^{13}C isotope chemistry in O and C-rich AGB star envelopes

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Introduction

An asymptotic giant branch (AGB) star is a low or intermediate mass star (< 8$M_\odot$) at a late evolutionary phase in its life. The star evolves into a degenerate C/O core, undergoes intense mass loss and injects dust and molecules into the surrounding regions, creating a circumstellar envelope (CSE). A schematic description[1] of AGB stars is shown in Figure 1. The molecular content, and also the grain types, in the CSEs of AGB stars are to a large extent determined by the C/O ratio of the central star. Depending on this ratio, AGB stars are divided into three different spectral types: C-rich AGB stars (C/O>1), O-rich or M-type AGB stars (C/O<1) and S-type AGB stars (C/O≈1).

In this work we present a new chemical model for the study of ^{13}C chemistry in the envelopes of AGB stars. Tracing the radial evolution of ^{12}C/^{13}C in AGB star envelopes is crucial for the interpretation of single-dish and interferometric observations, which will help determine the intrinsic nucleosynthetic ratio of the star vs. the molecular ratio of the envelope. Improved knowledge of these isotopic ratios is expected to provide insight into the contributions of evolved star ejecta into the Galaxy and how it may influence Galactic chemical evolution, as well as isotopic anomalies found in meteoritic samples.

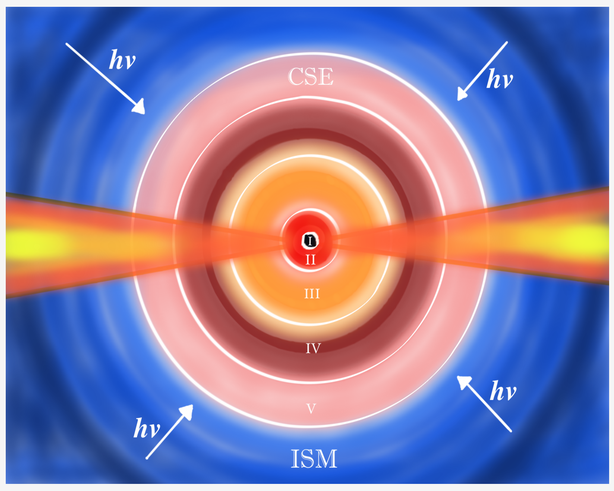


Figure 1 : Schematic structure of the CSE for an AGB star, which is divided into 6 regions: (I) a degenerate C/O core and He/H burning shell, (II) a convective shell, (III) a stellar atmosphere where parent species are formed, (IV) a dust formation shell with an expanding envelope, (V) an outer CSE where daughter species are formed.

The Chemical model

The chemical network, derived from a subset of the UMIST RATE12[2] database, contains 252 species coupled by 4839 reactions and is appropriate for use in both oxygen and carbon-rich envelopes. For the O-rich model the simulation starts at the inner envelope with the following set of parameters : the radius r_i = 2.0e15 cm, the molecular hydrogen number density n_{H2} = 5.2e5 cm^{-3}, the visual extinction A_v = 1.11 mag and the kinetic temperature of the gas T = 100 K. For the C-rich model : r_i = 2.0e15 cm, n_{H2} = 3.23e6 cm^{-3}, Av = 6.90 mag and T = 221 K. Figure 2 shows the evolution of these parameters in function of the radius. The Parent species (Table 1) injected at the inner radius have a ^{12}C/^{13}C ratio equal to 50 in the C-rich model , and have a ratio equal to 15 in the O-rich model. Our chemical network includes all singly and doubly ^{13}C-substituted isotopologues for species containing up to 2 C atoms.

Table 1 : Parent species and their respective initial abundances for the C-rich and O-rich models.

C-RICH MODEL		O-RICH MODEL	
Species	***Initial Ab.***	***Species***	***Initial Ab.***
CS	7.00(-7)	He	1.70(-1)
^{13}CS	1.40(-8)	CO	2.00(-4)
SiO	1.80(-7)	^{13}CO	1.30(-5)
SiS	1.30(-6)	H_2O	6.60(-5)
CO	6.00(-4)	N_2	1.50(-4)
^{13}CO	1.20(-5)	NH_3	2.00(-6)
CCH_2	8.00(-5)	HCN	4.40(-7)
$^{13}CCH_2$	3.20(-6)	H^{13}CN	2.90(-8)
HCN	2.00(-5)	CO_2	4.40(-9)
H^{13}CN	4.00(-7)	$^{13}CO_2$	2.90(-10)
CH_4	3.50(-6)	CS	8.00(-8)
$^{13}CH_4$	7.00(-8)	^{13}CS	5.30(-9)
NH_3	2.00(-6)	SiS	1.10(-5)
H_2O	1.00(-7)	SiO	1.60(-5)
CCH_4	2.00(-8)	SO	2.00(-6)
$^{13}CCH_4$	4.00(-10)	SO_2	2.00(-6)
H_2S	4.00(-9)	H2S	1.00(-8)
N_2	2.00(-4)	HS	2.30(-8)
He	1.00(-1)		
Outflow velocity (km/s)	18.0		14.5
Mass-loss rate ($M_\odot$)	3.0(-6)		1.5(-5)

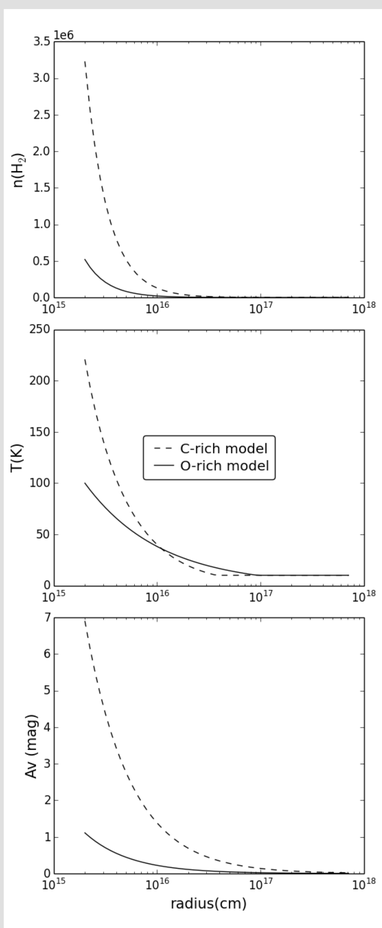


Figure 2 : Physical parameter profiles calculated as a function of the radius in the C-rich and O-model.

Results

Fractional Abundance profiles

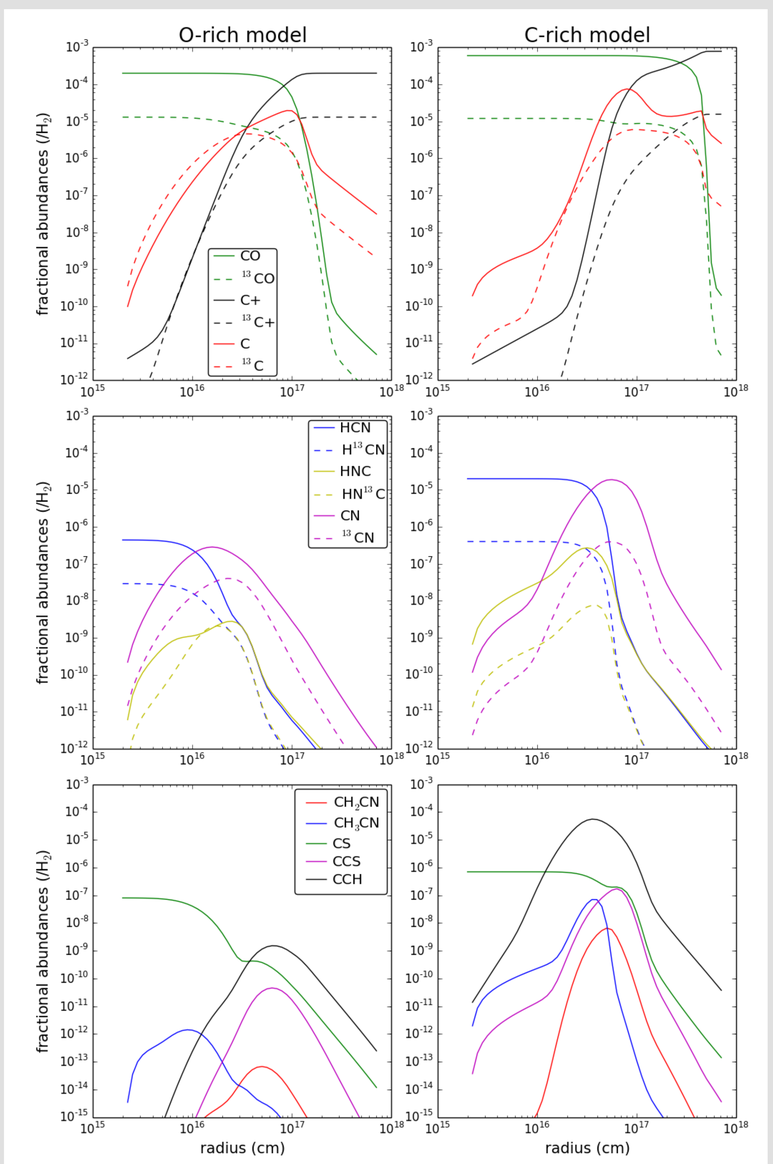


Figure 3 : Fractional abundance (log_{10}) profiles of some observable (and potentially observable) species and their isotopologues calculated in a C-rich and O-rich model.

^{12}C/^{13}C ratio profiles

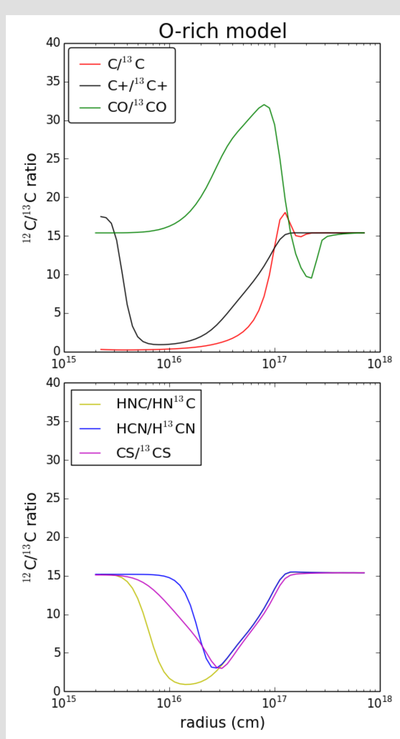


Figure 4 : ^{12}C/^{13}C ratio profiles of some observable species calculated in our O-rich model.

The main source of ^{13}C fractionation in both cases is the selective photodissociation of ^{13}CO in the inner parts of the circumstellar envelope, where ^{12}CO is self-shielded. This results in an enriched source of atomic ^{13}C for the ensuing chemistry. The following fractionation reactions also play a significant role:

$^{13}C^+ + CO \rightarrow C^+ + {}^{13}CO$

$^{13}CCH + H \rightarrow C^{13}CH + H$

$^{13}CCS + S \rightarrow C^{13}CS + S$

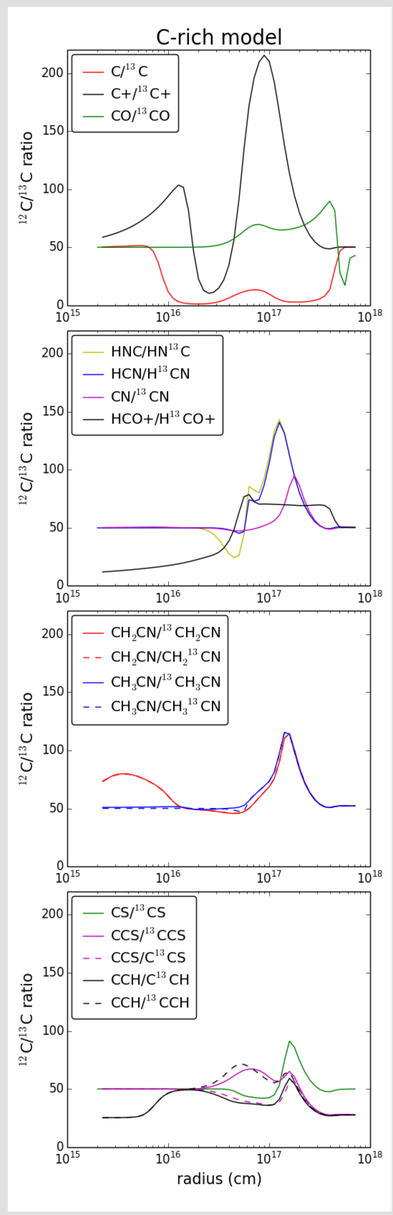


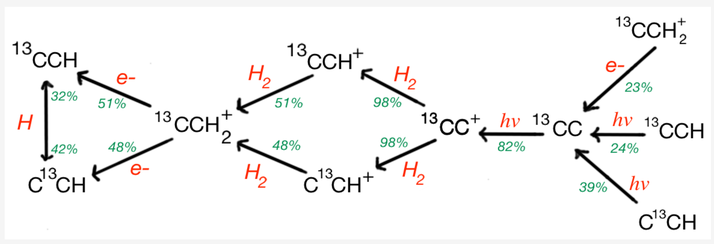
Figure 5 : : ^{12}C/^{13}C ratio as a funciton of radius for some observable species in our C-rich model.

Discussion

Using our simplified chemical network, the ^{12}C species fractional abundances relative to H_2 calculated with C-rich and O-rich models show similar results to some previous studies, such as X. Li et al.[3] in the O-rich case (IK Tau) and Agundez et al.[4] in the C-rich case (IRC+10216). Our models predict variations in the ^{12}C/^{13}C ratio as a function of radius for C^+, CO, CN, HCN, HNC, CS, HCO^+, CH_2CN, CH_3CN and others, many of which should be detectable using existing or future mapping observations.

The fractional abundance profiles in Fig.3 obtained in both models can be explained by analyzing the formation and destruction paths of each species and their isotopologues. The H^{13}CN fractionation in the O-rich model and the ^{13}CCH fractionation in the C-rich model result from the following pathways:

$$^{13}CO \xrightarrow{hv} {}^{13}C \xrightarrow{hv} {}^{13}C^+ \xrightarrow{NH} {}^{13}CN \xrightarrow{H_2} H^{13}CN^+ \xrightarrow{H_2} H^{13}CNH^+ \xrightarrow{e-} H^{13}CN$$



The ^{12}C/^{13}C ratio profiles in Fig.4-5 can be explain by looking at the fractional abundances. For example in the O-rich model the ^{12}CO/^{13}CO ratio, showing the higher value in Fig.4, begins to increase at a close radius ~10^{16} cm due to the photolysis of ^{13}CO, up to a maximum at 8.2x10^{16} cm, then C^+ and $^{13}C^+$ become the main carbon reservoir; ^{12}CO/^{13}CO decreases to a minimum at 2.1x10^{17} cm. For the others species ratios in this figure, except atomic carbon, we obtained ratios significantly different from the initial (parent) ^{12}C/^{13}C ratios in the molecular envelope at a radius 3x10^{15} cm to 10^{17} cm, due to the incorporation of atomic ^{13}C as a result of neutral-neutral chemistry in this range. The ^{12}C/^{13}C ratio value is low at the inner envelope until ~10^{17} cm, due to a greater atomic ^{13}C fractional abundance (from ^{13}CO photolysis). Another example, in the C-rich model, the increasing H^{12}CN/H^{13}CN around 10^{17} cm is due to an increase in $^{12}CH_2$/$^{13}CH_2$ in the following pathway:

$$^{13}CO \xrightarrow{hv} {}^{13}C \xrightarrow{hv} {}^{13}C^+ \xrightarrow[20\%]{H_2} {}^{13}CH_2^+ \xrightarrow{H_2} {}^{13}CH_3^+ \xrightarrow{e-} {}^{13}CH_2 \xrightarrow{N} H^{13}CN$$

Future Work

1. Expand the chemical network to include ^{13}C fractionation chemistry for species with 3 or more C atoms, including polyynes and cyanopolyynes.
2. Generate models for ^{18}O and ^{15}N chemistry in circumstellar envelopes
3. Comparison of models with interferometric (and single-dish) observations will provide new insights into the origins of the observed isotope abundances. Mapping ^{12}CO/^{13}CO will provide a test for our models.
4. Improved accuracy will be obtained by inclusion of more detailed radiative transfer and self-shielding calculations.

References : [1] X. Li, PhD, Leiden University ; [2] D. McElroy and al, 2013, A&A, 550, A36 ; [3] X. Li et al, 2015, A&A, 588, A4 ; [4] M. Agundez and J. Cernicharo, 2006, ApJ, 650:374-393

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