Modelling of the chemistry of protoplanetary disks

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Introduction

Adapted from Semenov & Henning 2013
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New framework which combines a thermo-chemical disk model and an full gas-grain chemical model (Ruaud & Gorti, submitted to ApJ)

Adapted from Semenov & Henning 2013
Thermo-chemical disk model

Iterations to get density and temperature structure at vertical hydrostatic equilibrium

- Dust collisions
- X-rays & UV
- \(H_2\) pump/form
- Chemical reactions
- ...
Gas-grain chemical model

**Time-dependent three-phase chemical model** (~500 species and ~7000 reactions)

- **Surface** and **mantle diffusion**
- **Reactions** through the Langmuir-Hinshelwood process
- **Surface and sub-surface photoprocessing** by stellar and interstellar photons and cosmic-rays generated photons
- **Desorption** restricted to the **top two monolayers** (thermal desorption, chemical desorption and photodesorption)
- **Grain growth** by accretion of molecules

Three phase model: gas, ice surface and ice mantle (Ruaud et al. 2016)
Results obtained with a typical disk

\[ M_{\text{disk}} = 0.005 M_\odot - \frac{\Sigma_d}{\Sigma_g} = 0.01 \]

\[ M_{\text{disk}} \sim \text{mean disk mass derived from surveys in Taurus and Lupus regions (Ansdell et al. 2016)} \]
Ice mainly consists of simple molecules: H$_2$O, CO, CO$_2$, CH$_4$, CH$_3$OH, HCN, …
Complex molecules efficiently form in the inner disk ~0.1-1% relative to water.
Chemistry of the midplane

Three chemically distinct regions in the disk midplane:

(1) Inner disk midplane (r<100 au):
- low UV flux
- $T_d>15$ K

Efficient formation of COMs: radicals diffuse at the surface of grains
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(2) Outer disk midplane (r>100 au):
- Substantial UV
- $T_d$<15 K → Hydrogenation reactions dominate the chemistry
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   - Substantial UV
   - $T_d<15$ K
   - Hydrogenation reactions dominate the chemistry

3. **Interface molecular layer/midplane or water condensation front**:
   - Important UV
   - $T_d\geq15$ K
   - Important photoprocessing of the ice
Impact of ice photochemistry on gas-phase composition

Photo-processing of the ice near the water condensation front:
- Photodesorption
- Photodissociation and re-formation at the surface of the ice: promotes chemical desorption
Efficient formation of $sCO_2$ near water condensation front impacts the location of the vertical CO snowline: shifts higher up from the disk midplane

\[
sH_2O + h\nu \rightarrow sOH + sH
\]
\[
sOH + sCO \rightarrow sCO_2 + sH (\Delta E = 150K)
\]
\[
\rightarrow sHOCO (\Delta E = 150K)
\]
Impact on the emission of CO isotopologues

Predicted line emissions can decrease by a factor of ~10
(work in progress)

Full model
No CO for T<20K

Full gas-grain chemistry +
Selective photodissociation
Summary

• **Chemistry in the midplane** depends mainly on the *radial and vertical gradients* of the *dust temperature* and on *photoprocesses*
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- **The disk interior can be divided into three chemically distinct regions:**
  1. Inner disk midplane where the dust is warm enough for radical mobility
  2. The outer disk midplane where hydrogenation reactions dominate the chemistry
  3. The interface between the molecular layer and the midplane where grain surface chemistry is driven by photoprocessing of ices
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• Interface between the molecular layer and the midplane:
  - Photoprocessing of ices has a significant impact on the gas-phase abundance of several molecules
  - Efficient conversion of CO to CO$_2$ ice which impacts the location of the vertical CO snowline: moves higher up in the disk midplane. Important impact on the predicted emission lines of CO isotopologues.
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Thank you for your attention!
Chemistry of the midplane

• Radial CO snowline also impacted:
  - Move closer to the star as a function of time
  - Conversion driven by cosmic rays

• Impacts N\textsubscript{2}H\textsuperscript{+}: tracer of CO snowline

\[
\begin{align*}
N_2 + H_3^+ & \rightarrow N_2H^+ + H_2 \\
CO + N_2H^+ & \rightarrow HCO^+ + N_2
\end{align*}
\]

$T_{\text{kin}}$=39K from N\textsubscript{2}H\textsuperscript{+} J=1-0 and J=4-3
(Schwarz et al. 2019)
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Impact on the composition of the gas
Two-phase vs three-phase approximation

- **Two-phase approximation over predicts gas-phase abundances:** all the mantle is available for desorption

- **Most disk chemical models use the two-phase approximation**

- **Could explain the systematic overestimation of cold water lines as compared to observations:** depletion factors of ~100 for oxygen have been invoked (Du et al. 2017)