Observational Properties of Protoplanetary Disks

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• Today:
  • Molecular spectroscopy basics
  • Molecular abundances
  • Molecular line observations of disks: kinematics, turbulence, mass
Questions from yesterday

• More on dust traps
  • Just heard from Phil, more this afternoon

• More on Lab Experiments
  • See Testi et al. 2014 PPVI review
  • Specific on laboratory experiments: Blum & Wurm 2008, ARAA
Part VIII
Molecular Spectroscopy
molecular spectroscopy

- Molecular lines:
  - Rotation
  - Vib (Stretching and Bending)
  - Electronic
Molecular rotational lines

- Molecular lines:
  - Rotational spectra of molecules (simplified)

\[
E_{\text{rot}} = \frac{\hbar^2}{2 \mu R_e^2} J(J + 1) = B_e J(J + 1)
\]

\[
\Delta E_{\text{rot}} (J) = 2 B_e (J + 1)
\]

\[
B_e = \frac{\hbar^2}{2 \mu R_e^2}
\]

- Selection rules:
  - Permanent dipole moment (H\textsubscript{2}, C\textsubscript{2}, O\textsubscript{2}, CH\textsubscript{4}, C\textsubscript{2}H\textsubscript{2} not ok)
  - DJ=1 (only adjacent levels)
  - Symmetric molecules => quadrupole transitions (DJ=2)
Molecular rotational lines

- Examples of diatomic molecules: CO (m=7) and H₂ (m=0.5)

- CO levels are closely spaced
  - Smaller DE => long wavelength transitions, low excitation
  - J=1-0 -> n=115GHz, l=2.7mm
  - J=2-1 -> n=230GHz, l=1.3mm
  - J=3-2 -> n=345GHz, l=0.87mm

- H₂ levels are further away, only quadrupole transitions allowed
  - MIR, high excitation lines
Molecular lines: symmetric top rotators

- Molecules with an axis of three-fold or higher symmetry
- Examples: NH$_3$, CH$_3$CN, CH$_3$CCH
- Quantum numbers: J and projection on axis K (K<=$J$)
- Selection rules: $DJ=1$ (only adjacent levels), $DK=0$
- $K=J$ levels are metastable
- Example: ammonia inversion transitions
Molecular rotational lines

- Molecular lines: asymmetric rotators
  - Quantum numbers: J and projections on two axes $K_-$ and $K_+$
  - Complicated spectra
  - Example: $\text{H}_2\text{O}$
Molecular abundances

- Molecular abundances in molecular clouds and YSOs
Part IX
Molecular gas in disks
Molecular gas

Gas has to dominate the disk mass

- From geometry: $H/R \sim 0.1$ at 1 AU

Direct measurements:

- Cold gas CO, … (outer disk)
- Warm gas $H_2$, CO, $H_2O$ (inner disk)
- Indirect: Accretion and Jets

\[
\frac{1}{\rho} \frac{\partial p}{\partial z} \sim \frac{p}{\rho z} = \frac{GM_*z}{R^3}
\]

\[
\rho(z) = \rho(0) \exp(-z^2/2H^2)
\]

\[
H/R = (T_d/T_g)^{1/2} (R/R_*)^{1/2}
\]
Gas in protoplanetary disks (van Dishoeck 2014)
Outer disks structure and kinematics

(de Gregorio Monsalvo+2013; Mathews+2013)
Molecular gas

- Calculation of the CO emission assuming thermalised gas

\[ I_\nu = \int_{0}^{\infty} S_\nu(s) e^{-\tau_\nu(s)} K_\nu(s) ds \]

\[ \tau_\nu(s) = \int_{0}^{s} K_\nu(s') ds' \]

\[ K^d_\nu(s) = \rho(s) \cdot k_\nu \]

\[ K^{CO}_\nu(s) = n_l(s) \cdot \sigma_\nu(s) \]

\[ n_l(s) = \chi_{CO} \frac{\rho(s)}{m_0} \cdot \frac{g_l e^{-E_l/k T_{CO}(s)}}{Z(T_{CO}(s))} \]

\[ S_\nu(s) = B_\nu(T_{CO}(s)) = \frac{2\hbar \nu^3}{c^2} \frac{1}{\exp(h\nu/k T_{CO}(s)) - 1} \]

\[ T_{CO}(r) = T_{CO}(r_0)(r/r_0)^{-q} \]

(Isella et al. 2007)
Molecular gas

- Simulated CO profiles and maps

(Isella et al. 2007)
Outer disks structure and kinematics

(Qi et al. 2012)
Gas properties and evolution

- Kinematics
  - Disk-outflow interaction
  - Possible evidence for non-Keplerian motions
- Physical properties
  - Temperature, density structure
  - Abundance, gas to dust ratio
- Chemical properties
  - Formation of complex molecules
  - Chemical differentiation in different regions of the disk

CO isotopes depletion factors:

\[ ^{13}\text{CO} \Rightarrow \sim 10 \quad ([^{13}\text{CO}]/[\text{H}_2] \sim 10^{-7}) \]

\[ ^{18}\text{C} \Rightarrow >60 \]
HD163296 as seen by ALMA

- Extent of the CO disk is much larger than that of the mm-grains disk
- Consistent with expectations from viscous spreading and migration of the larger grains
HD 163296 as seen by ALMA

- Evidence for a CO disk wind
HD 163296 as seen by ALMA

- Direct measurement of disk flaring and CO depletion on the mid plane

(Rosenfeld+2013)
5 min pause

- Why CO is our prime probe of gas?

- With $[\text{CO}]/[\text{H}_2] \approx 10^{-4}$, why should it be a better trace of mass than dust ($[\text{d}]/[\text{H}_2] \approx 0.01$)?

- What are the difficulties in using gas as tracer?
Gas kinematics

- Not exactly Keplerian
- Largest effect is the pressure term 5%, self gravity 0.1-0.5%

Potentially a direct measurement of the disk self-gravity

(Rosenfeld et al. 2013)
Turbulence provide an additional line broadening term

Measureable with ALMA: high S/N and resolution
Turbulence - pre-ALMA

- High S/N spectra limit turbulence to
  - < 40 m/s for TW Hya
  - ~300 m/s for upper layers of HD163296 disk (0.4 Mach)

- DM Tau: 0.4-0.5 Mach at intermediate layers (Guilloteau et al. 2012)

- Important for planet-formation models; mixing of material

Hughes et al. (2011)
HD163296 as seen by ALMA

• Chemical measure of CO snowline

(Mathews et al. 2013, Oberg et al. 2012)
Masses from CO and isotopomers

- CO isotopomers may be good tracers of the gas mass, if treated very carefully
- Taking into account: freeze-out and (selective) photodissociation
Direct measurement from HD

- HD has been detected with Herschel in the nearest disk. This may be a good constraint on the gas mass in disks.
Take home points

• Molecular spectroscopy is potentially a very powerful tool to study disk kinematics, physics and chemistry
  • Complex modelling
  • Missing/uncertain key data: collision rates, reaction rates

• ALMA will be the prime tool to study
  • kinematics and chemistry of disks