Modeling of Astrochemistry during Star Formation

1/ Deuterium chemistry

2/ Grain surface processes
Interstellar matter is heterogeneous and active

In interstellar cloud
By mass: 1 % grain
99 % gas
(by number: grain/gas = 10^{-12})

Molecular cloud
\(~10^{4-5} \text{ cm}^{-3}, \sim 10 \text{ K}\)

Prestellar core
\(~10^{16} \text{ cm}^{-3}, \sim 1,000 \text{ K (inner core)}\)

Protostar
\(~10^{24} \text{ cm}^{-3}, \sim 10^5 \text{ K}\)
(inner core)

Protoplanetary disk
\(~10^{9-12} \text{ cm}^{-3}, \sim 10^{1-3} \text{ K}\)

Stellar system
Modeling tool: gas grain chemical code

I - GAS PHASE

Main reactions: ion - neutral
neutral - neutral

2 body reactions

~500 to ~1000 species
~4000 to ~110,000 reactions

II - GRAIN SURFACE

adsorption
reaction
diffusion
desorption
dissociation

UV photons & Cosmic ray

~200 to ~500 species
~2,000 to ~9,000 reactions
Modeling tool: gas grain chemical code

- Chemical network: $\text{chemical network (A+B → C+D)}$
- Medium properties: $\text{medium properties (T,n...)}$
- Grain properties: $\text{grain properties (T,r...)}$
- Species properties: $\text{species properties (m,E_d...)}$
- Chemical composition: $\text{chemical composition} = \text{function(time)}$
- Initial & elemental abundance: $\text{initial & elemental abundance}$
1/ Deuterium chemistry

Deuterium fractionation

Key Reaction & Spin states

\[ \text{H}_3^+ + \text{HD} \rightleftharpoons \text{H}_2\text{D}^+ + \text{H}_2 \]

Ceccarelli et al. 2014 Protostar and Planets VI
1/ Deuterium chemistry : new network

- Low & high Temperature chemistry
  10 to 800 K
- Low & high Density chemistry
  \(10^4\) to \(10^{12}\) cm\(^{-3}\)
- Up to triply deuterated species
- Ortho, para, and meta spin states of H\(_2\), D\(_2\), H3+, H2D+, D2H+, and D3+

\(~1,600\) species linked by \(~120,000\) reactions

Spin state effects: abundances can be reduced by several orders of magnitude (see ↑)

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Condition 1</th>
<th>Condition 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2</td>
<td>initial H2 o/p = 3</td>
<td>initial H2 o/p = 0</td>
</tr>
<tr>
<td>H2D+</td>
<td>initial H2 o/p = 3</td>
<td>initial H2 o/p = 0</td>
</tr>
</tbody>
</table>
1/ Deuterium chemistry: HDO/H2O in high mass star forming region

Source: hot molecular core G34.26+0.15
Modeling: Molecular cloud condition followed by a 1D static physical structure of the core

- Observations reproduced. Lower abundance of HDO in the inner core (o/p effect?)
- Important reactions with H, HCO+ (destruction), H3O+, H2DO+ (formation)
- Chemical simulations gives constraints on the source age: \(\sim 10^5\) yrs

*Coutens, Vastel, Hincelin, Herbst et al 2014*  
*vander Tak et al 2013*
2/ Grain surface processes: Desorption due to H2 coverage

- Desorption energy of H2 on a water substrate: 440 K [1]
- Desorption energy of H2 on a H2 substrate: 23 K [1]
  → Desorption of H2 when on top of H2 substrate (called “encounter desorption”)
  
  \[ T = 10 \text{ K} ; n = 10^4 \text{ cm}^{-3} \]

2/ Grain surface processes:
Desorption due to H2 coverage

Basic idea: Microscopic Monte-Carlo models can reproduce this effect, but are still very time consuming.

How to apply for complex star formation modeling?
One solution: Use rate equation model

Method:
1/ Add g-H2 + g-H2 → g-H2 + H2(gas) in rate equation models
2/ Use a formalism for diffusion and reaction on grain surface \[2\]
3/ Give a correct rate to this “reaction” that depends on:
   - surface abundance of H2
   - competition between desorption & diffusion
   - desorption energy from H2 substrate

Results: Good reproduction of Microscopic Monte-Carlo models
Very low CPU time consuming

Summary

➢ New chemical network for deuterium chemistry 
  (Hincelin et al 2014 in prep.)

➢ HDO/H2O in high mass star forming region 

➢ Grain surface processes : desorption due to H2 coverage 
  (Hincelin, Chang, Herbst 2014 in prep.)

• Perspective :
  - Coupling of deuterium chemistry and encounter desorption with 
    complex 3D physical structure of star in formation 
    (3 Dimensional Radiative Magneto Hydrodynamics, see Hincelin et al. 2013)
  - Application to Low and High mass star formation

Thank you for your attention :-)  
Ugo Hincelin – University of Virginia