Effects of grain growth on the chemistry in protostars

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Grain Growth during the Star Formation

- Building blocks of planets
- mm-size grains & possibly cm-size grains in protoplanetary disks (Natta et al. 2007, Li et al. 2014)

Image: A. Maury
Grain growth in class 0/I protostars

- Small dust opacity spectral index $\beta (< 1)$ in envelopes of class 0 protostars (Kwon et al. 2009)

- Also in class I protostars to mm-size grains (Miotello et al. 2014, Testi et al. 2014)

Image: A. Maury
Chemistry in Protostars

CO, HCN
unsaturated molecules

CN, C₄H, HC₃N

N₂H⁺

CH₃OH

CO

CH₃OCH₃

CO, HCN
saturated molecules

CH₃OH, CH₃OCH₃, HCOOH

Prestellar phase

Protostellar phase

Pre-main sequence phase

Time
Chemistry in Protostars

Key Questions

1) How does the chemistry change with the effects of grain growth?

2) Which species are good tracers of grain growth?

Chemical Abundance Calculation
Physical model

- Radiation hydrodynamic code to form protostars from prestellar cores by Masunaga & Inutsuka (2000).

- Traces chemistry for each layer in temperature & density (Aikawa et al. 2008).

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prestellar core  \rightarrow collapse  \rightarrow compressional heating and formation of the 1st core  \rightarrow new-born protostar and infalling envelope (protostellar core)
Physical model

The diagrams illustrate the temperature and density changes over time for different values of $r_{\text{final}}$. The temperature is shown on a logarithmic scale, while the density is on a linear scale.

- **Temperature**
  - $r_{\text{final}} = 2.5$ AU
  - $r_{\text{final}} = 15$ AU
  - $r_{\text{final}} = 125$ AU
  - $r_{\text{final}} = 1000$ AU

- **Density**
  - $r_{\text{final}} = 2.5$ AU
  - $r_{\text{final}} = 15$ AU
  - $r_{\text{final}} = 125$ AU
  - $r_{\text{final}} = 1000$ AU

The time axis is denoted as $t_{\text{final}} - t$ (yr), with values ranging from $10^{-5}$ to $10^{1}$.
Chemical model

- Nautilus

- 8335 gas & grain reactions, 684 species

- A time-dependent model

- Initial conditions taken from a cloud formation model by Furuya et al. (2015), and inserted a quiescent phase for $10^6$ yrs.
Treatment of grain growth

- Chemistry change due to the total surface area
  - Single size $\rightarrow S_{gg}/S_{init} \propto (a_{gg}/a_{init})^{-1}$
  - MRN: $dn(a)/da \propto a^{-3.5}$
- Assume $a_{min}$ stays the same
  - $\rightarrow S_{gg}/S_{init} \propto (a_{gg}/a_{init})^{-0.5}$
- Change the dust-to-gas mass ratio to represent the change in surface area. Keep the grain size ($a=0.1 \, \mu m$)
  - $f_{gg}=0.01, 3\times10^{-3}, 1\times10^{-3}, 3\times10^{-4}$
    fiducial case             grain growth case
Results: fiducial case - S species

$r_{\text{final}} = 15\ \text{AU}, f_{gg}=0.01$
without grain growth

$r_{\text{final}} = 15\ \text{AU}, f_{gg}=3\times10^{-4}$ grain growth (x1000)

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gas phase

.... ice
Results: grain growth case - S species

- Less abundances of H$_2$S

- S(ice) + H(ice) $\rightarrow$ HS(ice)

- HS(ice) + H(ice) $\rightarrow$ H$_2$S(ice)

- Less efficient grain formation

- Remaining S species

  - S + OH $\rightarrow$ SO + H

  - SO + OH $\rightarrow$ SO$_2$ + H
Results: fiducial case - C species

\[ r_{\text{final}} = 15 \text{ AU}, f_{gg}=0.01 \]
without grain growth

\[ r_{\text{final}} = 15 \text{ AU}, f_{gg}=3 \times 10^{-4} \]
grain growth (x1000)

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gas phase

\[ \cdots \cdots \text{ ice} \]
Results: C species

- Destruction of CO ice
  - CO(ice) + OH(ice) → CO$_2$(ice) + H(ice)
- CH$_3$OH Formation
  - CO (ice) + H (ice) → HCO(ice)
  - HCO(ice) + H(ice) → H$_2$CO(ice)
  - ...
  - CH$_2$OH(ice) + H(ice) → CH$_3$OH(ice)
Results: fiducial case - organic molecules

\[ r_{\text{final}} = 15 \text{ AU}, f_{gg}=0.01 \]

without grain growth

\[ r_{\text{final}} = 15 \text{ AU}, f_{gg}=3 \times 10^{-4} \]

grain growth (x1000)
Results: grain growth case - COMs

- $\text{CH}_3\text{CN}$ formation
  - $\text{CH}_3(\text{ice}) + \text{CN}(\text{ice}) \rightarrow \text{CH}_3\text{CN}(\text{ice})$
  - $\text{CH}_2\text{CN}(\text{ice}) + \text{H}(\text{ice}) \rightarrow \text{CH}_3\text{CN} (\text{ice})$

- $\text{HCOOH}$ formation
  - $\text{O}_2^+ + \text{CH}_4 \rightarrow \text{CH}_3\text{O}_2^+ + \text{H}$
  - $\text{CH}_3\text{O}_2^+ + \text{e}^- \rightarrow \text{HCOOH} + \text{H}$
Results: Radial dependence S species

- $t = t_{\text{final}}$

<table>
<thead>
<tr>
<th>Gas phase</th>
<th>Ice</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$_2$S</td>
<td></td>
</tr>
<tr>
<td>H$_2$S(ice)</td>
<td></td>
</tr>
<tr>
<td>SO</td>
<td></td>
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<tr>
<td>SO$_2$</td>
<td></td>
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</tbody>
</table>
Results: Radial dependence COMs
Observations of S species

- IRAS 16293-2422

- A well-studied class 0 protostar (Source A & B)

SMA Observations
Beam ~ 1”x2” = 120 - 240 AU

Chandler et al. (2005)
Comparisons with Observations

\[ < X_i > = \frac{\int_{r_{\text{max}}} r^2 dr \cdot 4\pi n(r) X_i(r)}{\int_{r_{\text{max}}} r^2 dr \cdot 4\pi n(r)} \]

- \( f_gg = 3 \times 10^{-4} \)
- \( f_gg = 1 \times 10^{-3} \)

Observation:

- \( f_gg = 3 \times 10^{-3} \)
- \( f_gg = 1 \times 10^{-2} \)
Comparisons with Observations

- NGC 1333 - IRAS 2A: A class 0 protostar
- PdBI observation (Taquet et al. 2015)

<table>
<thead>
<tr>
<th>Species</th>
<th>Observed</th>
<th>Modeled fractional abundances</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>$f_g = 1 \times 10^{-2}$</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>$(2.5 \pm 0.9) \times 10^{-7}$</td>
<td>7.3e-07</td>
</tr>
<tr>
<td>CH$_3$CN</td>
<td>$(2.0 \pm 0.4) \times 10^{-9}$</td>
<td>3.5e-08</td>
</tr>
<tr>
<td>CH$_3$OCH$_3$</td>
<td>$(8.2 \pm 3.3) \times 10^{-9}$</td>
<td>6.6e-10</td>
</tr>
<tr>
<td>HCOOH</td>
<td>...</td>
<td>1.2e-09</td>
</tr>
</tbody>
</table>

- CH$_3$OH & CH$_3$CN - Overabundant in models
- CH$_3$OCH$_3$ - Underabundant in models
Caveats

- Does the grain grow as fluffy or spherical grain?

- How does the distribution of grain change with grain growth? (MRN: \( \frac{dn(a)}{da} \propto a^{-3.5} \))
Summary

- Grain growth can vary the surface area, so it can affect the chemistry.

- Sulfur species are sensitive probes of grain growth. (H2S: Band (5), 6, SO: Bands 3-, SO2: Bands 3-)

- Comparisons of modeling with observations of sulfur species shows good agreement with grain growth of a factor of 10-100 in $a_{\text{max}}$.

- The disagreement of complex organic molecules in the model and observations cannot be solved by inclusion of grain growth.