Chemistry in Disks –
an Observational Perspective
A.K.A. Chemical composition and distribution of molecules in low mass protostellar disks

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Chemical structure of protoplanetary disks

Bergin et al. PPV
Molecules in Disks

- CO and its isotopologues: CO, $^{13}$CO, C$^{18}$O
- HCO$^+$, H$^{13}$CO$^+$, DCO$^+$,
- HCN, CN, DCN
- H$_2$CO, N$_2$H$^+$, C$_2$H
- HDO, H$_2$D$^+$, D$_2$H$^+$, CH$_3$OH and CS?

See Dutrey et al. 1997, 2007; Thi et al. 2004; Bergin et al. PPV Poster by Semenov et al.
TW Hya

• **isolated** classical T Tauri star
  
  – southern sky: dec -35
  
  – Herbig (1978): K7Ve (Li), young Sun-like star, but far (13 degrees) from any dark cloud
  
  – Ruciniski & Krauter (1983): near-ir excess
  
  – Zuckerman et al. (1995): circumstellar CO(1-0)

• **distance** $56 \pm 7$ pc (*Hipparcos* 1997)
  
  – 2.5x closer than Taurus, Ophiucus, Chamaeleon, ...

• **age** estimate 5 to 15 Myr
  
  – interesting for disk dissipation, planet formation
SMA TW Hya Images

- CO 2-1
- $^{13}$CO 2-1
- HCO$^+$ 3-2
- DCO$^+$ 3-2
- HCN 3-2
- CN 2-1
Two model approaches

• The gas kinetic temperature is determined from CO line analysis, and the radial density distribution from the fit of the mm continuum images. Molecular line radiative transfer calculations based on escape probability and 1-D radiative transfer. Method used by Dutrey, Guilloteau and collaborators.

• The kinetic temperature and density structures are determined by modeling the SED of the dust disk. Full 2-D Monte-Carlo radiative transfer code are used for molecular line radiative transfer calculations.

See details in the review of Dutrey et al. in Protostars and Planets V
Check poster by A. Isella, O. Panic and D. Semenov.
Spectral line models

- Adopt the physical model (density and temperature structure) by D’Alessio, Calvet et al. to match the SEDs.
- Use 2D accelerated version of Michiel Hogerheijde’s Monte Carlo Model to calculate the radiative transfer and molecular excitation.
- Produce a grid of models with a range of disk parameters and select synthetic visibility observations at the observed \((u,v)\) spacings to simulate the molecular emission.
TW Hya Spectral Energy Distribution

- **far-ir/mm**: usual outer disk with grain growth: $F_{mm} \sim \lambda^{-2.6} \sim \kappa_{dust} \lambda^{-2}$
- **near-ir**: gap, cleared inner disk with gas and small amount $\sim \mu m$ dust
  - “wall” at $\sim 4$ AU ($T \sim 130$ K) = inner edge of outer disk
- Spitzer IRS finding similar systems (Uchida et al. 2004)
Temperature and density structure of TW Hya
TW Hya disk parameters

- Chi-square analysis in the \((u,v)\) plane
- Parameters including \(M_*\) (0.6 \(M_{\odot}\)), inclination \(i\) (7 degrees), \(R_{\text{out}}\) (170 AU), \(R_{\text{in}}\) (4 AU), \(V_{\text{turb}}\) (0.08 km s\(^{-1}\)) and various molecular fractional abundances.

New distribution parameters

- Radial distribution. Radial distribution highly correlated with $R_{\text{out}}$.
- Vertical distribution
  The vertical distributions at different radii similar as a function of the hydrogen column density measured from the disk surface.

$$\sum_{21} \equiv \frac{\sum H}{1.59 \times 10^{21} \text{cm}^{-2}}$$

Next talk by H. Nomura
Vertical distribution

![Graph showing vertical distribution with a peak at midplane and labels for surface and midplane.](image-url)
TW Hya CO 3-2
TW Hya $^{13}$CO 2-1

- Assuming $^{13}$CO and CO share the same distribution including $R_{out}$.
- $\text{CO}/^{13}\text{CO} = 40 \pm 5$
Models with different column density radial distributions ($^{13}$CO)
Data vs Models with different column density radial distributions ($^{13}$CO)
TW Hya $C^{18}O$ 2-1

- $\frac{CO}{C^{18}O} = 200 \pm 50$
TW Hya HCO\textsuperscript{+} 3-2 and H\textsuperscript{13}CO\textsuperscript{+} 4-3

HCO\textsuperscript{+} 3-2

MODEL

DATA

H\textsuperscript{13}CO\textsuperscript{+} 4-3

HCO\textsuperscript{+}/H\textsuperscript{13}CO\textsuperscript{+} = 50\pm10
• The abundance of DCO$^+$ is found to increase with increasing radius till 70 AU.
• The distribution of DCO$^+$ clearly doesn’t follow that of HCO$^+$. 
Models with different vertical column density distributions (DCO⁺)
Data vs Models with different vertical column density distributions (DCO⁺)
TW Hya HCN/DCN 3-2

• First detection of DCN in disks.
• DCN/HCN=2×10⁻³
  — Consistent with the observation of comets.
• The outer radius of HCN is much smaller than that of CN, probably due to the photochemistry in the outer disk. HCN can be photolyzed by Ly $\alpha$ emission, while CN cannot.
Radial Distribution of Molecular Column Densities in the Disk of TW Hya (Best Fit Model)

- CO/^{13}CO=40\pm5
- CO/^{18}O=200\pm50
- HCO^+/^{13}CO^+=50\pm10
- DCN/HCN=2\pm0.5 \times 10^{-3}
Concluding Remarks I

• By combining self-consistent physical models and 2D radiative transfer code, along with high spatial resolution mm/submm molecular images, we are starting to investigate the radial and vertical distribution of molecules in disks.
  – TW Hya:
    • The outer radius of $^{13}$CO/$^{18}$O is not necessarily smaller than that of $^{12}$CO, provided the decrease of CO column density with radius is sufficiently steep.
    • The distribution of DCO$^+$ clearly doesn’t follow that of HCO$^+$, where DCO$^+$ is found to increase with increasing radius till 70 AU, owing to the decreasing temperature and CO depletion in the outer disk; following the prediction of chemical models.
    • The outer radius of HCN is much smaller than that of CN, probably due to the photochemistry in the outer disk. HCN can be photolyzed by Ly$\alpha$ emission, while CN cannot.
Concluding Remarks II

• What we expect:
  – **ALMA**: more disk samples; more lines.