Probing the composition of the planet-building reservoir in protoplanetary disks

what we have learned from comets and ALMA?

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Our astrochemical origins

Inheritance?
Disk formation?
Disk processing?
Delivery?

What is the provenance of planetary system building material?
Protoplanetary disks have a history

To what degree does chemical processing modify interstellar material?

From clouds to disks to comets

Comets are frozen relics of planet-building material in the Solar System.
Our astrochemical origins

Is chemistry useful?

Can I trust chemistry? It's complicated!

What can chemistry tell us about physics?

Credit: ESO/T. Preibisch
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</table>

Our astrochemical origins

Protoplanetary disk molecules/volatiles?

25* and counting …

* not including isotopologues

Adapted from the Cologne Database for Molecular Spectroscopy: http://www.astro.uni-koeln.de/cdms
Our astrochemical origins

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Example Tracers</th>
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<tbody>
<tr>
<td>Mass</td>
<td>$^\text{x}C\text{yO}$, HD</td>
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<tr>
<td>Temperature</td>
<td>$^\text{x}C\text{yO}$, CH$_3$CN</td>
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<td>Density</td>
<td>CS, H$_2$CO, HC$_3$N</td>
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<td>Kinematics</td>
<td>$^\text{x}C\text{yO}$, HCO$^+$</td>
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<td>Photodissociation</td>
<td>CN, HCN, C$_2$H</td>
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<td>Ionisation</td>
<td>HCO$^+$, N$_2$H$^+$, CH$^+$</td>
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<td>Deuteration</td>
<td>DCO$^+$, N$_2$D$^+$, DCN</td>
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<td>Turbulence</td>
<td>$^\text{x}C\text{yO}$, CS, HC$_3$N</td>
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<td>C/N/O fractionation</td>
<td>$^\text{x}C\text{yO}$, $^\text{x}$C$^z$N, $^\text{H}$x$^\text{C}$,$^\text{z}$N</td>
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<td>Snow lines</td>
<td>$^\text{x}C\text{yO}$, N$_2$H$^+$, DCO$^+$, HCO$^+$</td>
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<tr>
<td>Grain-surface processes</td>
<td>Complex molecules</td>
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$x = 12, 13; y = 16, 17, 18; z = 14, 15$

Adapted from Henning & Semenov 2013, Chem. Rev., 113, 9016
What has ALMA revealed about disk composition and chemistry?
Chemical tracers of snowlines

TW Hya
$N_2H^+$

$N_2 + H_3^+ \rightarrow N_2H^+ + H_2$
$CO + N_2H^+ \rightarrow HCO^+ + N_2$

im Lup
$DCO^+$

$HD + H_3^+ \rightarrow H_2D^+ + H_2$
$CO + H_2D^+ \rightarrow DCO^+ + H_2$

Chemical tracers of snowlines

$R_{\text{snow}} = 20.5 \pm 1.3 \, \text{au}; \ T_{\text{snow}} = 27 \pm 3 \, \text{K}; \ CO/H_2 \sim 10^{-6}$

Chemical tracers of snowlines

Chemical models of disk midplanes with gas and ice chemistry predict a chemical conversion of CO into a less volatile form: CO$_2$, C$_x$H$_y$, COMs

Results in a “fake” CO snowline which evolves in time
The gas-phase CO in the outer disk is also depleted over time
What is happening to the CO?

What does a systematic exploration using single-point chemical models tell us?

If the gas and dust are moderately warm, CO is chemically converted to other species on ~ 1 Myr timescales.
What is happening to the CO?

What does a systematic exploration using single-point chemical models tell us?

If the gas and dust are moderately warm, CO is chemically converted to other species on ~1 Myr timescales.

$T = 25 \text{ K}; \ n \sim 10^{11} \text{ cm}^{-3}$

Bosman et al. 2018; Schwarz et al. 2018
CO as a tracer of gas mass?

ALMA survey of Lupus star-forming region
Low gas-to-dust mass ratios? Or low CO/H$_2$ abundance ratios?

Ordered by increasing dust mass

No clear trend

Low disk gas masses also inferred for Chameleon I and Upper Sco

How does this compare with comets?

% abundance relative to H$_2$O

Based on radio observations

Bockele-Morvan & Biver 2017
First detection of $^{13}\text{C}^{17}\text{O}$
First detection of $^{13}\text{C}^{17}\text{O}$

We can do these weak lines with ALMA
Suggests 3-4 times more gas mass than previous analyses

HCO$^+$ tracing real-time ionisation

Multi-epoch observations of H$^{13}$CO$^+$ in IM Lup

Confirmation of real-time stellar variability in ionisation in the disk atmosphere

What is ALMA revealing about the chemical complexity of protoplanetary disks?
Searching for complex molecules

Cyanides (-CN) play a role in the synthesis of amino acids

\[ \text{CH}_3\text{CN}/\text{HCN} \approx 5 - 20\% \]

MWC 480
\[ T_{\text{eff}} \approx 8000 \text{ K} \]

Credit: B. Saxton (NRAO/AUI/NSF)
How does this compare with comets?

% abundance relative to $\text{H}_2\text{O}$

Based on radio observations

Bockelee-Morvan & Biver 2017
Searching for complex molecules

TW Hya
$T_{\text{eff}} \sim 4000 \text{ K}$
CH$_3$CN in TW Hya

Obs. $N_T = 1.45^{+0.19}_{-0.15} \times 10^{12}$ cm$^{-2}$

Obs. $T_{rot} = 32.7^{+3.9}_{-3.4}$ K

Model $N_T = 1.49 \times 10^{12}$ cm$^{-2}$

Model $T_{rot} = 36.6$ K

CH$_3$CN in TW Hya

Chemical models fail to reproduce cometary CH$_3$CN abundance in the midplane: another indicator of inheritance?

CH$_3$CN in TW Hya

Searching for complex molecules

Methanol is an interstellar ice molecule and a feedstock for more complex molecules.

$\text{CH}_3\text{OH}/\text{H}_2\text{O} \sim 1\% - 5\%$

How does this compare with comets?

Based on radio observations, Bockelee-Morvan & Biver 2017

% abundance relative to H₂O

CH₃OH

JFC
HFC
DO
DN

Bockelee-Morvan & Biver 2017
Problem: CH$_3$OH ice fragments when photodesorbing

CH$_3$OH in TW Hya

HCOOH in TW Hya

$T_{\text{eff}} \sim 4000$ K

HCOOH/CH$_3$OH $\sim 1$

Comets $\sim 0.01 - 1$

Chemical complexity in protoplanetary disks

Next steps?
Next steps?

Cycle 2
Methanol
TW Hya

Next steps?

Cycle 4
Methanol
TW Hya

Next steps?

Compact CH$_3$OH emission ($< 60$ au): following the large dust grains?

Next steps?

Cycle 4 data: lines with low $E_{up}$ only detected (< 38 K)

Can we observe molecular emission on planet-forming scales?
DSHARP: Disk Substructure at High Angular Resolution Project
Resolved molecular emission in the ringed disk around HD 97048

The data cannot be fit by a fixed abundance ratio between HCO$^+$/H$^{13}$CO$^+$.

There is mounting evidence that gas-phase chemistry is strongly influenced by the dust evolution in the disk (see also Bergin et al. 2016).

Chemical evidence of planets?

Detection of SO in HD 100546: SO is a known shock tracer

Could this be a disk wind? Or an accreting protoplanet?
Need a “high” abundance of S to match the line flux: \( \sim 10^{-6} \) wrt \( \text{H}_2 \)

MAPS: Molecules with ALMA on Planet-forming Scales

Credit: J. Bergner, CfA

Aikawa, Bergin, Guzmán, Öberg, Walsh
Chemistry is useful!

Not only as a tracer of composition of ice and gas ....

... also as a sensitive tracers of physics, ...

..., and other molecules are available!

Happy to share chemical codes: c.walsh1@leeds.ac.uk