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MOLECULAR FORMATION THE INNERMOST REGION OF O-RICH AND C-RICH AGB STARS

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Abstract. Evolved cool stars are important in the recycling of matter in the universe. They provide strong mechanical, chemical, and radiative feedback on their host environment. The composition of the recycled/feedback material depends on the elemental C/O ratio at the stellar surface. Typically, molecules in circumstellar envelopes are mostly formed at the stellar atmosphere under chemical equilibrium or in the outer expanding layers due to the action of photochemistry. The presence of most of the molecules detected is relatively well understood. However, there are a few molecules for which their origin is not clear at all. For example, the observed abundances of H_2O and PH_3 in the inner regions of C-rich envelopes are a few orders of magnitude above the predictions from chemical equilibrium. A similar situation is observed in O-rich stars, where the abundances of HCN, CS, and NH_3 derived from observations are higher than expected. In this work, we want to compare the abundance of a sample of molecules in O-rich stars, to reveal the differences between the interferometer observations and equilibrium chemistry models. Such study allows us to add more constraints on the models to reproduce those unexpected abundances. The differences could be explained by non-equilibrium chemistry such as shocks or UV photons which are not considered in classic models for isolated, smoothing pulsating AGB stars.

Keywords: astrochemistry - molecular processes - stars:AGB - radiolines: stars

1 Introduction

Evolved stars provide strong mechanical, chemical, and radiative feedback on their host environment (Habing 1996; Höfner & Olofsson 2018). The chemical and dynamical evolution of AGB stars is a complex unsolved problem in stellar astrophysics. Some molecules are formed in the inner region of the envelope, warmer and denser, and controlled by chemical equilibrium (Tsuji 1973; Agúndez et al. 2020), or in the outer expanding layers due to the action of photochemistry (Glassgold et al. 1986; Nejad & Millar 1987; Cherchneff 2006). The molecular composition of the CSE depends heavily on the carbon over oxygen ratio C/O at the stellar surface (Agúndez et al. 2009; Decin et al. 2010). The presence of most of the molecules detected is relatively well understood. There are a few molecules for which their origin is not clear at all (Ziurys 2006; Agúndez et al. 2020). For example, the abundance of HCN, CS, and NH_3 in the inner regions of O-rich envelopes, can be orders of magnitude above the predictions from chemical equilibrium (Agúndez et al. 2020) and also, only form from a certain distance from the star. In this study, we want to reproduce high angular resolution ALMA data with a non-LTE radiative transfer code.

2 Method

We want to model two O-rich stars: R Crt and IK Tau, with low/intermediate mass-loss rates. To reproduce the HCN (J=4-3) and $\nu_2 = 1$ (J=4-3) lines, we used a non-LTE radiative transfer code based on the Large Velocity Gradiente (LVG) formalism, including infrared pumping to excited vibrational states (Agúndez et al. 2012). Initial parameters have been estimated observationally (size of the radio photosphere, 3.3 stellar radii $R_\star$ for R Crt, $2.6R_\star$ for IK Tau, from ALMA continuum observations at 354 GHz), by literature (pressure at

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the radio-photosphere) or with ad-hoc law, for the density. We used the radiative transfer code DUSTY (Ivezic & Elitzur 1997) to reproduce the SED of our two stars, which is used to determine the dust temperature profile and the gas-to-dust ratio. Finally, we used a LVG code to find the gas mass loss rate of the star. Once all the properties of the dusty component of the envelope are determined, the LVG was applied to the HCN lines to reproduce and characterize the molecular line emissions and estimate the HCN abundance profile. Finally, this profile will be compared with the output of our chemical model at the end of this on-going work.

3 Results

With the LVG code, we can reproduce the HCN emission coming from the envelopes. We find that some parameters, such as the density at the photosphere and the size of the radiophotosphere, do not have a big impact on the brightness radial distribution of HCN lines. Models predict low HCN abundances in the innermost shells of O-rich. Observations should indicate the presence of a void or hole in the brightness distribution of HCN in O-rich stars. The LVG model with a hole in the abundance of HCN in the 1-5 $R\star$ region reproduces the shape of the ALMA observation (Fig. 1). The line intensity ratio between the J=4-3 line in the vibrationally excited state $\nu_2 = 1$ and ground state allows also to constrain the initial radius of HCN, when trying to reproduce the observations.

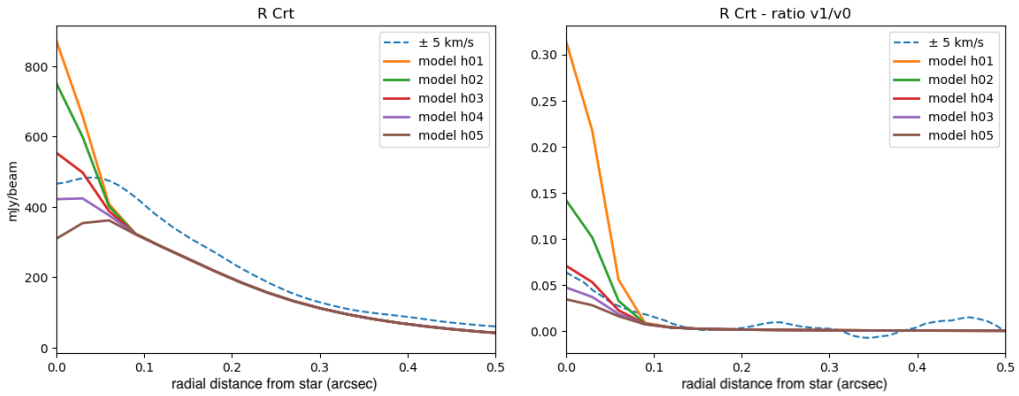

Fig. 1. Axially averaged HCN line emission around the systemic velocity the envelope of R Crt. The dotted lines are the ALMA observations integrated between -5 and +5 km/s. The solid lines are the models with a hole between 1 and 5 $R_\star$ in the abundance of HCN (named model h0X, with X the size of the hole). The left panel shows the emission of the J=4-3 ground vibrational state line and the right panel is the ratio of the $\nu_2 = 1$ and the ground vibrational state line.

4 Discussion and Conclusions

With the models, we were able to reproduce the emission radial profile of HCN and constrain to the formation region of the molecule to 4 $R\star$ which best reproduces the ALMA observations, an inner hole. This void in abundance profile should be explained by non-equilibrium chemistry such as shocks due to the stellar pulsation and convective motions or internal UV photons which are not considered in classic models.

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