Lecture:

CIRCUMSTELLAR CHEMISTRY

G. Haro School on Molecular Astrophysics, 11-20 October 2016
The term “circumstellar chemistry” refers in this case to the chemical processes occurring in the ejecta of an evolved star. However, you could consider also the processes that transform e.g. the chemical nature of a cloud of gas and dust surrounding young stars.
Circumstellar chemistry depends on the carbon-to-oxygen ratio:

Most stars are O-rich (C/O<1) like the Sun. However, dredge-up processes may invert this ratio: C-rich (C/O>1). There are also stars with C/O~1 (S-type stars).

\[
\log\left(\epsilon_H\right) = 12.00
\]
\[
\log\left(\epsilon_x\right) = \log\left(\frac{N_x}{N_H}\right) + 12
\]

Asplund et al., 2009
After $H_2$, CO is the most abundant species formed (independent of the C/O ratio):

It is a very stable molecule (Dissociation energy of the ground state: $89462 \text{ cm}^{-1} = 11.09 \text{ eV}$, $\lambda < 1118 \text{ Å}$)

Thus, all the possible CO is formed and then, depending on which element is in excess (C/O) C- or O-bearing molecules will be formed

<table>
<thead>
<tr>
<th></th>
<th>Tracing molecules</th>
<th>Dust grains</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>C-rich (e.g. IRC+10216)</strong></td>
<td>$C_2H$, $SiC$, $HC_xN$...</td>
<td>Carbonaceous</td>
</tr>
<tr>
<td><strong>O-rich (e.g. IK Tau)</strong></td>
<td>$SO$, $SO_2$, $NO$, $OH$ ...</td>
<td>Silicates, Metal oxides</td>
</tr>
<tr>
<td><strong>S-type (e.g. $\chi$ Cyg)</strong></td>
<td>Mixed</td>
<td>Mixed</td>
</tr>
</tbody>
</table>

However, O-bearing molecules are found in C-rich CSEs and vice versa
Molecular formation under TE conditions in the atmosphere of the star:

High densities ($n > 10^{12} \text{ cm}^{-3}$)

Temperatures ($T_{\text{kin}} = 2000-3000$)

Example: dissociation of $H_2$

$$H_2 \rightleftharpoons H + H$$

$$p = p_{H_2} + p_H$$  \textit{(Partial pressures)}

Dissociation constant can be calculated using thermodynamical properties (see bibliography and additional slides)

$$\frac{p_H^2}{K_p} + p_H - p = 0$$

$$p_H = \frac{-1 + \sqrt{1 + 4p/K_p}}{2/K_p}$$

$$p_{H_2} = p - \left(\frac{-1 + \sqrt{1 + 4p/K_p}}{2/K_p}\right)$$
Thermodynamical equilibrium: general case

- For each molecule in our system, we can write:
  \[
  \underbrace{X_x Y_y Z_z}_{i} \implies xX + yY + zZ
  \]
  \[
  K_{p,i} = \frac{(p_X)^x (p_Y)^y (p_Z)^z}{p_i}
  \]

- For each element in our system, we can write these conservation equations:
  \[
  n^0_{H} = n_H + x \ n_{AH_x} + y \ n_{BH_y} + z \ n_{BH_z} + \ldots
  \]
  \[
  n^0_{C} = n_C + x \ n_{AC_x} + y \ n_{BC_y} + z \ n_{BC_z} + \ldots
  \]
  \[
  n^0_{O} = n_O + x \ n_{AO_x} + y \ n_{BO_y} + z \ n_{BO_z} + \ldots
  \]
  \[
  \ldots
  \]

- You can write this densities as a function of H density:
  \[
  n^0_{C} = \epsilon_C n^0_{H}
  \]

... and make use of the ideal gas law
Thermodynamical equilibrium: computational model

- We have a system of equations as follows:

\[ \varepsilon_i k T = p_i + \sum_{n=1}^{N} \frac{(p_i)^h_n (p_j)^c_n (p_k)^o_n \cdots}{K_{p,n}} \]

The system of non-linear algebraic equations can be solved by using a Newton-Raphson method, with a set of initial abundances, a temperature, and the dissociation constants.

Tsuji, 1973

Molecular Abundances in Stellar Atmospheres. II.

T. Tsuji*
Observatoire de Paris-Meudon

Received March 31, revised September 22, 1972

Summary. Chemical equilibria of 36 elements are solved for the physical conditions of cool stellar atmospheres. It is found that the molecular species formed (monoxide, dioxide, halide etc.) and the degree of molecular association, (i.e. the fraction of atoms locked in molecules) are well correlated with the position of each element (both Group and atomic weight) in the periodic table.

In the atmospheres of carbon-rich stars, molecular formation is generally less important than in oxygen-rich atmospheres except for some carbon compounds. The metal oxides in oxygen-rich atmospheres are generally replaced by metal carbides, especially by dicarbides, in carbon-rich atmospheres. The formation of carbides in carbon-rich atmospheres, however, is less effective than that of the corresponding metal oxides in oxygen-rich atmospheres. In carbon stars, it is shown that the Si/S ratio plays a critical role just like the C/O ratio.

Key words: equilibrium constants – chemical equilibrium – molecular abundance – atmospheres of cool stars
These are the results of chemical modelling for a C-rich and an O-rich CSE:
### Types of reactions

- **Chemical reactions occurring in a CSE are similar to those occurring in the ISM:**

<table>
<thead>
<tr>
<th>Type</th>
<th>Example</th>
<th>Units of $k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CR direct processes</td>
<td>$\text{H}_2 + \zeta \rightarrow \text{H}_2^+ + e^-$</td>
<td>$\text{s}^{-1}$</td>
</tr>
<tr>
<td>Neutral-neutral</td>
<td>$\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$</td>
<td>$\text{cm}^3 \text{ s}^{-1}$</td>
</tr>
<tr>
<td>Ion-neutral</td>
<td>$\text{CH}^+ + \text{H}_2\text{O} \rightarrow \text{HCO}^+ + \text{H}_2$</td>
<td>$\text{cm}^3\text{s}^{-1}$</td>
</tr>
<tr>
<td>Radiative association</td>
<td>$\text{Si} + \text{O} \rightarrow \text{SiO} + \gamma$</td>
<td>$\text{cm}^3 \text{ s}^{-1}$</td>
</tr>
<tr>
<td>Dissociative recombination</td>
<td>$\text{HCO}^+ + e^- \rightarrow \text{CO} + \text{H}$</td>
<td>$\text{cm}^3 \text{ s}^{-1}$</td>
</tr>
<tr>
<td>Mutual neutralisation</td>
<td>$\text{H}_2\text{CO}^+ + e^- \rightarrow \text{H}_2\text{CO} + \gamma$</td>
<td>$\text{cm}^3 \text{ s}^{-1}$</td>
</tr>
<tr>
<td>3-body reactions</td>
<td>$\text{H} + \text{H} + \text{H}_2 \rightarrow \text{H}_2 + \text{H}_2$</td>
<td>$\text{cm}^6 \text{ s}^{-1}$</td>
</tr>
<tr>
<td>Thermal dissociation</td>
<td>$\text{CH} + \text{H} \rightarrow \text{C} + \text{H} + \text{H}$</td>
<td>$\text{cm}^3 \text{ s}^{-1}$</td>
</tr>
<tr>
<td>$\gamma$-induced reactions</td>
<td>$\text{HCN} + \gamma \rightarrow \text{CN} + \text{H}$</td>
<td>$\text{s}^{-1}$</td>
</tr>
</tbody>
</table>

$\zeta$: Cosmic ray.  $\gamma$: Photon.

*And also photoprocesses induced indirectly by cosmic rays*
**Chemical kinetics: description**

- **A simple reaction:** \( A + B \rightarrow C + D \)

\[
v = \frac{-dn(A)}{dt} = \frac{-dn(B)}{dt} = \frac{dn(C)}{dt} = \frac{dn(D)}{dt} = kn(A)n(B)
\]

**Rate constant, \( f(T) \)**

- **Arrhenius law:**

\[
k = A \exp\left(-\frac{E_a}{kT}\right) \quad \rightarrow \quad k(T) = A \alpha(T/300)^\beta \exp\left(-\frac{\gamma}{T}\right)
\]

- \( E_a \): activation energy = minimum energy of the reactants system to form the products
- \( A \): pre-exponential factor = fraction of collisions that have \( E \geq E_a \)
Chemical kinetics: generalisation and computational model

- For a first order reaction:

\[ \frac{dn_i}{dt} = -k_i n_i \rightarrow n_i = n_{0,i}e^{-k_it} \]

- We must consider all the species in our system, a chemical reactions network, an initial guess of the abundances, and a physical model \((T(r), n(H_2), \text{mass loss rate, } A_v, \text{cosmic-ray ionisation rate...})\):

\[
\frac{dn_i}{dt} = \sum_{j=1}^{N_f} k_j \prod_{l=1}^{N_{i,\text{reac}}} n_{j,l} - \sum_{m=1}^{N_{d}} k_m n_i \prod_{s=1}^{N_{m,\text{reac}}} n_{m,s}
\]

- Formation of \(i\) \quad Destruction of \(i\)

- Using the physical model of the corresponding CSE, and as initial abundances, you can start using the output from a TE model or observational constraints

The system of non-linear ODEs can be solved by using a Runge-Kutta method, with a set of initial abundances, a physical model \((T(r), n(r))\), and the reaction rates for the chemical network considered.
Chemical kinetics: an example

- Consider pure hydrogen gas in expansion:

  $T = 2000 \text{ K}$  \hspace{1cm}  $n = 10^{12} \text{ cm}^{-3}$

  
  \[
  \text{Initial state: Hydrogen gas at } P_0 \text{ and } T_0, \text{ with } n_H \text{ and } n_{H_2} \text{ at chemical eq.}
  \]

  \[
  \text{Final state: adiabatic expansion (} P \text{ and } T \text{ decrease), abundances will evolve according to chemical kinetics}
  \]

- Chemical network and rates:

  \[
  \begin{align*}
  H + H + H &\rightarrow H_2 + H \\
  H + H + H_2 &\rightarrow H_2 + H_2 \\
  H_2 + H &\rightarrow H + H + H \\
  H_2 + H_2 &\rightarrow H + H + H_2
  \end{align*}
  \]

  \[
  \begin{align*}
  k_{M,H} &= 8.82 \times 10^{-33} \text{ cm}^6\text{s}^{-1} \\
  k_{M,H_2} &= 2.65 \times 10^{-31}T^{-0.6} \text{ cm}^6\text{s}^{-1} \\
  k_{d,H} &= 1.11 \times 10^{-9}T^{0.36}e^{-52043/T} \text{ cm}^3\text{s}^{-1} \\
  k_{d,H_2} &= 3.32 \times 10^{-8}T^{-0.24}e^{-52043/T} \text{ cm}^3\text{s}^{-1}
  \end{align*}
  \]

- System of equations:

  \[
  \begin{align*}
  \frac{dn_H}{dt} &= (2k_{d,H}n_{H_2}n_H + 2k_{d,H_2}n_H^2) - (2k_{M,H}n_H^3 + 2k_{M,H_2}n_H^2n_{H_2}) \\
  \frac{dn_{H_2}}{dt} &= (k_{M,H}n_H^3 + k_{M,H_2}n_H^2n_{H_2}) - (k_{d,H}n_{H_2}n_H + k_{d,H_2}n_{H_2}^2)
  \end{align*}
  \]
Chemical kinetics: example results

• Consider pure hydrogen gas in expansion:

Initial state \[ H_2 \]

Final state \[ H + H \]

\[ H_2 \rightleftharpoons H + H \]

\[ \nu_{exp} = 10^{12} \ell/\text{s} \]

\[ \nu_{exp} = 10^9 \ell/\text{s} \]

\[ \nu_{exp} = 10^6 \ell/\text{s} \]
**Dust formation**

- **Dust formation:**

  A species will condense if its partial pressure is larger than its vapor pressure.

  ![Graph showing dust formation](image)

  Grain growth through condensation and aggregation of species.

  Water ice mantles observed in some OH/IR sources (Justtanont et al. 2006)
Other chemical processes: dust grains and shocks

- **Dust grains chemistry:**
  - Adsorption
  - Desorption
  - Grain-surface (catalytic) reactions

- **Shock-induced chemistry:**
  - Gas compression and heating

Shocks can produce different effects on the chemistry, which are difficult to characterise:
  - Dissociating or not?
  - UV radiation
  - Molecular reformation after shock passage
Circumstellar chemistry: general ideas

- Studied because physical conditions are well-constrained
- Importance of chemical and dynamical times:

Chemical kinetics depends on time. As the gas of the CSE expands, molecules have to re-adapt their abundances to the new physical conditions \((n, T)\) encountered during the expansion. If the dynamical time \((t_d=r/v_{\text{exp}})\) is shorter than the chemical time (i.e. the characteristic time of a given reaction), the abundances will remain constant during the expansion. This is called frozen chemistry.

- Parent and daughter species:

**Parent molecules:** abundant species that have been formed in the innermost parts of a CSE and are injected into the intermediate envelope in gas phase.

**Daughter molecules:** molecules that are formed in the outermost parts of a CSE, as a result of chemical reactions involving parent species. Daughter species are usually distributed in a hollow shell.
Circumstellar chemistry: chemical regions of a CSE

- **Standard scenario:**

![Diagram of circumstellar chemistry](image)

- **Chemical regions:**
  - **Chemical Equilibrium**
  - **Frozen Chemistry**
  - **Photochemistry**

- **Markers:**
  - \( R \), \( r_0 \), \( r_c \), \( r_{PH} \)

- **Species:**
  - \( \text{CO, H}_2\text{O, SiO} \)
  - \( \text{C}_2\text{H}_2, \text{HCN} \)

- **Reactions:**
  - \( \text{H}_2\text{O} \rightarrow \text{OH} + \text{H} \)
  - \( \text{SiO} \rightarrow \text{Si} + \text{O} \)
  - \( \text{C}_2\text{H}_2 \rightarrow \text{C}_2\text{H} + \text{H} \)
  - \( \text{HCN} \rightarrow \text{CN} + \text{H} \)

- **Parameters:**
  - \( r \) [cm]: \( 10^{13}, 10^{14}, 10^{15}, 10^{16}, 10^{17}, 10^{18} \)
  - \( T \) [K]: 3000, 1000, 100, 20
  - \( n \) [cm\(^{-3}\)]: \( 10^{15}, 10^{12}, 10^8, 10^5, 10^3, 10 \)
Circumstellar chemistry: C-rich CSE

- Chemical models:
  - Agúndez et al., 2010
  - Millar, T., 2016

2.5% photons are able to penetrate deep in the CSE
Circumstellar chemistry: C-rich CSE

- The case of IRC+10216:

<table>
<thead>
<tr>
<th>10^{-3}</th>
<th>CO</th>
<th>1(-3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10^{-4}</td>
<td>C_2H_2</td>
<td>8(-5)</td>
</tr>
<tr>
<td></td>
<td>HCN</td>
<td>2(-5)</td>
</tr>
<tr>
<td>10^{-5}</td>
<td>CH_4</td>
<td>3.5(-6)</td>
</tr>
<tr>
<td></td>
<td>C_2H</td>
<td>3(-6)</td>
</tr>
<tr>
<td></td>
<td>NH_3</td>
<td>2(-6)</td>
</tr>
<tr>
<td></td>
<td>C_4H</td>
<td>2.5(-6)</td>
</tr>
<tr>
<td></td>
<td>CN</td>
<td>1.7(-6)</td>
</tr>
<tr>
<td></td>
<td>C_2</td>
<td>1(-6)</td>
</tr>
<tr>
<td></td>
<td>HC_3N</td>
<td>1.4(-6)</td>
</tr>
<tr>
<td>10^{-6}</td>
<td>C_3N</td>
<td>4(-7)</td>
</tr>
<tr>
<td></td>
<td>CS</td>
<td>5(-7)</td>
</tr>
<tr>
<td>10^{-7}</td>
<td>H_2O</td>
<td>1(-7)</td>
</tr>
<tr>
<td></td>
<td>C_5</td>
<td>1(-7)</td>
</tr>
<tr>
<td></td>
<td>HNC</td>
<td>1(-7)</td>
</tr>
<tr>
<td></td>
<td>OH</td>
<td>4(-8)</td>
</tr>
<tr>
<td></td>
<td>C_6H</td>
<td>4(-8)</td>
</tr>
<tr>
<td></td>
<td>C_5H</td>
<td>3(-8)</td>
</tr>
<tr>
<td></td>
<td>CH_3CN</td>
<td>3(-8)</td>
</tr>
<tr>
<td></td>
<td>SiC</td>
<td>4(-8)</td>
</tr>
<tr>
<td></td>
<td>C_3H_2</td>
<td>3(-8)</td>
</tr>
<tr>
<td></td>
<td>CH_3C_2H</td>
<td>3(-8)</td>
</tr>
<tr>
<td></td>
<td>c-C_3H</td>
<td>2(-8)</td>
</tr>
<tr>
<td></td>
<td>HC_7N</td>
<td>2(-8)</td>
</tr>
<tr>
<td>10^{-8}</td>
<td>H_2CO</td>
<td>1.3(-8)</td>
</tr>
<tr>
<td></td>
<td>H_2C_4</td>
<td>1.4(-8)</td>
</tr>
<tr>
<td></td>
<td>C_3S</td>
<td>1.2(-8)</td>
</tr>
<tr>
<td></td>
<td>CP</td>
<td>1(-8)</td>
</tr>
</tbody>
</table>

More molecules found:

- Si_2C
- CCN
- SiHC_3N
- NCCP
- MgCCH
- C_5S
- HMgNC
- FeCN
- KCN
- CN^-
Circumstellar chemistry: C-rich CSE

* The case of IRC+10216:

Lucas et al., 1995

Agúndez et al., 2015
Circumstellar chemistry: C-rich CSE

- The case of IRC+10216:

\[ SiS \quad J=15-14 \]

\[ NaCN \]
\[ SiS \]
\[ CS \]
\[ HC_5N \]
\[ SiC_2 \]
\[ NaCl \]
\[ MgNC \]
\[ CN \]
\[ HNC \]
\[ C_2H \]
\[ C_3H \]
\[ C_4H \]

Velilla Prieto et al., 2015
Observational studies of O-rich CSEs:

O-rich CSEs are not so well studied. Most observational works are limited to CO and maser emission (SiO, H$_2$O, and OH), and single-dish observations of other species (e.g. SiO or HCN).

Castro-Carrizo et al., 2010
Circumstellar chemistry: O-rich CSE

- **Chemical models:**

  Agúndez et al., 2010

  ![Graphs showing chemical composition](image1)

  Li et al., 2016:
Circumstellar chemistry: chemical routes

- Chemical models:

Li et al., 2016:

**Inner e\(^{-}\) source: (both C- and O-rich):**

\[
H_2 + \text{crp} \rightarrow H_2^+ + e^-
\]

**\(\text{H}_3^+\) its very important:**

\[
\begin{align*}
\text{H}_3^+ + O & \rightarrow H_2O^+ + H \\
H_2O^+ + H_2 & \rightarrow H_3O^+ + H
\end{align*}
\]

**Example of neutrals reaction:**

\[
N + OH \rightarrow NO + H
\]

**Example: formation of HNCO:**

\[
\begin{align*}
\text{CN} + \text{OH} & \rightarrow \text{NCO} + H \\
\text{H}_3^+ + \text{NCO} & \rightarrow \text{HNCO}^+ + H_2 \\
\text{HNCO}^+ + H_2 & \rightarrow \text{HNCOH}^+ + H \\
\text{HNCOH}^+ + e^- & \rightarrow \text{HNCO} + H
\end{align*}
\]
• **Presence of O-bearing molecules in C-rich CSEs and vice versa:**

*TE models do not predict high abundances of water vapor in C-rich CSEs:*

_Melnick et al. 2001, detected the $o$-$H_2O \, 1_{1,0}-1_{0,1}$ line (556.9 GHz) toward IRC+10216:*
Water in C-rich CSEs

Presence of O-bearing molecules in C-rich CSEs and vice versa:

Water vapor lines were detected toward different C-rich CSEs with HIFI-HSO (Neufeld et al. 2011):

Black spectra represent the o-H$_2$O $1_{1,0}$-$1_{0,1}$ and p-H$_2$O $1_{1,1}$-$0_{0,0}$ lines at 556.9 and 1113.3 GHz, respectively. The blue spectra represent the scaled CO $J=10-9$ line (when available). Units are in antenna temperature (K) and velocity ($\text{km} \cdot \text{s}^{-1}$).

There should be a kind of universal mechanism to form H$_2$O in the CSEs of C-rich AGB stars.
Willacy & Millar (1997) proposed CH$_4$ as a parent molecule in O-rich CSEs. Their model predicts the formation of CH$_3$OH and C$_2$H. Marvel (2005) did not detect emission of these molecules, estimating upper limits to their abundances lower than the predicted values by Willacy & Millar (1997).

**Species** | **Model**
--- | ---
HCN | 1.4 (-7)
HNC | 2.0 (-8)
SiS | 3.5 (-6)
CS | 2.9 (-7)
SiO | 3.2 (-5)
SO | 9.1 (-7)
SO$_2$ | 2.2 (-7)
H$_2$S | 1.3 (-5)
HCO$^+$ | 3.9 (-8)
CH$_3$OH | 4.5 (-8)
C$_2$H | 2.3 (-7)

Recent observation of the O-rich CSE IKTau evidenced the presence of C-bearing molecules with abundances that are not compatible with predictions by chemical models. (Velilla Prieto et al. 2016).
Circumstellar chemistry: evolving toward the post-AGB phase

*Shock-induced chemistry: The peculiar object OH231.8+4.2*
Shock-induced chemistry: The peculiar object OH231.8+4.2

**Formation of ions:**

- \( \text{HOC}^+ + \text{H}_2 \rightarrow \text{HCO}^+ + \text{H}_2 \)
- \( \text{CO}^+ + \text{H}_2 \rightarrow \text{HCO}^+ + \text{H} \)
- \( \text{C}^+ + \text{H}_2\text{O} \rightarrow \text{HCO}^+ + \text{H} \)
- \( \text{S}^+ + \text{OH} \rightarrow \text{SO}^+ + \text{H} \)
- \( \text{SO} + \text{h}_\nu \rightarrow \text{SO}^+ + e^- \)
- \( \text{C}^+ + \text{SO}_2 \rightarrow \text{SO}^+ + \text{CO} \)
- \( \text{H}_3^+ + \text{N}_2 \rightarrow \text{N}_2\text{H}^+ + \text{H}_2 \)
- \( \text{N}_2^+ + \text{H}_2 \rightarrow \text{N}_2\text{H}^+ + \text{H} \)
- \( \text{HCO}^+ + \text{N}_2 \rightarrow \text{N}_2\text{H}^+ + \text{CO} \)

**HCO+ (1-0):** gray scale and solid contours

**CO (1-0):** dotted contours

*Its molecular content is similar to L1157*
Laboratory work: reaction rates

- **The problem:**

  \[ k = \text{cm}^3\text{molecule}^{-1}\text{s}^{-1} \]

  **Std. laboratory conditions (T~300 K)**

  **Extrapolation**

  \( T=10 \text{ K} \)

  **OH + CH\textsubscript{3}OH**

- **Cryogenic cooling:** if \( P>P_{sv} \) the gas will eventually condense on the walls of the vessel

\[ k(T=210-866K) = 6.38 \times 10^{-14} T^2 \exp(-144/T) \]

\[ k_{\text{OH}}(T) \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1} \]

\[ T/ \text{K} \]

\[ 0 \quad 100 \quad 200 \quad 300 \quad 400 \quad 500 \]

\[ 0.01 \quad 0.1 \quad 1 \quad 10 \]

\[ \text{This work, Pulsed Laval nozzle} \]
\[ \text{Shannon et al. (2013), Pulsed Laval nozzle} \]
\[ \text{Gómez-Martín et al. (2014), Flow tube} \]
\[ \text{Gómez-Martín et al. (2014), Pulsed Laval nozzle} \]
\[ \text{IUPAC Recommendation} \]

\[ k(T=210-866K) = 6.38 \times 10^{-14} T^2 \exp(-144/T) \]
Laboratory work: reaction rates

- The solution: CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme)

Density of gas in the jet: $10^{16}-10^{17} \text{ cm}^{-3}$

Thermal equilibrium

This technique allows to estimate reaction rates at temperatures as low as a ~20 K. Such low temperatures are representative of ISM environments (like CSM).
Chemical databases: where to...

- **UMIST**: http://udfa.ajmarkwick.net/
  
  UMIST RATE2012 / astrochemistry.net
  
  Welcome to the 2012 edition of The UMIST Database for Astrochemistry
  
  This is the 5th public release of the database.
  
  The database download files and the paper are available from the [download](http://udfa.ajmarkwick.net/) section.

  **Recent updates**

  21/03/16: Python scripts by Paul Woods that take output from UDfA chemical models and generate input files for popular radiative transfer codes. Available in the [download](http://udfa.ajmarkwick.net/) section.

- **KIDA**: http://kida.obs.u-bordeaux1.fr/

  KIDA is a database of kinetic data of interest for astrochemical (interstellar medium and planetary atmospheres) studies.

  ![KIDA search](http://kida.obs.u-bordeaux1.fr/)

  Indicate a species (ex: H3O+) or a couple of species (ex: C + H2)
  
  Warning: Second letter of 2-letter elements have to be lowercase, eg Si
Circumstellar chemistry: open questions

- Clumpy envelope? Binarity?
- Shock-induced and dust grains chemistry?

\[
\begin{align*}
CO + h\nu & \rightarrow C + O \\
O + H_2 & \rightarrow OH + H \\
OH + H_2 & \rightarrow H_2O + H
\end{align*}
\]
BIBLIOGRAPHY

- Agúndez, M., 2009, PhD Thesis
- Asplund et al., 2009, ARAA, 47, 481
- Decin, L., Agúndez, M., Barlow, M.J., et al. 2010, Nat, 467, 64
Chemical thermodynamical equilibrium:

\[ K_p(T) = (p^0)^{\Delta \nu} \exp\left\{ -\Delta G_r^0(T)/RT \right\} \]

\[ \Delta G_r^0(T) = \Delta H_r^0(T) - T \Delta S_r^0(T) \]

\[ \Delta H_r^0(T) = \sum_{i=1}^{N_{\text{prod}}} \Delta H_{f,i}^0(T) - \sum_{j=1}^{N_{\text{reac}}} \Delta H_{f,j}^0(T) \]

\[ \Delta S_r^0(T) = \sum_{i=1}^{N_{\text{prod}}} S_i^0(T) - \sum_{j=1}^{N_{\text{reac}}} S_j^0(T) \]
G. Haro School on Molecular Astrophysics, 11-20 October 2016