Chemical conditions of gas in planet-forming disks

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Big questions

• What is the gas mass and the gas:dust ratio?
• What is the chemical inheritance for the ISM & star formation process?
• What is the balance between ice and gas? What is the role of snow lines?
• Where do the elements like C,O,N reside?
• Where/how do organics form?
• (How) does the chemistry reflect the underlying disk structure?
Disk structure

- Basic structure of the disk
  - Radial surface density profile (gas, dust)
  - Vertical hydrostatic scale height
  - Irradiation by stellar spectrum
- Assumption: small (~µm) grains coupled (thermally, hydrodynamically) to gas
- Spectral Energy Distribution fitting provides overall disk structure

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Figure 1. Near-IR scattered light image of the protoplanetary disk around the Herbig Ae star MWC 758 obtained with the Subaru telescope by the Strategic Exploration of Exoplanets and Disks (SEEDS) collaboration. Reprinted with permission from ref 18. Copyright 2013 American Astronomical Society.

Figure 2. Sketch of the physical and chemical structure of a ∼1−5 Myr old protoplanetary disk around a Sun-like star.
$T(R,z), G_0(R,z)$

- Radial and vertical temperature gradient
- (Inter)stellar ultraviolet radiation attenuated by small grains $\rightarrow$ photo-dissociation layer
- Stellar X-rays, cosmic rays penetrate to midplane $\rightarrow$ secondary ionization
  - Do stellar winds shield Cosmic Rays effectively from the disk?
  - Short-lived radioactive nuclei also (may) provide secondary ionization


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Figure 2. Sketch of the physical and chemical structure of a $\sim 1-5$ Myr old protoplanetary disk around a Sun-like star.
Gas:Dust

- Dust mass estimates good to ~factor of a few
- Complications: dust evolution, migration
- Gas mass estimates uncertain
  - CO generally observed to be depleted (... see next slides...)
  - H₂ only observable in warm/hot surface, inner disk (weak lines)
- HD detected in TW Hya
  - With thermal structure (+chemistry) → large gas mass estimates (0.05 Mₖₚ), gas:dust~100:1 (~ISM)
  - Model uncertainties? Unresolved contributions from hot material? Generalization to other disks?
CO depletion

• Consistently observed to be depleted (Dutrey et al. 1997, ...)

• Freeze out in cold disk interior

• Photodissociation of CO in UV-irradiated surface, outer region
  • Isotope-selective photodissociation: $^{13}$CO, $^{18}$C$^1$O, C$^{17}$O

• With appropriate model: reliable gas masses
  • e.g., Lupus survey gas:dust <100 (Ansdell et al. 2016)

![Diagram](Miotello et al. (2014))
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  • e.g., Lupus survey gas:dust <100 (Ansdell et al. 2016)

Williams & Best (2014)
Snow lines

- Radial temperature gradient $\rightarrow$ snow lines for major volatiles: H$_2$O, CO, N$_2$?

- Directly traced via CO isotopes

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**Image credit: NASA/JPL**

Qi et al. (2011)
Snow lines

- Radial temperature gradient → snow lines for major volatiles: H₂O, CO, N₂?

- ...or indirectly via N₂H⁺

production: H₃⁺ + N₂ → N₂H⁺ + H₂
H₃⁺ + CO → HCO⁺ + H₂

destruction: N₂H⁺ + CO → HCO⁺ + H₂

Qi et al. (2013, 2015)
Snow lines

- Radial temperature gradient → snow lines for major volatiles: H₂O, CO, N₂?
- ...or indirectly via N₂H⁺

Caution: CO snow line is not sharp. It is a gradient. N₂H⁺ may not show up until well outside the point where the CO freeze-out temperature is reached (’t Hoff et al. in prep)

production: H₃⁺ + N₂ → N₂H⁺ + H₂
H₃⁺ + CO → HCO⁺ + H₂

destruction: N₂H⁺ + CO → HCO⁺ + H₂

Qi et al. (2013, 2015)
Snow surface

- Vertical temperature gradient → snow surface
- Traced by
  - CO isotopes and different transitions
  - In channel maps for inclined disks

Fig. 3. Snow surface trace at different velocity channels for HD 163296. The red boxes indicate the location of the bisector for each channel. The color bar represents the level of emission, with red indicating higher intensity.
UV irradiated outer regions

- Interstellar radiation field penetrates outer disk
- Extended CN emission compared to HCN

Guzmán et al. (2015)

See also Chapillon et al. (2012) for more results on HCN, CN, HC$_3$N
UV irradiated outer regions

- Interstellar radiation field penetrates outer disk
- Extended CN emission compared to HCN
- Photodesorption (rather than thermal desorption) sets up a second, outer snow line

TABLE 1

<table>
<thead>
<tr>
<th>Molecular Line</th>
<th>Rest freq.</th>
<th>Log 10(Aij)</th>
<th>Eu</th>
<th>beam (PA)</th>
<th>Integrated flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>DCO+ J=3–2</td>
<td>216.1126</td>
<td>-2.62</td>
<td>20.7</td>
<td>0.′′65 × 0.′′48</td>
<td>(-71°)4 5 0 ± 45</td>
</tr>
<tr>
<td>C18O J= 2 – 1</td>
<td>219.5604</td>
<td>-6.22</td>
<td>15.8</td>
<td>0.′′68 × 0.′′47</td>
<td>(-60°)1 4 6 0 ± 150</td>
</tr>
<tr>
<td>H13CO+ J=3–2</td>
<td>260.2553</td>
<td>-2.87</td>
<td>25.0</td>
<td>0.′′68 × 0.′′59</td>
<td>(89°)4 8 4 ± 48</td>
</tr>
</tbody>
</table>

Fig. 1.—Continuum and integrated emission maps of C18O J = 2 – 1, H13CO+ J = 3–2 and DCO+ J = 3–2 toward IM Lup (top row), integrated emission in two velocity bins (middle row) and deprojected azimuthally averaged profiles (bottom row).

The integrated emission maps and average radial profiles reveal two significant morphological features. First, all three molecular species show a clear central depression. The C18O and DCO+ emission each peak at a radius of 0.′′6, or ∼90 AU, and the H13CO+ line peaks at 0.′′8 (∼125 AU). Second, DCO+ exhibits a large second ring at 2′′, near the outer edge of the continuum emission. No such ring is observed in C18O, H13CO+ or the continuum. However, the H13CO+ emission “plateaus” around the same radius and C18O exhibits a subtle slope change.

4. DISK CHEMISTRY MODELING
4.1. Model Description

Öberg et al. (2015)
Volatiles

- Other detected volatiles
  - H₂O in several disks
  - gas-phase production / evaporation in inner disk

Carr & Najita (2008); Salyk et al. (2008, 2015); Pontoppidan et al. (2010); Meijerink et al. (2009); Zhang et al. (2013); Fedele et al. (2012); Riviere-Marichalar et al. (2012)
Volatiles

- Other detected volatiles
  - $\text{H}_2\text{O}$ in several disks
  - gas-phase production / evaporation in inner disk
  - photodesorption in outer disk
    - much lower amount than expected → most ices settled in the midplane on larger grains?
  - $\text{NH}_3$ in TW Hya

Hogerheijde et al. (2011), Salinas et al. (2016), Hogerheijde et al. (in prep), Du et al. (in prep)
Depletion of volatiles

- CO, C, and H$_2$O depleted in many disks
- TW Hya in particular
- Locked up in the midplane

Kama et al. (2016), Du et al. (2015, in prep)
Deuterated molecules are enriched in cold gas

- $\text{H}_3^+ + \text{HD} \leftrightarrow \text{H}_2\text{D}^+ + \text{H}_2$
- $\text{H}_2\text{D}^+ + X \rightarrow \text{XD}^+ + \text{H}_2$

N$_2$D$^+$ in HD163296

Salinas et al. (in prep)
Deuteration

- Deuterated molecules are enriched in cold gas
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  - $\text{H}_2\text{D}^+ + X \rightarrow \text{XD}^+ + \text{H}_2$
- High(er) temperature deuteration
  - $\text{CH}_3^+ + \text{HD} \leftrightarrow \text{CH}_2\text{D}^+ + \text{H}_2$
  - $\ldots + \text{O} \rightarrow \text{DCO}^+ + \ldots$

See also Favre et al. (2015) and Salinas et al. (in prep)
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DCO$^+$ is not as much a CO snow line tracer as it is an ionization tracer (cf. Teague et al. 2015; Guilloteau et al. 2016 for HCO$^+$, DCO$^+$)

see also Favre et al. (2015)
Deuterated molecules are enriched in cold gas

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  - $\ldots + \text{O} \rightarrow \text{DCO}^+ + \ldots$
  - $\ldots + \text{N} \rightarrow \text{DCN} + \ldots$

See also Öberg et al. (2012)

Salinas et al. (in prep)
Organics

• Simple organics are being detected in disks
  • HC$_3$N and CH$_3$CN in MWC480
  • H$_2$CO across the disks of DM Tau, TW Hya, HD163296

Qi et al. (2013)

See also: HC$_3$N, Chapillon et al. (2012)

Öberg et al. (2015)

Loomis et al. (2015)
Organics

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Carney et al. (in prep):
- $\text{H}_2\text{CO} \, 3_2-2_2$ detected via matched filtering (Loomis et al., in prep)
- additional reservoir of $\text{H}_2\text{CO}$ outside $\sim 300$ au: UV photodesorption?
Organics

- Simple organics are being detected in disks
  - HC$_3$N and CH$_3$CN in MWC480
  - H$_2$CO across the disks of DM Tau, TW Hya, HD163296

Walsh et al. (in press)
- (stacked) CH$_3$OH detected in TW Hya
- see talk by Nomura
Gaps

- Fair fraction of disks are transitional: large (dust) gaps
- (Reduced amount of) gas fills the gaps
- Photodissociation effects?

Canovas et al. (2016)

see also Carmona et al. (2014), Bruderer et al. (2014), ...

Perez et al. (2015)  
vanders Marel et al. (2015)
Inheritance

- Models of disk chemistry:
  - gas-phase & grain-surface formation; full or reduced networks
  - freeze out & evaporation
  - photodesorption by UV
  - ionization by UV, CR, X-rays, short-lived radionuclides
  - steady state, time dependent, or fully coupled with hydrodynamic solution and/or grain evolution

Inheritance

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• How about initial conditions?
  • How much of the chemistry is inherited from the ISM, protostellar phase?
  • How much is reprocessed during star /disk formation, esp. ices/volatiles
  • Influence of episodic heating?
Inheritance

• Tracers of embedded disks
  • e.g., L1527
  • c-C$_3$H$_2$ shows rotation & infall: envelope
  • SO shows solid-body rotation: accretion shock at centrifugal barrier

• Alteration of ice/gas at point of entry into the disk

Sakai et al. (2014)
Disks in 2016

• So far, disk structure taken from SED modeling
  • Radial, vertical gradients in density and temperature
    • Freeze out & snow lines, deuteration, photodesorption...
  • (Large) gaps in transitional disks
    • Often seen to be filled with (reduced amounts of) gas
  • Accretion shocks at centrifugal barrier of forming disks
• HL Tau, TW Hya (how general?)
  • Disks are series of rings, gaps, wiggles
  • Traced in millimeter-sized grains
• Underlying gas surface density distribution?
• Associated distribution of μm-sized grains (⇔UV, ionization)?

ALMA Partnership, Brogan et al. (2015); Andrews et al. (2016)
ALMA

• This talk has been ALMA-centric

  • Great progress in the last few years, and many exciting results to come

• Fundamental limitation

  • Sensitivity to small-scale structure in thermal continuum will always be larger than to small-scale structure in gas emission lines

  • Weak lines require very good bandpass calibration and very accurate continuum subtraction

  • Inner, densest regions become optically thick in dust continuum at all/many ALMA wavelengths

• Other ways to probe gas in (inner) disks

  • Long-slit spectroscopy

  • MATISSE

  • JWST