Chemistry in protoplanetary disks
Outline

• Molecules as disk probes

• Observations of molecules in disks

• Disk chemical structure

• Toward chemo-dynamical disk models
Disks are birth sites of planetary systems

- Planet formation
- Primordial atmospheres
- Primitive bodies
- Genesis of organic molecules

Molecules are probes:
- Physical conditions
- Kinematics
- Chemical complexity
Protoplanetary disks in Orion: optics, Hubble
Protoplanetary disks: IR, Hubble
Advantages of millimeter observations

- Optically thin dust emission: direct measure of mass
- Rotational transitions of molecules
- High frequency resolution: $\sim 10^6$ (~0.05 km/s)
- Sensitive to cold regions $\sim 10$–20 K
- Interferometers: sub-arsec resolution (<100 AU at 100 pc)
(Sub-)millimeter telescopes

• Single-dish telescopes:
  IRAM 30m, JCMT 15m, CSO 10m, APEX 12m, HHT 10m
  - Typical beam sizes 10–30": 1000–3000 AU at 100 pc

• Interferometers:
  IRAM 6×15m, CARMA 6×10m+9×6m, SMA 8×6m, Nobeyama 6×10m, early ALMA: 32×12m
  - Beam sizes 0.5–5": 50–500 AU at 100 pc
Detecting molecular lines

Depends on physical conditions and distribution of molecules
Analysis of spectral lines is challenging.
Molecules in space (~170)

Detected in disks: CO, HCO\(^+\), DCO\(^+\), CN, HCN, DCN, HNC, N\(_2\)H\(^+\), HC\(_3\)N, H\(_2\)CO, CS, HDO, C\(_2\)H\(_2\), CO\(_2\), OH, H\(_2\)O, Ne, Fe, Si, H\(_2\)

http://www.astrochymist.org/astrochymist_mole.html
http://www.astro.uni-koeln.de/cdms/molecules
Molecular emission: diagnostics

Plane-parallel infinite, homogeneous slab of turbulent gas:
- LTE and low optical depth, intensity scales with column density $N_u$:

$$I = \frac{A_{ul} \, N_u \, h \nu_{ul}}{4\pi}$$

- LTE and high optical depth, intensity scales with $T$ and line width $b$:

$$I \simeq B(T) \frac{\nu b}{c}$$

From molecular emission lines:
- Line strength: column densities
- Line ratios (ladder): temperatures, densities
- Line profiles: kinematics
## Molecules as probes

<table>
<thead>
<tr>
<th>Tracer</th>
<th>Properties</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}$CO</td>
<td>Optically thick lines</td>
<td>Temperature</td>
</tr>
<tr>
<td>$\text{H}_2$, $\text{NH}_3$</td>
<td>Symmetric species</td>
<td></td>
</tr>
<tr>
<td>$^{13}$CO, $\text{C}^{18}$O, CS, $\text{H}_2\text{CO}$</td>
<td>Large dipole moment</td>
<td>Density</td>
</tr>
<tr>
<td>$\text{HCO}^+$, $\text{N}_2\text{H}^+$, $\text{C}^+$, $\text{Ne}^+$, OH$^+$, $\text{H}_2\text{O}^+$, $\text{H}_3\text{O}^+$</td>
<td>Charged species</td>
<td>Ionization</td>
</tr>
<tr>
<td>$\text{H}_2\text{CO}$, organics</td>
<td>Complex species</td>
<td>Surface processes</td>
</tr>
<tr>
<td>$\text{DCO}^+$, DCN, $\text{H}_2\text{D}^+$</td>
<td>Deuterated species</td>
<td>Deuterium fractionation</td>
</tr>
</tbody>
</table>

Semenov et al. (2010)
Disk structure & evolution

- Conservation & redistribution of angular momentum
- Gas viscosity due to turbulence
- Gravity
- Pressure
- Initial mass
- Initial angular speed of a cloud

Characteristics: $R_{\text{disk}}$, $M_{\text{disk}}$, $T_{\text{dust}}$, $T_{\text{gas}}$, surface density, accretion rate, ...
Disk vertical structure

- Equation of state: \( P = c_s^2 \rho \)

- Hydrostatic equilibrium: \( \frac{dP}{dz} = \rho \Omega_K^2 z \)

- Assuming isothermal structure in z-direction:

  - Density profile: \( \rho = \rho_0 \exp\left(-\frac{z^2}{H^2}\right) \)

  - Disk pressure scale height: \( H = \sqrt{2}c_s \Omega_K^{-1} \)

  - \( H \sim 0–5 \)
Disk shape

- Power-law model for temperature: \( T \propto r^{-q} \), \( c_s \propto r^{-q/2} \)
- Keplerian rotation: \( \Omega_K = \sqrt{GM_*/r^3} \propto r^{-3/2} \)
- Aspect ratio: \( H/r = \sqrt{2c_s/r\Omega_K} \propto r^{(1-q)/2} \)

- Flaring disks when \((1-q)/2 > 0\), \(q < 1\)
- A typical disk with \(q = 1/2\): \( H/r \propto r^{1/4} \)

Young disks have a shallow density profile:

\[ \Sigma(r) \propto r^{-1} \]
Surface density: Power-law with tapered edge

Dimensionless time

Start

End

\( \frac{\Sigma \pi R_o^2}{m} \)

\( \tau = 0.004 \)

\( \tau = 0.016 \)

\( \tau = 0.064 \)

\( \tau = 0.256 \)
Disks around Sun-like stars

T Tauri stars (G, K, M):
Age: <10 Myr
$T_{\text{eff}} = 3000–6000 \, \text{K}$,
X-ray luminosity: $\sim 10^{31} \, \text{erg/s}$,
At 100 AU UV intensity is $x500$ compared to the interstellar UV

Herbig Ae/Be stars (A, B):
Age: <1–10 Myr
$T_{\text{eff}} = 8000–15000$ K,
X-ray luminosity: <10$^{30}$ erg/s,
At 100 AU UV intensity is > $\times 10000$ compared to the interstellar UV field

- Disks around Herbig Ae/Be stars are warmer than T Tauri disks
- $T_{\text{gas}} > T_{\text{dust}}$ in upper disk layers
Observational campaigns to study disks

• "Chemistry in Disks" (CID): Europe, USA, Taiwan:
  Plateau de Bure Interferometer

• "DISCS" program in USA:
  Submillimeter Array

• Herbig Ae: CO, HCO\(^+\), CN, HCN

• T Tau: CO, HCO\(^+\), HCN, N\(_2\)H\(^+\), CCH, CS, H\(_2\)CO,
  DCO\(^+\), DCN

Dutrey et al. (2007), Schreyer et al. (2008), Henning et al. (2010), Öberg et al. (2010-11)
Mm-observations: outer disk regions

- Strong CO lines: 10–30 min per source
- Other molecules: ~3–10 hours per source
- Thus, only several brightest disks are studied
- Less lines are detected in Herbig Ae disks
Mm-observations: outer disks

- Less molecules in the gas in disks: freeze-out and photodissociation

Bergin et al. (2007), Dutrey et al. (2007), Semenov et al. (2010)
Mm-observations: outer disks

- Photo-dominated chemistry
- Ices: H$_2$O, NH$_3$, CH$_4$, H$_2$CO, CH$_3$OH
- Temperature gradients
- Cold CO, CCH, CN, HCN
- Keplerian rotation
- Non-thermal line broadening

Bergin et al. (2007), Dutrey et al. (2007), Semenov et al. (2010)
Weighting the stars: kinematics from molecular lines

- $M^*$ can be determined from Keplerian velocity law: accuracy is up to 5%

Simon et al. (2000)
Resolved surface density & $T$: DM Tau

Density & temperature from CO isotopologues:

- $^{12}\text{CO}/^{13}\text{CO} \sim 20$ (Earth value is $^{12}\text{C}/^{13}\text{C} = 80$)
- Cold CO, HCO$^+\sim 10$–15K

Pietu et al. (2007)
Temperature in T Tau and Herbig Ae disks

- "Warm" Herbig Ae disks: $T_{\text{kin}} > 20$–$100$K
- "Cool" T Tauri disks: $T_{\text{kin}} \sim 10$–$30$K
- No gradient in LkCa 15: inner hole of $\sim 45$ AU
- Are transitional disks peculiar?

Pietu et al. (2007)
Chemistry in T Tau vs Herbig Ae disks

<table>
<thead>
<tr>
<th>Molecule</th>
<th>AB Aur (A0) N(X)/N(13CO)</th>
<th>DM Tau (M1) N(X)/N(13CO)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2</td>
<td>1.5 (6)</td>
<td>1.0 (7)</td>
</tr>
<tr>
<td>$^{13}$CO</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>HCO$^+$</td>
<td>1.5 (-4)</td>
<td>2.0 (-3)</td>
</tr>
<tr>
<td>HCN</td>
<td>1.3 (-5)</td>
<td>7.0 (-4)</td>
</tr>
<tr>
<td>CS</td>
<td>&lt;8 (-5)</td>
<td>3.0 (-4)</td>
</tr>
<tr>
<td>CCH</td>
<td>&lt;5 (-4)</td>
<td>1.0 (-3)</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>&lt;2 (-1)</td>
<td>0</td>
</tr>
</tbody>
</table>

- Less molecules more complex than CO in AB Aur disk:
  - warmer AB Aur disk has no CO-chemistry on dust surfaces
  - less X-rays from AB Aur lead to slower destruction of CO via $\text{CO} + \text{He}^+ \rightarrow \text{C}^+ + \text{O} + \text{He}$

Schreyer et al. (2009), Öberg et al. (2010-11)
IR revolution: molecules in planet-forming zones

- NeII, FeII, OI, H$_2$, OH, H$_2$O, CO$_2$, HCN and C$_2$H$_2$
- Warm gas: $T \gtrsim 100 – 5000$ K
- No depletion
- Non-Keplerian profiles: disk wind?
- Herbig Ae disks appears to be deficient in H$_2$O and organics

(Lahuis ++ 06, Pascucci ++ 07-11, Salyk ++ 08-11, Pontoppidan ++ 07-11, Carr & Najita 08, Kamp++11)
Pause
Zone of ions and radicals (atmosphere)

- Intense UV and X-rays
- Low densities
- High temperatures
- High ionization degree
- Limited gas-phase chemistry
Zone of molecules (intermediate layer)

- Partly shielded from UV and X-rays
- Moderate densities
- Moderate temperatures
- Oasis of rich chemistry: gas-surface cycling, photoprocessing of ices
- Most molecular lines are excited here
Zone of ices (midplane)

- Only cosmic rays can penetrate
- High densities
- Low temperatures
- Molecules are frozen out
- Rich chemistry on dust surfaces
Inner, planet-forming zone

- High n, T
- Reactions with barriers
- 3-body collisions
- X-ray-driven processes
- No freeze-out
- Fast grain evolution
Chemical kinetics equations

\[ \frac{\partial n_i}{\partial t} = \sum_{j,k \neq i} k_{jk} n_j n_k - n_i \sum_{l} k_{ln} n_l + \nabla D n_H \nabla (n_i/n_H) - \nabla U n_i \]

Evolution = Formation - Destruction + Diffusion + Advection

[ Chemistry ] [ Dynamics ]

- Physical conditions
- Initial abundances of molecules
- Grain properties
- Reaction data
- Chemical code

Performance:
- Laminar model: \( \sim 0.1-1 \) hour
- 2D-chemo-dynamical model: \( \sim 12 \) hours – 7 days
Modeling chemistry with dynamics

Evidence:
• Isotopic homogeneity of Solar nebula (<10–20 AU)
• Crystalline silicates in comets and outer disk regions
• Viscous evolution driven by turbulence

Model:
• 5 Myr, 10–800 AU, $M_{\text{disk}} = 0.055M_{\text{Sun}}$
• Diffusion coefficient: $\alpha=0.01, \sim 10^{18} \text{ cm}^2/\text{g}$
• ALCHEMIC chemical model

## Timescales: chemistry vs dynamics

<table>
<thead>
<tr>
<th>Process @ 250 AU</th>
<th>Midplane</th>
<th>Warm layer</th>
<th>Atmosphere</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mixing</td>
<td>1 000 000 yr</td>
<td>250 000 yr</td>
<td>150 000 yr</td>
</tr>
<tr>
<td>Gas-phase</td>
<td>1 yr</td>
<td>1 yr</td>
<td>3 yr</td>
</tr>
<tr>
<td>Photoreaction</td>
<td>&gt;1 000 000 yr</td>
<td>1 000 000 yr</td>
<td>30 yr</td>
</tr>
<tr>
<td>Freeze-out</td>
<td>27 yr</td>
<td>180 yr</td>
<td>2300 yr</td>
</tr>
<tr>
<td>Desorption</td>
<td>1 000 000 yr</td>
<td>4 yr</td>
<td>0 yr</td>
</tr>
<tr>
<td>Surface reaction</td>
<td>&gt; 1 000 000 yr</td>
<td>&gt; 1 000 000 yr</td>
<td>150 000 yr</td>
</tr>
</tbody>
</table>

- Gas-phase chemistry is faster than mixing
- Ice chemistry is slower than mixing
Steadfast species

- Fast gas-phase formation and destruction
- Example: CO, OH, H$_2$O ice, CCH, C$^+$, CN, HCN
**Sensitive species**

<table>
<thead>
<tr>
<th>Laminar</th>
<th>Slow Mixing</th>
<th>Fast Mixing</th>
<th>Column Densities</th>
</tr>
</thead>
</table>

- Slow surface formation and photoprocessing
- Example: hydrocarbons (C<sub>2</sub>H<sub>2</sub>), organics (HCOOH), SO, SO<sub>2</sub>, C<sub>2</sub>S, C<sub>3</sub>S,...
### Observations vs Predictions: DM Tau

<table>
<thead>
<tr>
<th>Species</th>
<th>Observed, cm(^{-2})</th>
<th>Laminar</th>
<th>Mixing</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>3.0 (17)</td>
<td>3.0 (17)</td>
<td>3.0 (17)</td>
</tr>
<tr>
<td>HCO(^+)</td>
<td>1.7 (13)</td>
<td>8 (12)</td>
<td>2.5 (13)</td>
</tr>
<tr>
<td>H(_2)CO</td>
<td>1-2 (13)</td>
<td>6.2 (12)</td>
<td>4.0 (12)</td>
</tr>
<tr>
<td>N(_2)H(^+)</td>
<td>4 (11)</td>
<td>3.4 (11)</td>
<td>1.2 (12)</td>
</tr>
<tr>
<td>CS</td>
<td>4 (12)</td>
<td>8.1 (10)</td>
<td>5.6 (11)</td>
</tr>
<tr>
<td>CN</td>
<td>4 (13)</td>
<td>1.4 (13)</td>
<td>1.8 (13)</td>
</tr>
<tr>
<td>HCN</td>
<td>8 (12)</td>
<td>1.2 (13)</td>
<td>2.7 (13)</td>
</tr>
<tr>
<td>HNC</td>
<td>3 (12)</td>
<td>1.0 (13)</td>
<td>2.4 (13)</td>
</tr>
<tr>
<td>CCH</td>
<td>3 (13)</td>
<td>1.1 (13)</td>
<td>1.4 (13)</td>
</tr>
<tr>
<td>Agreement</td>
<td>7/8</td>
<td>6/8</td>
<td></td>
</tr>
</tbody>
</table>

- Laminar & mixing model are OK
- Agreement with observations of cometary ices
ALMA: The Brave New World

Specifications:
• 66 antennas: 5000 m²
• 0.005-0.3”
• 86 – 950 GHz, <0.05 km/s

Science:
• Complex molecules
• Isotopologues: $^{15}$N, $^{34}$S, $^{17,18}$O, D
• Surveys

Vast flow of data to be interpreted
⇒ new models are needed
ALMA is working: TW Hya disk

Science Verification observations of TW Hya at 345 GHz
Conclusions

- Handful of molecules are detected
- Large observational & modeling campaigns
- UV/X-ray radiation
- Freeze-out (depletion)
- Different chemistry in T Tauri vs Herbig Ae disks?
- Dynamical processes!
- Models qualitatively agree with observations
- ALMA revolution!
The End
1) Which angular resolution is needed (approximately) to resolve molecular emission from nearby protoplanetary disks:
   a) with radius of 1000 AU at a distance of 140 pc (DM Tau)?
   b) with radius of 200 AU at a distance of 60 pc (TW Hya)?

2) Assuming that intensity of an optically thick line is of the order of the local gas kinetic temperature, calculate the measured line intensity from a disk with a radius of 1000 AU at 140 pc when observed with an angular resolution of:
   a) 1" (typical temperature is 50K)
   b) 10" (typical temperature is 20K)
   c) 30" (typical temperature is 20K)
3) How large could the molecular line width (in km/s) be if we are observing molecular emission arising from 10–1000 AU in a disk with Keplerian rotation profile $V(r) = \left(\frac{GM}{r^3}\right)^{1/2}$, observed at inclination angle of:
a) 0 deg (face-on orientation),
b) 10 deg,
c) 90 deg (edge-on orientation).
(Assume turbulent broadening of 0.1 km/s and thermal broadening of 0.5 km/s).
Suggested literature

• A. G.G.M. Tielens, "The Physics and Chemistry of the ISM" (2007), CUP

• "Protoplanetary Dust" (2010), eds. D. Apai & D. Lauretta, CUP

• "Protostars & Planets V" (2005), Part VI, eds. B. Reipurth et al., Univ. Arizona P.