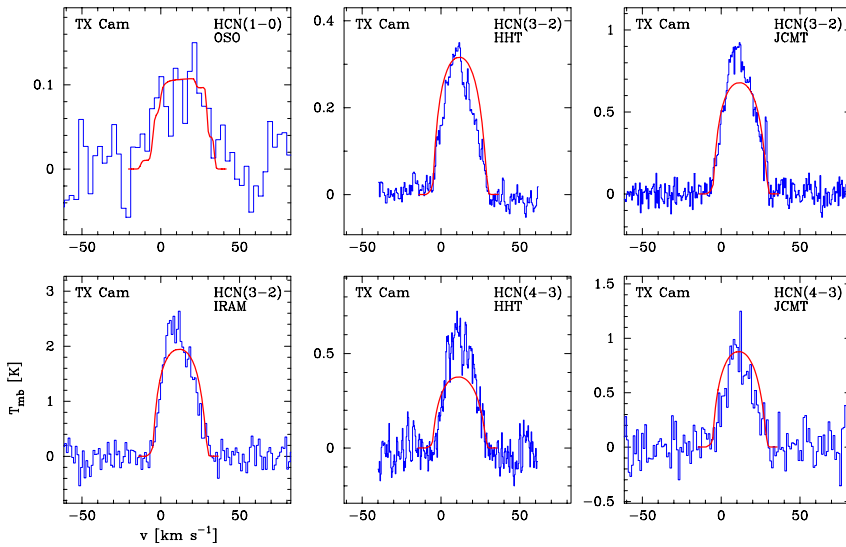


Figure 1. Multi-transition spectra (histograms) of HCN line emission toward the M-type AGB star TX Cam (HHT data from Bieging *et al.* 2000). Spectra from the best-fit single-dish model (assuming a Gaussian abundance distribution) using a fractional HCN abundance $f_0 = 3.5 \times 10^{-7}$ and an envelope size $r_e = 2.0 \times 10^{16}$ cm are also shown (solid lines). The hyperfine splitting of the $J = 1 \rightarrow 0$ transition significantly broadens the line. This effect is explicitly taken into account in the modelling. The calibration uncertainty in the observed spectra is $\pm 20\%$. (Schöier *et al.*, in prep.)

2. Circumstellar chemistry

Most of the published abundance estimates are carried out for limited samples, based on rather simple methods, and are typically order of magnitude estimates. At this level, chemical modeling does a reasonable job in explaining many of the observed abundances (Millar 2003). However, there are some notable exceptions such as the detection of H_2O , H_2CO and NH_3 toward the carbon star IRC +10216 (Melnick *et al.* 2001, Ford *et al.* 2004, Hasegawa *et al.* 2006) in amounts significantly higher than predicted by stellar equilibrium chemistry. Processing by shocks does not seem to increase these abundances any further. A possible explanation for these high abundances could be catalytic processes (Willacy 2004) or, in the case of H_2O , evaporation of Kuiper-belt like objects (Melnick *et al.* 2001). The detection of carbon bearing species such as CN, CS and HCN in envelopes of M-type AGB stars is also somewhat surprising. In the atmospheres of M-type AGB stars the lack of any free carbon prevents them to form in equilibrium chemistry. However, as shown by Duari *et al.* (1999) non-equilibrium gas-phase chemistry can potentially produce significant amounts of carbon bearing molecules such as HCN and CO_2 .

3. Results and discussion

3.1. SiO and SiS

The first more detailed studies of circumstellar abundances in larger samples of sources have been performed by Gonzalez-Delgado *et al.* (2003), Schöier *et al.* (2006a) and Schöier *et al.* (2007). Average SiO and SiS fractional abundances were obtained from a detailed radiative transfer analysis of multi-transition single-dish observations. In the case of SiO (see also contribution by Ramstedt *et al.* in this proceeding) the M-type AGB stars have much lower fractional abundances than expected from photospheric equilibrium

chemistry. For the carbon stars the derived abundances can be up to two orders of magnitude higher than predictions based on equilibrium chemistries. A clear trend that the SiO fractional abundance decreases as the mass-loss rate of the star increases, as would be the case if SiO is accreted onto dust grains, is found. Further support for such a scenario comes from interferometric observations by Schöier *et al.* (2004) and Schöier *et al.* (2006b). In their analysis they found evidence of an inner compact component of high fractional abundance, consistent with predictions from stellar atmosphere chemistry in the case of the M-type objects but several orders of magnitude larger than expected for the carbon star IRC +10216, indicating also the importance of non-LTE chemical processes. These conclusions are further corroborated by recent chemical modeling by Cherchneff (2006). In contrast, for SiS the derived fractional abundances depend critically on the photospheric C/O-ratio and are more in line with expectations from LTE chemistries. There are also indications of adsorption of SiS onto dust grains in individual sources. In addition to constraining photospheric and circumstellar chemistry, it has become evident that the line emission also has the potential to probe the formation and evolution of dust grains in CSEs, as well as CSE dynamics.

3.2. HCN

In Figure 1 we show a best-fit to the available HCN single-dish data towards the M-type AGB star TX Cam. In order to obtain good constraints on the abundance distribution multi-transitional observations are required, By combining low-excitation ($\sim 5\text{--}20$ K) rotational transitions at 3 mm with high-excitation transitions ($\sim 50\text{--}200$ K) in the sub-millimeter regime a large radial range in the circumstellar envelope can be probed and existing chemical gradients can be detected. This is illustrated in Figure 2 (left panel) for the M-type AGB star TX Cam, where a good fit to the available observational data can be obtained using a Gaussian distribution ($f = f_0 \exp[-(r/r_e)^2]$) for the fractional abundance of HCN relative to H_2 . In addition, available interferometric observations provide further constraints (Figure 2, right panel). Here, f_0 is sensitive to the chemistry occurring in and near the photosphere whereas r_e provide constraints on photodissociation models.

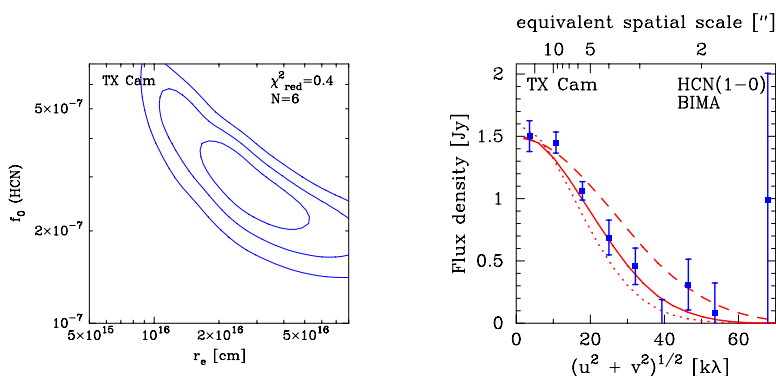


Figure 2. **left** – χ^2 -map showing the quality of the fit to available HCN multi-transitional single-dish data for the M-type AGB star TX Cam when varying the adjustable parameters, f_0 and r_e , in the model. Contours are drawn at the 1, 2, and 3 σ levels. Indicated in the upper right corner are the reduced χ^2 of the best-fit model and the number of observational constraints used, N . **right** – Visibilities, averaged over 2 km s^{-1} around the systemic velocity, obtained for TX Cam using the BIMA interferometer (Marvel 2005). The observations are overlaid by model results using various abundance distributions: $f_0 = 1.1 \times 10^{-6}$ and $r_e = 1.1 \times 10^{16}$ cm (dashed line); $f_0 = 5.0 \times 10^{-7}$ and $r_e = 1.6 \times 10^{16}$ cm (solid line); $f_0 = 4.0 \times 10^{-7}$ and $r_e = 2.1 \times 10^{16}$ cm (dotted line) (Schöier *et al.*, in prep.).

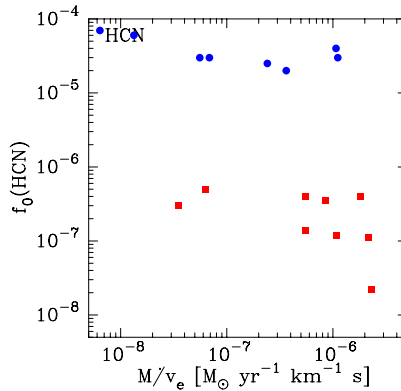


Figure 3. HCN fractional abundance (f_0) obtained from an excitation analysis, as a function of a density measure (\dot{M}/v_e), for carbon stars (filled circles) and M-type (O-rich) AGB stars (filled squares) (Schöier *et al.*, in prep.).

The observations will also help to put constraints on the photochemistry that involves HCN and occurs further out in the envelope.

The HCN abundance is expected to be highly sensitive to non-equilibrium chemical processes, in particular for the M-type AGB stars and S-stars (Cherchneff 2006) leading to fractional abundances similar to those for carbon stars. The importance of non-equilibrium processes is supported by our preliminary results for a sub-sample of the sources detected in HCN. However, there is still a distinct sensitivity to the C/O ratio (Figure 3) where carbon stars have on average about two orders of magnitude higher fractional abundances of HCN than the M-type AGB stars.

Our knowledge of the relative importance of freeze-out onto dust grains, grain surface reactions, photodissociation, and circumstellar chemistry is still rudimentary. There exists as yet no detailed chemical modeling including all these processes, but it is important to observationally determine the relation between abundant and chemically interesting molecules such as SiO, SiS, HCN, CS and CN.

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Discussion

CECCARELLI: How did you deal with the gas temperature with respect to the dust temperature? Do you assume that they are the same?

SCHÖIER: No, we derived the kinetic temperature by solving the energy balance equation for the gas, and for the dust temperature we calculated from the DUSTY model.

CECCARELLI: Did you find the coupling between the dust and gas, and in what regions?

SCHÖIER: Not temperature wise, because the heating of the gas is essentially due to the fact that the dust stream through the gas and heat the dust. So there's no immediate connection between the dust temperature and the gas temperature, and they do differ.

TENENBAUM: So to determine the mass loss rate, you assume the CO abundance. Where did you get that number and how uncertain is it? Does that uncertainty propagate into your results?

SCHÖIER: That uncertainty certainly propagates into our results. We simply adopt what people normally adopt. So we've somewhere around 10^{-3} for CO with respect to H_2 for carbon stars. And we used something like 2×10^{-4} for the M-type stars. So it does propagate, of course, to our determinations of the abundances.

ZIURYS: How well do you know all your molecular parameters in the model? For example, you know, the dipole-moment derivative, for the absorption of infrared radiation and all these different Einstein coefficients and so forth.

SCHÖIER: The basic molecular parameters they are known for these simple molecules. But of course there are other number uncertainties in the circumstellar model itself, which may also vary from star to star. For instance, for the SiO there is quite a spread in the abundances for a given density. We think that the uncertainty within the circumstellar model is less than that spread. But the uncertainty from circumstellar model to circumstellar model, we don't really know. It just showed how difficult it is to estimate reliable abundances.



From left to right: Ewine van Dishoeck, Hans Olofsson, Åke Hjalmarsen, and Bill Irvine at the reception.