## INVESTIGATING MOLECULAR CHEMISTRY IN THE COMPLEX WINDS OF EVOLVED STARS

Mark A. Siebert<sup>1</sup>

Anthony J. Remijan<sup>2</sup>

<sup>1</sup>Department of Astronomy, University of Virginia, Charlottesville, VA 22904, USA <sup>2</sup>National Radio Astronomy Observatory, Charlottesville, VA 22903, USA

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#### Abstract

The circumstellar envelopes of carbonrich AGB stars are known for their rich molecular inventories and their role in processing stellar material as it is returned to the interstellar medium. Recently, it has been revealed that binary interaction plays a prevalent role in shaping the dusty winds of these evolved stars and transitioning them to the planetary nebula phase. Recent interferometric surveys have shown that this interaction produces many characteristic morphologies including stable/expanding disks, bipolar outflows, and spiral wind patterns; however, the connection between these different structures and gas phase molecular content is not well-constrained. We present spectroscopic case studies of three known binary carbon star systems: IRC+10216, CIT 6, and V Hya, using archival ALMA observations at Bands 3, 6, and 7. We detect emission from over 20 molecules toward these sources, and present spatially resolved maps for the brightest tracers of carbonaceous chemistry (e.g.  $C_2H$ ,  $HC_5N$ ,  $C_3N$ , HNC). CIT 6, which has a spiralshaped outflow characteristic of a companion on a wide orbit, shows a high degree of photochemical and cosmic ray-driven processing. V Hya, which instead harbors a dynamically expanding circumbinary disk, is comparatively molecule-poor. Revealing these characteristics is crucial to our understanding of stellar recycling.

## 1 Introduction

Evolved stars have long been upheld as the major sites of chemical enrichment in the Universe. In the case of massive stars, this occurs in Type II supernovae that yield elements up to iron (fused in the star) and additional heavier elements through energetic r-process nuclear reactions (during the supernova). As for the more typical low-to-intermediate mass stars (< 10solar masses) which are not large enough to fuse elements up to iron, their enrichment of the interstellar medium (ISM) occurs over a longer period of time (about 1 million years), well after they have evolved off the main sequence and reached the end of the what is known as the asymptotic giant branch (AGB). Thermally pulsing AGB stars have a complex structure comprising an inert carbon/oxygen core, a periodically igniting helium shell, a hydrogen burning shell, and a convective envelope that extends out to the stellar photosphere.

In a process that is thought to be aided by stellar pulsations, material in the 2-10 stellar radii region undergoes high temperature reactions to form gas phase molecules, some of which condense and coagulate to form the seeds of silicate/carbonaceous dust grains. Radiation pressure then accelerates these grains over the local escape velocity and they are then pushed out into the interstellar medium along with gas phase material which is coupled to the dust through collisions. The result is significant mass-loss (on the order of  $10^{-8} - 10^{-4}$  solar masses per vear) in a large-scale wind of gas and dust that extends out to thousands of stellar radii, an object commonly known as a circumstellar envelope (CSE). These environments are well-known for their rich molecular chemistry, which can be studied using radio and submillimeter wavelength telescopes. Characterizing this chemistry is crucial to understanding the processing of stellar material as it is reintroduced into the ISM.

The general understanding of how chemistry proceeds in CSEs assumes precursor molecules (e.g. CO, HCN, SiO) form out of gas phase thermochemical equilibrium in the hot, dense inner envelope. Once they reach the outer regions where there is more ultraviolet light from interstellar radiation, these species then undergo photochemistry to form exotic product molecules (e.g.  $HC_5N$ , SiN, MgNC) (Ziurys 2006). However, recent leaps in observational capability have revealed that this picture may be much more complicated than previously thought. Agúndez et al. (2015) and Quintana-Lacaci et al. (2017) discovered that CH<sub>3</sub>CN and NaCN

are present in the inner wind (< 5") of the carbon star IRC+10216, despite their only known formation routes involving photochemistry.

An important aspect of AGB evolution that has become clear with the advent of ALMA is the prevalence of binary companion stars influencing mass loss and shaping circumstellar winds (Decin, 2021). Companions are difficult to detect directly in these systems, due to the intrinsic luminosity of the AGB star, and the high attenuation of visible light by their dusty envelopes. However, several recent studies of gas and dust kinematics have shown the perturbative effects binary companions can have on many AGB and proto-planetary nebula (PPNe) systems. Both small-scale asymmetries, such as density-enhanced clumps (e.g. Khouri et al., 2016; Agúndez et al., 2017; Leão et al., 2006), and large-scale structures, such as spirals (e.g. Mauron & Huggins, 2006; Maercker et al., 2016; Decin et al., 2015; Ramstedt et al., 2017), disk geometries (e.g Kervella et al., 2014; Homan et al., 2018, 2020), and bipolar outflows (e.g. Kim et al., 2015; Sahai et al., 2017; Lagadec et al., 2011) have been detected. In particular, the ALMA Large Program ATOMIUM (2018.1.000659.L, PI: Decin) has shown the widespread nature of these structures through a survey of numerous AGB outflows (Decin et al., 2020). It is now thought that influence from stellar and planetary companions is closely related to the stark morphological changes in circumstellar material during the transition between the AGB and PN stages of evolution (Sahai et al., 2007).

While their physical effects have been studied in detail, the chemical impact of companion stars embedded in CSEs and PPNe has not yet been observationally tested. IRC+10216, CIT 6, and V Hya are three carbon-rich AGB stars that all show different signs of binary influence, with envelopes harboring companion-induced shells, large-scale spiral arms and an expanding Keplerian disk (Decin et al., 2011; Kim et al., 2015; Sahai et al., 2022). Though considerable work has been done on the dynamical physics of these sources. detailed mapping efforts are needed to better constrain their chemistry. We conducted an archival interferometric line study of IRC+10216, CIT 6, and V Hya to constrain the abundance and distribution of product molecules in these sources, and determine how these vary with outflow morphology.

# 2 Observations and reduction

We utilize observations from six publicly available archival ALMA projects to map transitions of  $HC_3N$  toward IRC+10216. Projects 2016.1.00251.S, 2019.1.00507.S, and 2011.0.00229.S provide Band 7, 6, and 3 spectral scans of the carbon star which cover the J = 38 - 37, J = 28 - 27, and J = 30 - 29 transitions of HC<sub>3</sub>N. In the gas phase, this species is formed primarilv through the reaction between acetylene  $(C_2H_2)$  and the cyanide radical (CN), the latter of which is only available as a reactant when the flux of UV photons is large enough to efficiently dissociate the precursor molecule HCN (Agúndez et al., 2017). Because  $C_2H_2$  is an abundant precursor molecule and one of the main carriers of carbon in C-rich CSEs (Santoro et al., 2020), HC<sub>3</sub>N is one of the first product molecules to form out of UV-driven chemistry, making it useful in probing the photoprocessing of gas phase material in these objects.

For CIT 6 and V Hya, we use observations from project codes 2015.1.00271.S, 2016.1.00033.S, and 2018.1.01113.S. The first includes a molecular line survey of both sources spanning 80 – 110 GHz, covering numerous transitions of chemically relevant species. The latter provide Band 6 and 7 data, covering higher transitions of similar molecules that trace warmer regiions of each source.

All data were calibrated using CASA's standard calibration pipeline. Visibilities were transformed to a velocity resolution of  $0.5 \,\mathrm{km} \,\mathrm{s}^{-1}$ and deconvolution was performed using the tclean CASA task with briggs weighting.

# 3 <u>Results</u>

#### 3.1 Emission Maps

Toward CIT 6 and V Hya, we detect emission from over 12 molecules in addition to the HC<sub>3</sub>N lines observed toward IRC+10216. Figures 1 and 2 show examples of emission maps toward these sources, demonstrating their unique outflow shapes. CIT 6 shows a clear spiral pattern in both <sup>13</sup>CO and carbon chain species, while V Hva shows the characteristic velocity pattern of a rotating Keplerian disk. Moreover, CIT 6 shows distinct deviations between the brightness patterns of  $HC_3N$  and  $^{13}CO$ , indicating that the build up of cyanopolyynes is not isotropic in this source. Toward V Hya, we obtained a surprising detection of warm  $C_4H$  at Band 7, which suggests that radical species which typically only form in the cool outer regions of spherical envelopes are instead present in the  $\sim 200 \,\mathrm{K}$  disk of V Hya.



Figure 1: Map of various molecular emission lines toward CIT 6 with contours of <sup>13</sup>CO J = 3 - 2 overlaid. All maps were taken at the system velocity ( $V_{sys} = -2 \text{ km s}^{-1}$ ), and contours are shown at 3, 6, 9, and 12 times the rms noise of the <sup>13</sup>CO image.



Figure 2: Channel maps of  $HC_3N J = 11 - 10$  emission with contours of  $HC_5N$  maps overlaid. In the center bottom panel, the integrated map of HNC is shown, demonstrating the extent of the rotating disk of material around V Hya.

Maps of the studied HC<sub>3</sub>N lines toward IRC+10216 are shown in Figure 3. All images represent emission averaged  $0.75 \,\mathrm{km} \,\mathrm{s}^{-1}$ about the systemic velocity of IRC+10216 ( $V_{sys} = -26.5 \,\mathrm{km} \,\mathrm{s}^{-1}$ ). These maps show primary morphologies centered on the position of the AGB star extending out to 5". This represents the most compact emission of a cyanopolyyne molecule that has been observed toward an AGB star.

The distribution of the J = 28 - 27 transition shows an extended component reaching  $r = \sim 3$ " surrounded by density-enhanced arcs. The majority of this emission is entirely separate from that observed



Figure 3: Emission maps of three  $HC_3N$  lines toward IRC+10216 from separate archival ALMA observations. The yellow circle denotes a radius of 7.5". The synthesized beam is shown in the bottom-left corner of each panel.

in the J = 10 - 9 line by Agúndez et al. (2017), with the notable exception of a bright clump to the SW at a radius of 10". In the central component, the average brightness of the line is 10 mJy/beam, with asymmetric clumps in the N and SW. Although a central peak is seen at the position of the carbon star, we expect that this is contributed from an interloping transition of an unidentified molecule, which was noted in the single-dish survey conducted by He et al. (2008). Because this transition is sufficiently far away in frequency, we expect that its distribution is a point source, and only contaminates the central part of this map.

The J = 30 - 29 line also appears in a bright clump to the SW which is spatially coincident with those seen in the other transitions. However due to the poor uv-coverage and sensitivity of these observations, very little additional emission is seen in this map. If this line has a similar extended component as seen in J = 30-29, we would expect most of this flux to be resolved out by the interferometer given its maximum recoverable scale. Due to these observational limitations, we did not include this line in our radiative transfer analysis.

Finally, the J = 38 - 37 line also shows bright, spatially resolved emission that is entirely separate from the map in Agúndez et al. (2017). In contrast to J = 28 - 27, the distribution of this line is entirely concentrated within a radius of 4" and shows no central peak on the position of IRC+10216. The emission is again not azimuthally symmetric, and traces knots with an average brightness of 30 mJy/beam.

Figure 4 shows the maps of these  $HC_3N$  transitions as contours overlaid on a map

of <sup>13</sup>CO J = 3 – 2. Since <sup>13</sup>CO has constant abundance throughout circumstellar envelopes, it is useful as an indicator of the density structure of stellar outflows. With this in mind, we see that the bright arcs and knots traced by HC<sub>3</sub>N are spatially coincident with density enhancements that are a result of non-isotropic mass-loss.

## 3.2 Non-LTE Radiative Transfer Modeling

We employ a forward modeling approach consisting of simulated imaging with LIME (Brinch & Hogerheijde, 2010), and subsequent visibility sampling with vis\_sample<sup>1</sup>. LIME is a radiative transfer code used to simulate molecular excitation and radiation in astronomical environments. Given a 3D physical structure describing the density and temperature of a region along with the abundance distribution of a targeted molecule, LIME solves the populations and uses a ray-tracing algorithm to produce model image cubes of rotational lines. We then sample those images based on the uv-coverage of the observations to create model visibilities for each line. Those visibilities are then reimaged with the same parameters used to create the maps in Fig. 3.

Though LIME is capable of simulating 3D structures, we use a 1D approximation for the physical parameters of IRC+10216. Though there are clear asymmetries in the morphologies seen in Figures 3 and 4, these require computationally expensive hydrodynamical simulations to describe, and 1D approximations have been utilized successfully for chemical studies of IRC+10216 in the past (Agúndez et al., 2011).

Our model adopts the temperature and density profiles used in (Cernicharo et al., 2011). We also use a mass-loss rate of  $2.7 \times 10^{-5} \,\mathrm{M_{\odot}/yr}$ , which is the value obtained by Guélin et al. (2018) specific to regions within a radius of 10". The spectroscopic data for  $HC_3N$  was obtained from the LAMBDA database which uses the transition strengths and collisional rates from Faure et al. (2000). These rates were extrapolated to extend to include the J =45 rotational level. Additionally, we take into account the affect of pumping to vibrational states via infrared photons by including the  $\nu_5$  and  $\nu_6$  transition ladders which were obtained from the HITRAN  $database^2$ .

To apply this to  $HC_3N$ , we ran LIME for several abundance profiles. The shape of these profiles was motivated by the results of the chemical model by Agúndez et al. (2017). The resulting best fit profile is shown in Fig. 5, and its comparison with the observations is shown in the bottom two panels of Fig. 6. We find that a fractional abundance with respect to  $H_2$ of  $10^{-8}$  is needed to reproduce the average intensity in our maps, and that this abundance must be increasing with radius in this region to explain the distribution of the observed brightness. When compared with the results of previous chemical models, this represents a stark overabundance of at least one order of magnitude.

## 4 <u>Discussion</u>

Our many spectral line maps toward CIT 6 and V Hya show clear deviations from the typical model of AGB envelope chemistry. In the former, this was the asymmetric formation of carbon chains,

<sup>&</sup>lt;sup>1</sup>https://github.com/AstroChem/vis\_ sample

<sup>&</sup>lt;sup>2</sup>https://hitran.org/lbl/



Figure 4: Map of <sup>13</sup>CO J = 3 – 2 emission toward IRC+10216 with contours of HC<sub>3</sub>N maps overlaid. All maps were taken at the system velocity ( $V_{sys} = -26.5 \text{ km s}^{-1}$ ), and contours are shown at 3, 6, 9, and 12 times the rms noise of each respective image.

and the presence of hot  $HC_3N$  in a single blue-shifted clump of material. For V Hya, the Keplerian disk morphology clearly owes itself to the production of carbon chains and other complex species at high temperatures. This likely occurs because the inner regions are more exposed to the interstellar radiation field than in spherical sources, allowing photochemistry to occur readily at warm temperatures.

From our observations of IRC+10216, it is clear that  $HC_3N$  is forming more readily between distances of  $10^{15}$  and  $10^{16}$  cm from IRC+10216. One possible explanation for this behavior, in addition to the observed abundances of other photochemical products discussed previously, is that an embedded binary companion star could be supplying UV photons to the inner regions of this circumstellar envelope. Previous studies of IRC+10216 have concluded that it is part of a binary system (Guélin et al., 2018), and if its companion has a high enough temperature, its radiation could be enough to influence the chemistry of the envelope.

To test this hypothesis, we employed the photochemical model of Van de Sande

et al. (2021), which was built to predict molecular abundances in AGB envelopes with an internal source of UV radiation. This model was run using the same physical parameters of IRC+10216 discussed in Section 3.2. In addition, this chemical model uses a porosity formalism to describe the clumpiness of the outflow. The main components of this formalism are the clump volume filling factor  $(f_{vol})$  which describes the fraction of the envelope that is occupied by clumps, and the clumpinterclump density contrast  $(f_{ic})$ , which describes how overdense the clumps are. We ran this photochemical model for a wide range of companion scenarios.

In all models, a binary companion with surface temperature larger than 6000 K causes an increased abundance of HC<sub>3</sub>N within a radius of  $10^{16}$  cm relative to the companionless model. An example of this is shown in Fig. 5. While these models can reproduce the  $\sim 10^{-8}$  abundance feature constrained by our observations, there is a notable difference in the shape of the profiles. In the companion models we see a much shallower, almost constant slope at inner radii, whereas the observations suggests the abundance tapers off around  $10^{15}$  cm. This could be explained by some of the limitations and approximations of the chemical model, namely that all the companion photons are release instantaneously into the porous wind. So further investigation is needed to resolve these details.



Figure 5: The retrieved IRC+10216 HC<sub>3</sub>N abundance (black) together with the chemical modelling results. Gray, solid: smooth outflow without a stellar companion. Red, dotted: porous outflow (characterised by  $f_{\rm ic} = 0.40$ ,  $f_{\rm vol} = 0.50$ , and  $l_* = 2 \times 10^{13}$  cm) without a stellar companion. Orange, dashed: smooth outflow with a solar-like companion and dust condensation radius  $R_{\rm dust} = 5$  R<sub>\*</sub>. Blue, solid: porous outflow with a solar-like companion and  $R_{\rm dust} = 5$  R<sub>\*</sub>. The shaded red region represents the radii where the HC<sub>3</sub>N abundance is best sampled by the observations.

# 5 <u>Conclusions</u>

We conducted a study of the photochemical products toward the carbon stars IRC+10216, CIT 6, and V Hya using archival ALMA observations. Through rigorous simulations of the observed lines we identify a clear enhancement of this molecule within a radius of 5" from IRC+10216. We then compared these results with the predicted abundances of a specialized photochemistry model and find that the observations could be explained, in part, by a 6000 K stellar companion embedded near the dust formation region of IRC+10216. Toward CIT 6 and V Hya we also see anomalous distributions of chemical products, including but not limited to  $HC_3N$ ,  $HC_5N$ ,  $C_3N$ , and  $C_4H$ .

The implications of these results on how we understand stellar recycling are ex-In recent years, it has become citing. more clear the important role binary stellar companions of AGB stars play in their mass-loss and envelope morphology (Decin et al., 2020), but this is some of the first direct evidence we see of these unique orbital systems influencing the chemistry and processing stellar material as it is released into the ISM. Similar future astrochemical studies into IRC+10216, other binary AGB stars, and proto-planetary nebula will be instrumental in reframing how gas and dust are processed in stellar envelopes.

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Figure 6: Azimuthal averaged brightness distributions of  ${}^{13}$ CO (top), and the two HC<sub>3</sub>N lines we model with LIME. Dash-dotted lines correspond to the visibility sampled RT models using the abundance profile shown in Fig. 5. For  ${}^{13}$ CO, the visibility sampled result is shown (dashed) in reference to a plain convolution of the LIME image cube (dotted).

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