Molecular complexity around evolved stars

Marcelino Agúndez
Instituto de Física Fundamental, CSIC, Spain

The Cosmic Cycle of Dust and Gas in the Galaxy: From Old to Young stars
9-13 July 2018, Guy Nhon (Vietnam)
Large prevalence of organic molecules
≈3/4 (all with 6 or more atoms) contain at least one C atom

Large organic molecules around evolved stars:
- Presence of unsaturated carbon chains
- No saturated O-, N-bearing stable molecules

Metal-bearing molecules (Mg, Al, Ti, Fe, Na, K)
They are only found around evolved stars
<table>
<thead>
<tr>
<th>$10^{-3}$ CO</th>
<th>CARBON-RICH: The ~80 molecules detected in IRC+10216</th>
</tr>
</thead>
</table>
| $10^{-4}$ | $\begin{align*}
C_2H_2 & \quad \text{HCN} \\
\end{align*}$ |
| $10^{-5}$ | $\begin{align*}
\text{CH}_4 & \quad \text{NH}_3 \\
\text{C}_2H & \quad \text{CN} \\
\text{C}_4H & \quad \text{HC}_3\text{N} \\
\text{C}_2 & \quad \text{SiC}_2 \\
\text{C}_3 & \quad \text{SiS} \\
\end{align*}$ |
| $10^{-6}$ | $\begin{align*}
\text{C}_3\text{N} & \quad \text{CS} \\
\text{CH}_4 & \quad \text{HC}_3\text{N} \\
\text{CH}_3\text{CN} & \quad \text{C}_2\text{S} \\
c-C_3\text{H}_2 & \quad \text{HCP} \\
c-C_3\text{H} & \quad \text{HC}_7\text{N} \\
\text{C}_2\text{H}_4 & \quad \text{H}_2\text{CO} \\
\text{CH}_3 & \quad \text{C}_3\text{S} \\
\text{C}_6 & \quad \text{CH}_3\text{SiH}_3 \\
\text{H}_2\text{C}_4 & \quad \text{CP} \\
\text{H}_2\text{CO} & \quad \text{HF} \\
\end{align*}$ |
| $10^{-7}$ | $\begin{align*}
\text{H}_2\text{O} & \quad \text{C}_5 \\
\text{OH} & \quad \text{CN}^- \\
\text{C}_6\text{H} & \quad \text{CH}_3\text{CN} \\
\text{C}_5\text{H} & \quad \text{C}_2\text{S} \\
c-C_3\text{H}_2 & \quad \text{c-SiC}_3 \\
\text{CH}_3\text{C}_2\text{H} & \quad \text{H}_2\text{CS} \\
c-C_3\text{H} & \quad \text{SiN} \\
\text{C}_2\text{H}_4 & \quad \text{PH}_3 \\
\text{H}_2\text{C}_4 & \quad \text{MgNC} \\
\end{align*}$ |
| $10^{-8}$ | $\begin{align*}
\text{C}_8\text{H} & \quad \text{HC}_3\text{N} \\
\text{CH}_2\text{CN} & \quad \text{H}_2\text{CS} \\
\text{HC}_2\text{N} & \quad \text{SiN} \\
\text{C}_5\text{N} & \quad \text{CP} \\
\text{C}_7\text{H} & \quad \text{HCCNC} \\
\text{H}_2\text{C}_6 & \quad \text{C}_2\text{H}_3\text{CN} \\
\text{C}_6\text{H}- & \quad \text{H}_2\text{S} \\
\text{C}_3\text{O} & \quad \text{c-SiC}_3 \\
\text{C}_8\text{H}- & \quad \text{SiC}_4 \\
\text{H}_2\text{C}_3 & \quad \text{SiCN} \\
\text{C}_3\text{N}^- & \quad \text{SiNC} \\
\text{C}_6\text{H}- & \quad \text{PN} \\
\text{C}_3\text{O} & \quad \text{C}_2\text{P} \\
\end{align*}$ |
| $10^{-9}$ | $\begin{align*}
\text{HCO}^+ & \quad \text{HNCCC} \\
\text{C}_4\text{H}- & \quad \text{MgCN} \quad \text{HMgNC} \\
\end{align*}$ |
| $10^{-10}$ | $\begin{align*}
\end{align*}$ |
<table>
<thead>
<tr>
<th>Concentration (cm⁻³)</th>
<th>Species</th>
</tr>
</thead>
<tbody>
<tr>
<td>10⁻³</td>
<td>CO, H₂O</td>
</tr>
<tr>
<td>10⁻⁴</td>
<td>OH, H₂O</td>
</tr>
<tr>
<td>10⁻⁵</td>
<td>H₂O</td>
</tr>
<tr>
<td>10⁻⁶</td>
<td>SO₂, SO, SiO, SiS</td>
</tr>
<tr>
<td>10⁻⁷</td>
<td>H₂S, H₂CO, NH₃, CS, PN, NaCl</td>
</tr>
<tr>
<td>10⁻⁸</td>
<td>HCO⁺</td>
</tr>
<tr>
<td>10⁻⁹</td>
<td>NS, HNC</td>
</tr>
<tr>
<td>10⁻¹⁰</td>
<td></td>
</tr>
</tbody>
</table>
Circumstellar envelopes around AGB stars

IRC+10216 in V band (Leao et al. 2006)
IRC+10216 in CO (Cernicharo et al. 2015)
R Sculptoris in CO (Maercker et al. 2012)
IRC+10216 in CN (Agúndez et al. 2017)
standard scenario

chemical equilibrium
chemistry frozen
photochemistry

PARENT SPECIES
distribution:
concentric around star

DAUGHTER SPECIES
distribution:
hollow shell

\begin{array}{cccccc}
\text{r [cm]} & 10^{13} & 10^{14} & 10^{15} & 10^{16} & 10^{17} & 10^{18} \\
\text{T [K]} & 3000 & 1000 & 100 & 20 & \\
\text{n [cm}^{-3}] & 10^{15} & 10^{12} & 10^{8} & 10^{5} & 10^{3} & 10
\end{array}
Outline of the rest of the talk:

1) Some introduction (already done)

1) Chemistry in the inner layers

1) Chemistry in the outer envelope

1) Concluding remarks
The inner circumstellar layers
CW Leo observed in the MIR (11-14 μm) with IRTF/TEXES (Fonfría et al 2008)

Spectra shows absorption lines from C₂H₂ and HCN present in the inner circumstellar envelope
Single-dish millimeter observations

SiS (v=0-6) lines in IRC+10216 (Agúndez et al 2012)

A detailed model allows to derive the radial abundance profile
Gas-phase abundance of SiC$_2$ decreases with increasing density

Can be interpreted in terms of a more efficient formation of dust (and incorporation of SiC$_2$ on grains) at high densities
Legacy of Herschel on circumstellar chemistry

# H$_2$O around carbon stars

Inner-envelope origin

Widespread occurrence in carbon stars

Decin et al (2010)

Neufeld et al (2011)
Legacy of Herschel on circumstellar chemistry

# H₂O around carbon stars
   Inner-envelope origin
   Widespread occurrence in carbon stars

# Other hydrides around AGB stars
   NH₃  (Menten et al 2010; Schmidt et al 2016; Wong et al. 2018)
   HCl  (Cernicharo et al 2010; Agúndez et al 2011)
   HF   (Agúndez et al 2011)
   PH₃  (Agúndez et al 2014)
Comparison between observed abundances and calculated abundances at chemical equilibrium for the carbon star IRC+10216
chemical equilibrium

chemistry frozen

photochemistry

PARENT SPECIES
distribution: concentric around star

DAUGHTER SPECIES
distribution: hollow shell

standard scenario

stellar atmosphere
inner envelope
outer envelope

$R_*$ $r_0$ $r_C$ $r_{PH}$

r [cm]

$10^{13}$ $10^{14}$ $10^{15}$ $10^{16}$ $10^{17}$ $10^{18}$

T [K]

3000 1000 100 20

n [cm$^{-3}$]

$10^{15}$ $10^{12}$ $10^8$ $10^5$ $10^3$ 10
Small-scale distribution of parent species in IRC+10216

The arrival of ALMA

$^{29}\text{SiO J}=6-5$

$^{29}\text{SiS J}=15-14$


$\text{NaCl J}=21-20$

Quintana-Lacaci et al (2016)
Small-scale distribution of Ti and Al oxides in O-rich stars

Evaluating the role of TiO, TiO$_2$, AlO, and AlOH as gas-phase precursors for dust nucleation

The ALMA view of IRC+10216: a forest of U lines arises from the surroundings of the star

(Cernicharo et al 2013)
The outer circumstellar envelope
standard scenario

PARENT SPECIES distribution: concentric around star

DAUGHTER SPECIES distribution: hollow shell
IRAM Plateau de Bure (1990s)

Parent species: concentric around star
Daughter species: hollow shell at ≈15-20''
Parent species: concentric around star
Daughter species: hollow shell at ≈15-20''

$\text{CH}_3\text{CN}$ shows a peculiar distribution
The arrival of ALMA Cycle 2 3mm line survey of IRC+10216 Carbon chains maps (Agúndez et al 2017)

Carbon chain growth in IRC+10216

(Agündez et al 2017)
The growth of polyynes is driven by reactions involving \( \text{C}_2\text{H} \) and \( \text{C}_4\text{H} \) radicals

The growth of cyanopolyynes is driven by reactions involving \( \text{CN} \) and \( \text{C}_3\text{N} \) radicals

Low-temperature kinetics of these reactions studied with CRESU machines
Infrared detection of diacetylene ($C_4H_2$) in IRC+10216 (Fonfría et al 2018)

$C_4H_2$ is a non polar molecule, predicted to form abundantly in the outer envelope. Important observation because it allows to put constraints on the chemical model.

Derived abundance of cold (outer) $C_4H_2$ in good agreement with chemical model. Presence of hot (inner) $C_4H_2$ is puzzling.
Concluding remarks:

# Overall picture of the circumstellar chemistry around AGB stars well understood
  > parent molecules formed under LTE close to the star
  > daughter species formed by photochemistry in outer envelope

# Observations are revealing a growing number of aspects not well understood yet
  > Formation of H₂O in C-rich objects and other hydrides (NH₃, PH₃)
  > Relevance of non-equilibrium chemistry in the inner envelope
different small-scale distribution of molecules: (NaCl, KCl) vs (SiS, SiO) in IRC+10216
role of refractory molecules as precursors of dust grains
distribution of CH₃CN in IRC+10216
existence of hot C₄H₂ in IRC+10216
carriers of unidentified lines arising just close to the star
  > Discontinuous and non-isotropic mass loss

# Need to revise the current paradigm of circumstellar chemistry
  > Dust formation
  > Shocks driven by the stellar pulsation
  > Clumpiness
  > Spiral-like structures caused by binarity
The evolved stars team at IFF, Madrid

José Cernicharo  Luis Velilla Prieto  José Pablo Fonfría

Guillermo Quintana-Lacaci  Sarah Massalkhi  Jason Champion