Chemistry in Disks – an Observational Perspective

A.K.A. Chemical composition and distribution of molecules in low mass protostellar disks

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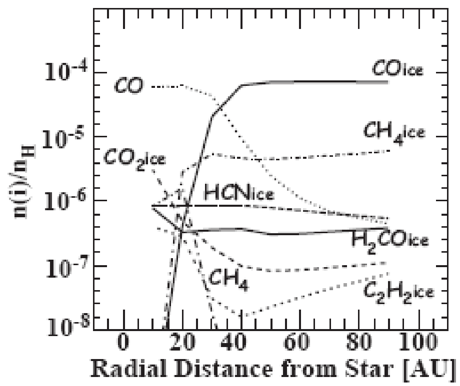
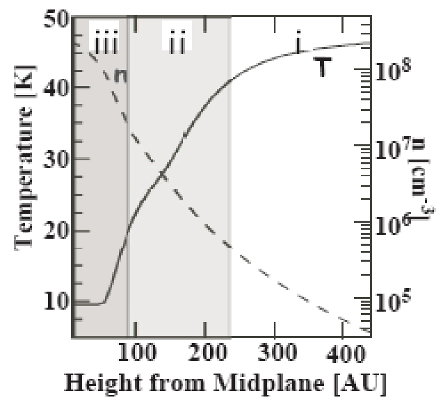
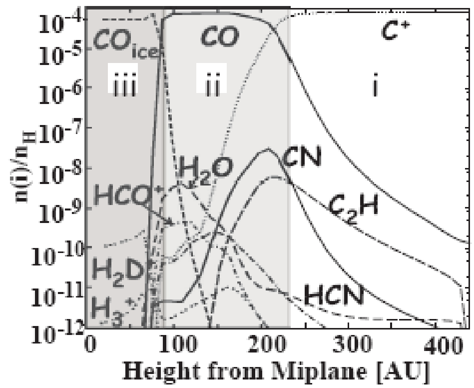
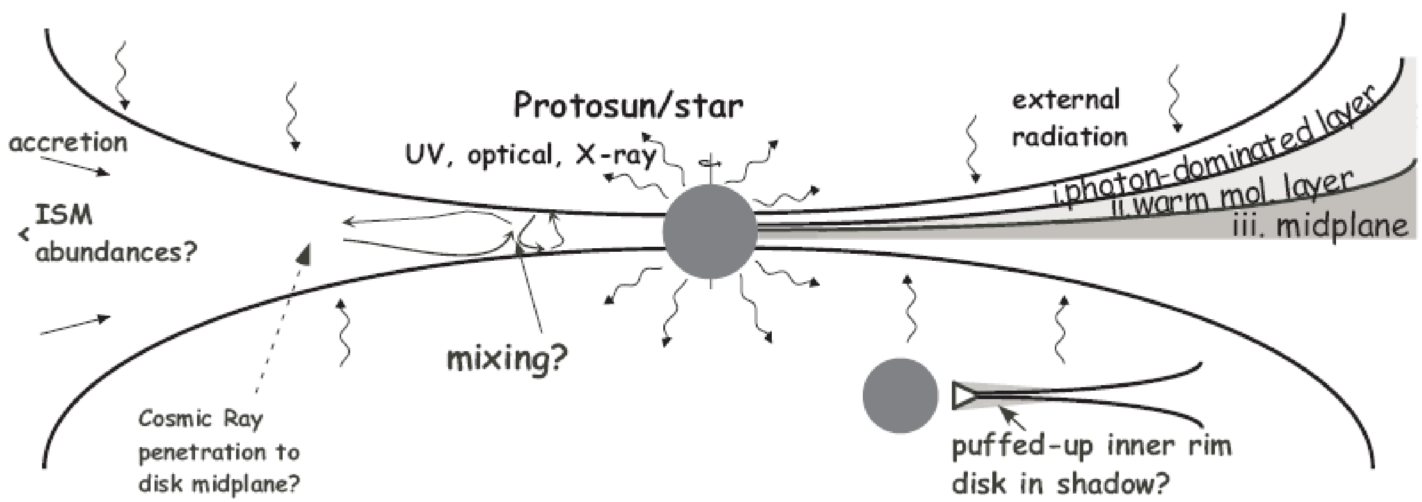
Chemical structure of protoplanetary disks









Bergin et al. PPV

Molecules in Disks

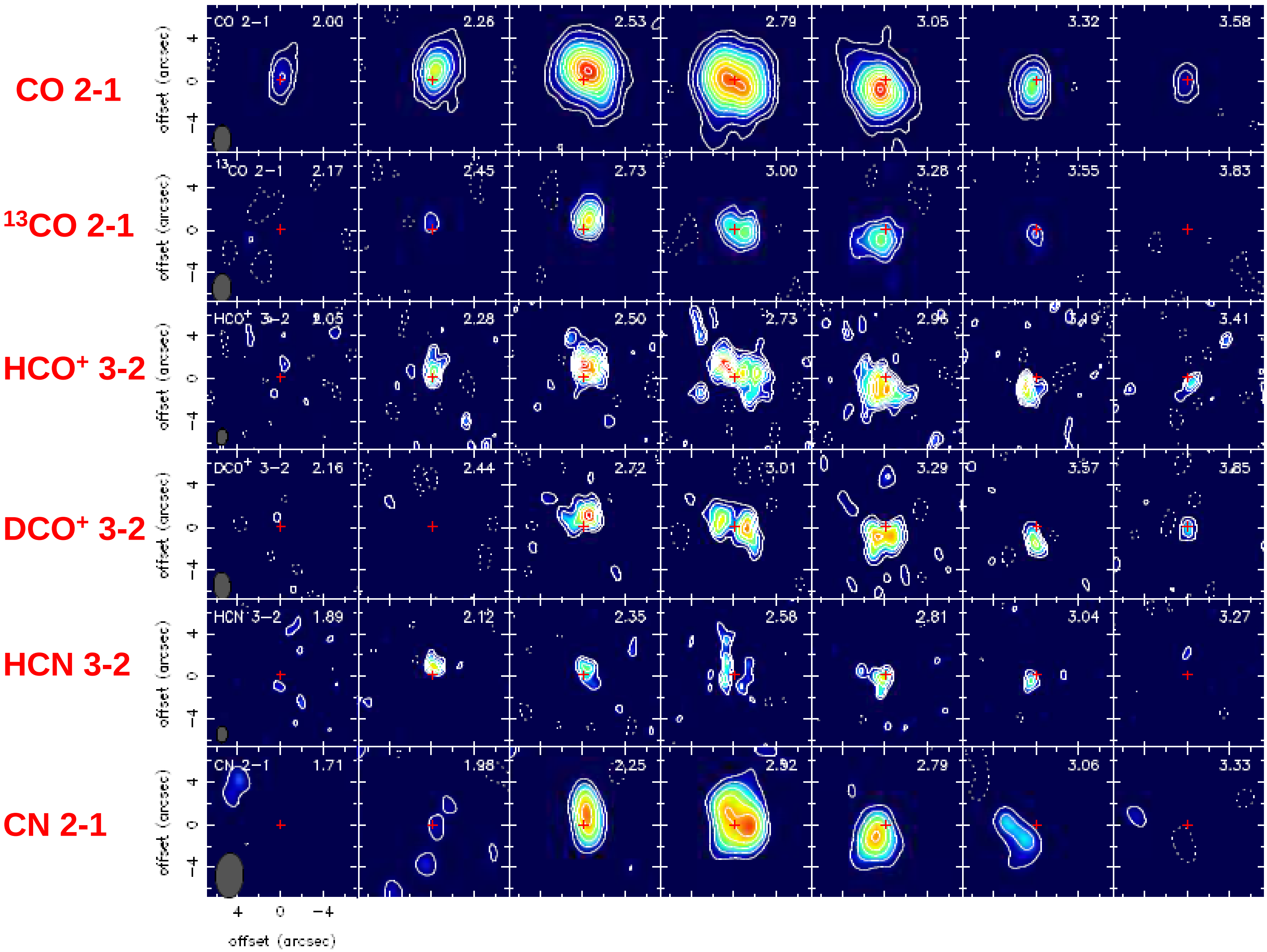
- CO and its isotopologues: CO, ^{13}CO, $C^{18}O$
- HCO^+, $H^{13}CO^+$, DCO^+,
- HCN, CN, DCN
- H_2CO, N_2H^+, C_2H
- HDO, H_2D^+, D_2H^+, CH_3OH and CS ?

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 ± 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



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.

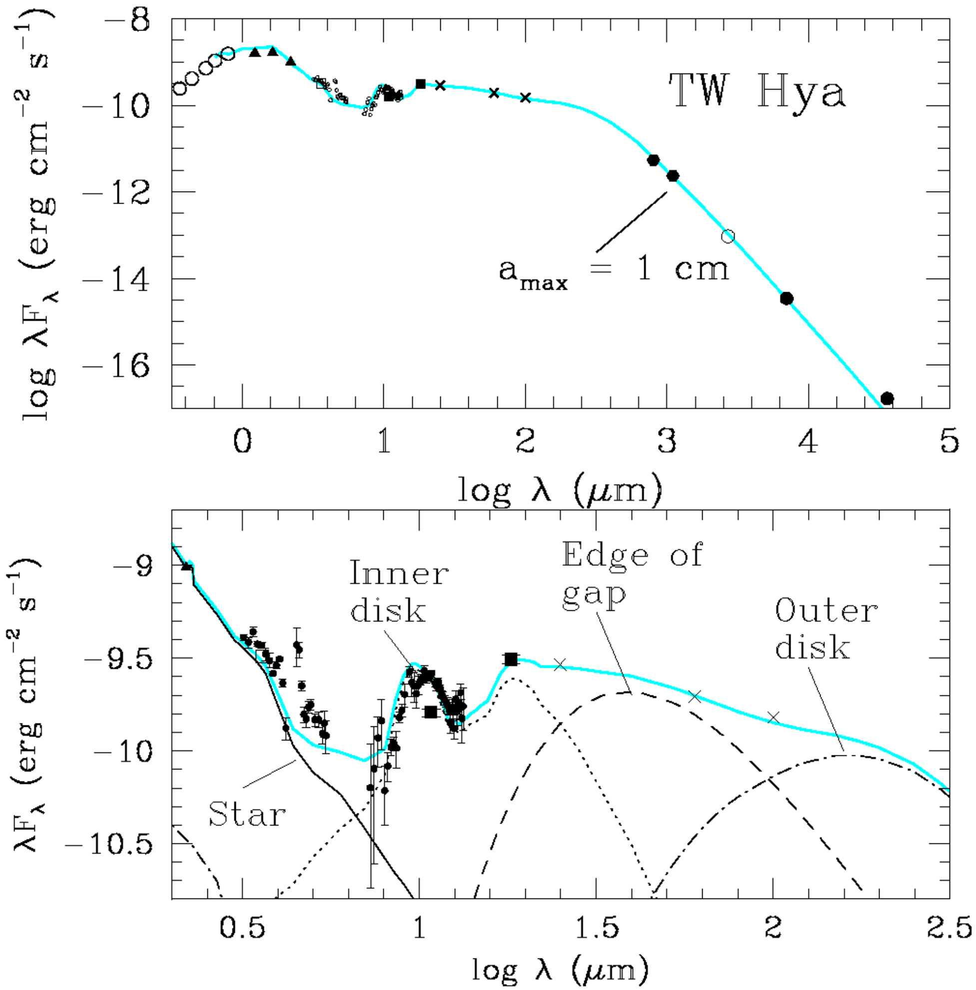
See details in the review of Dutrey et al. in Protostars and Planets V

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.

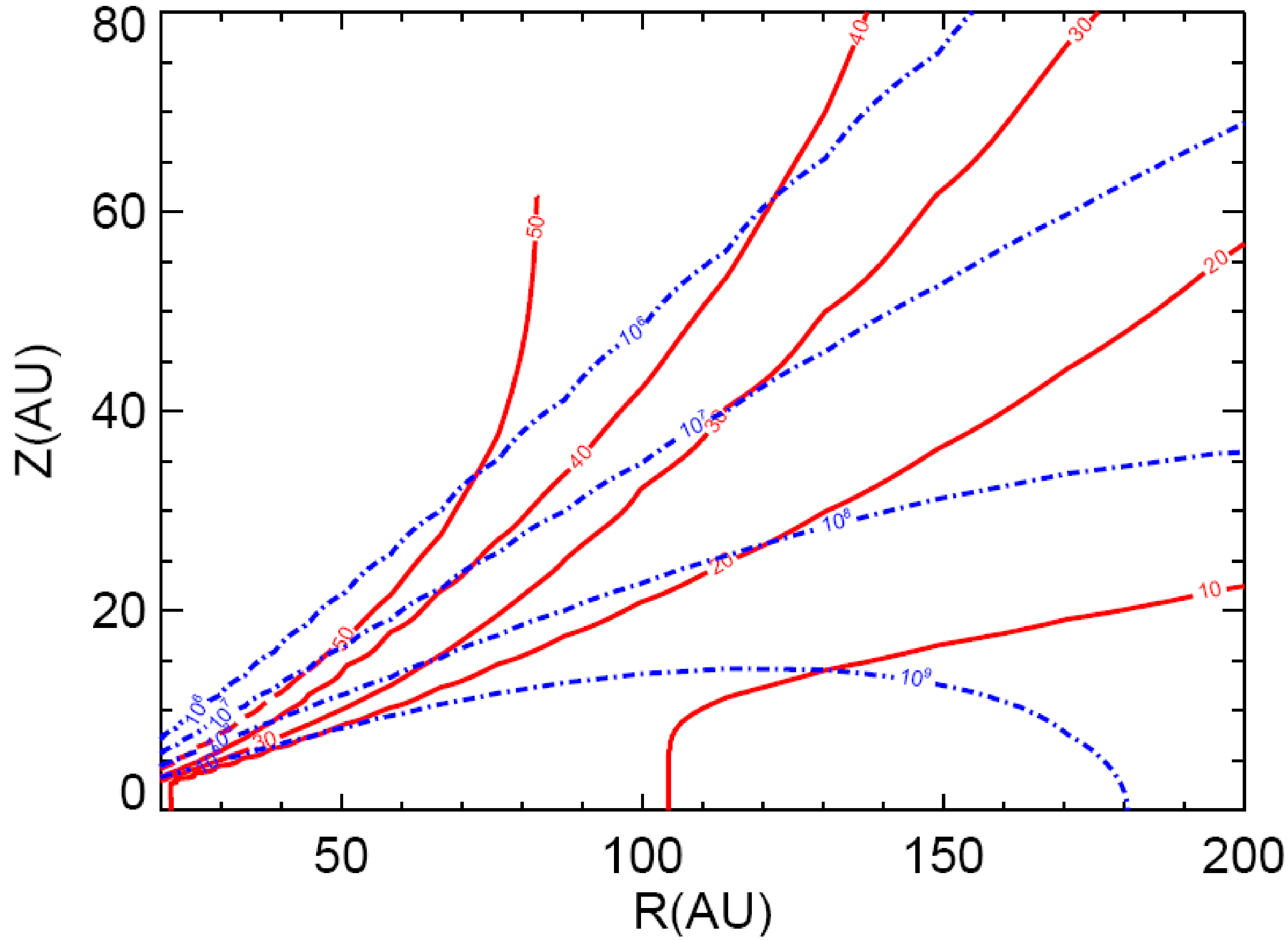
TW Hya Spectral Energy Distribution



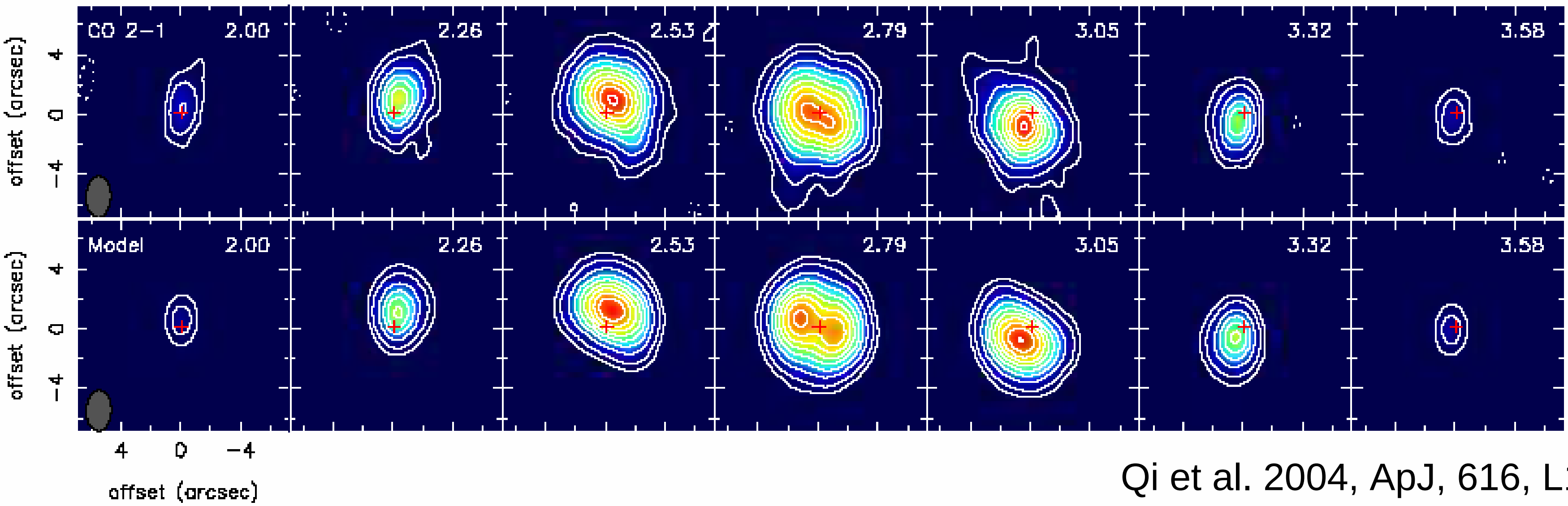
Calvet et al. 2002

- 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 ~μm dust
- "wall" at ~4 AU (T~130 K) = inner edge of outer disk
- Spitzer IRS finding similar systems (Uchida et al. 2004)

Temperature and density structure of TW Hya



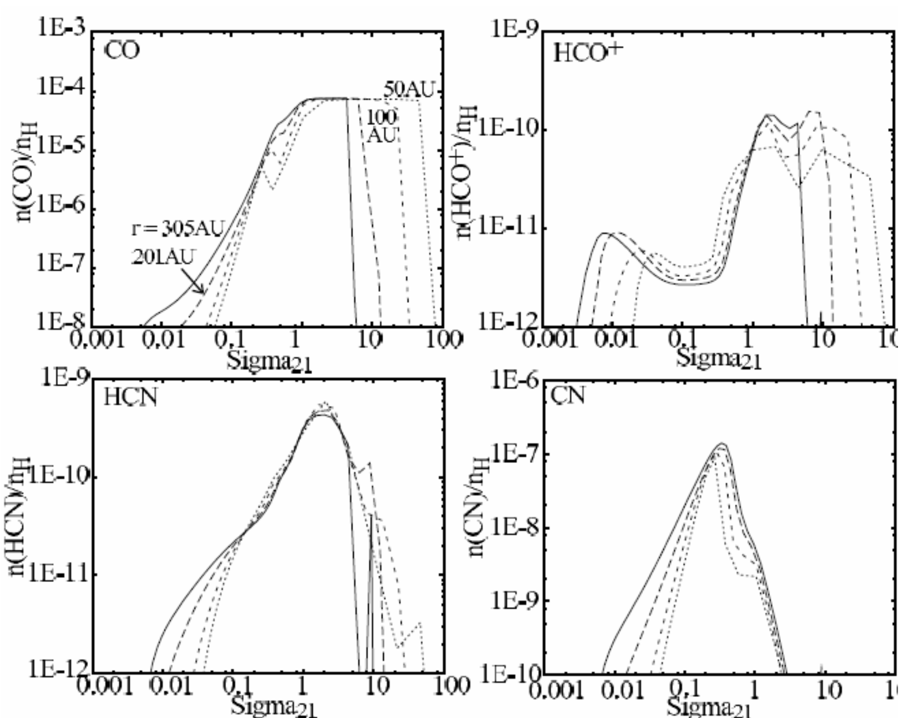
TW Hya disk parameters



Qi et al. 2004, ApJ, 616, L11

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

New distribution parameters



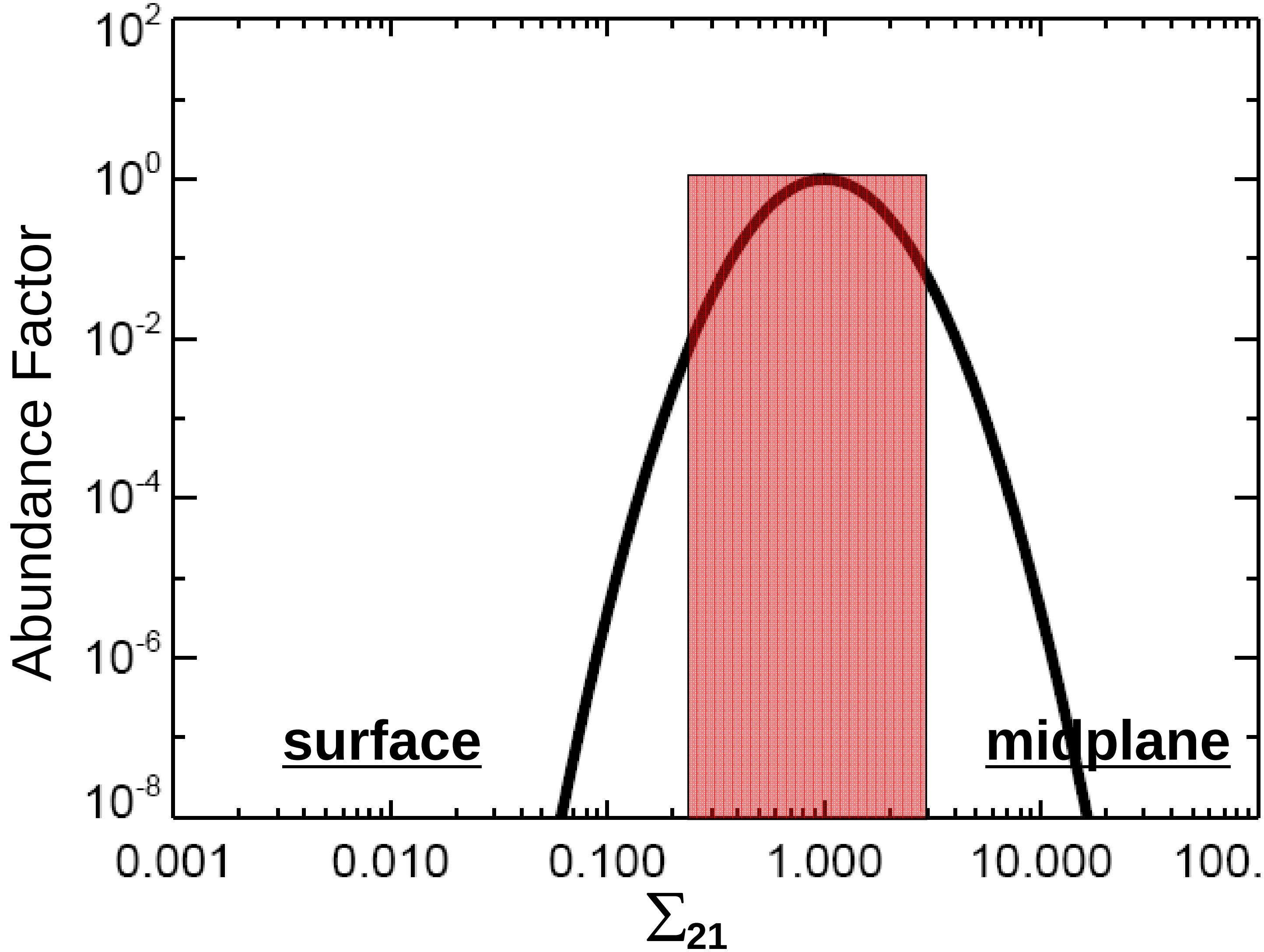
Aikawa & Nomura 2006

$$\sum_{21} \equiv \frac{\sum_H}{1.59\times10^{21}cm^{-2}}$$

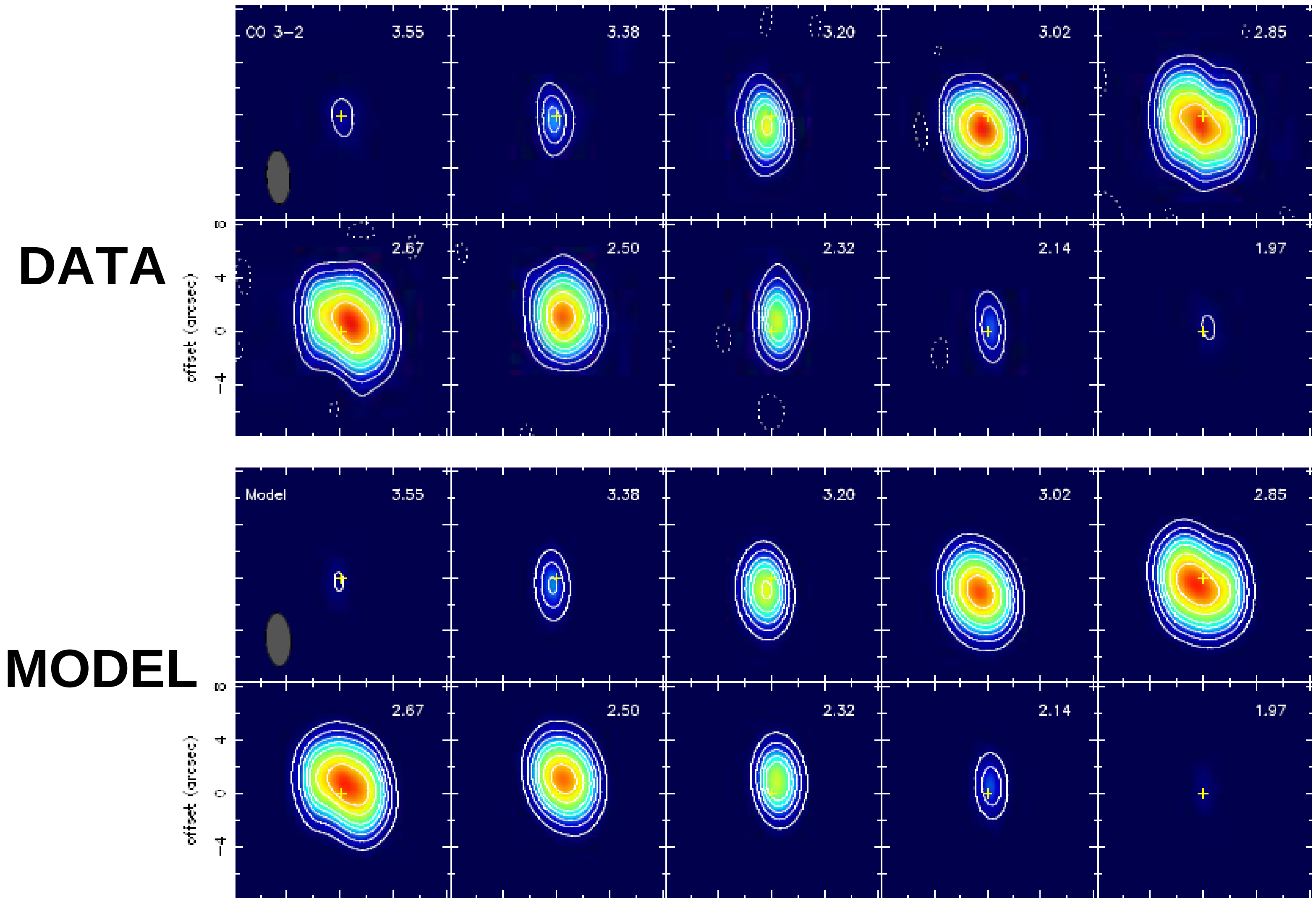
- Radial distribution.
  Radial distribution highly correlated with R_{out}.
- Vertical distribution
  The vertical distributions at different radii similar as a function of the hydrogen column density measured from the disk surface.

Next talk by H. Nomura

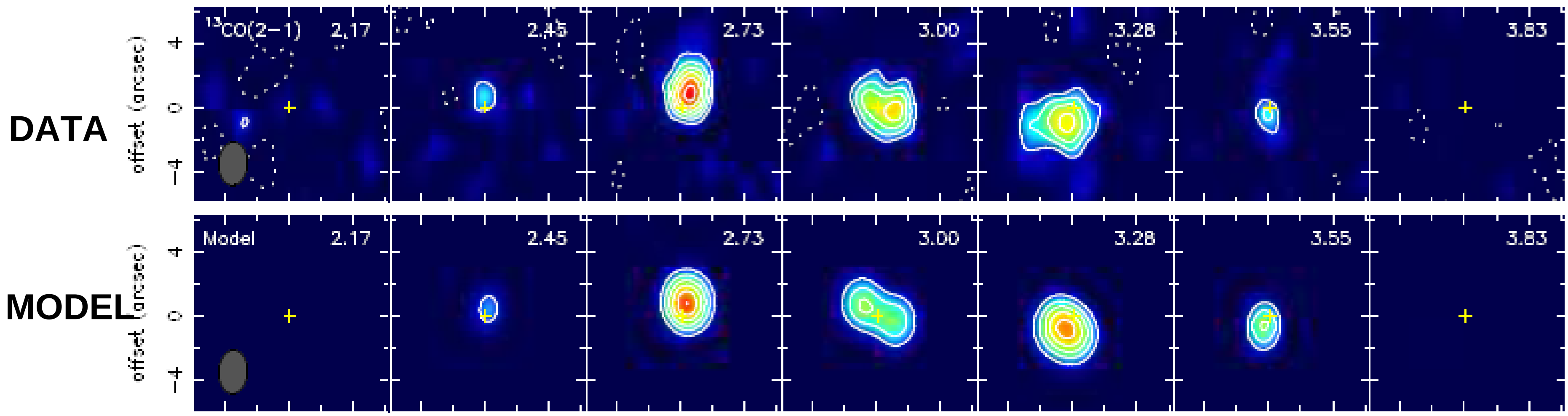
Vertical distribution



TW Hya CO 3-2

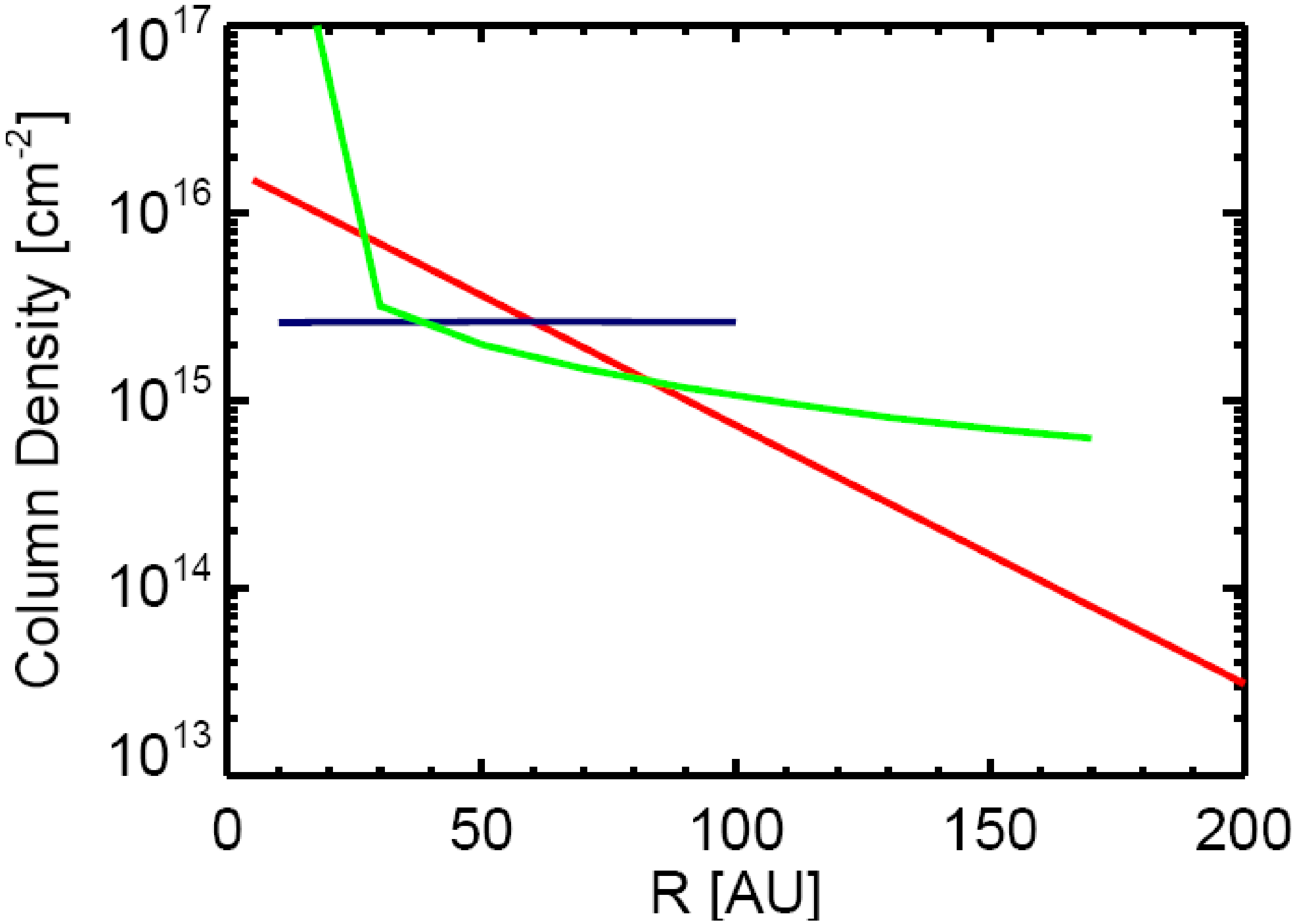

DATA
MODEL
CO 3–2
Model
3.55
3.38
3.20
3.02
2.85
2.67
2.50
2.32
2.14
1.97
offset (arcsec)
8
4
0
−4

TW Hya ^{13}CO 2-1

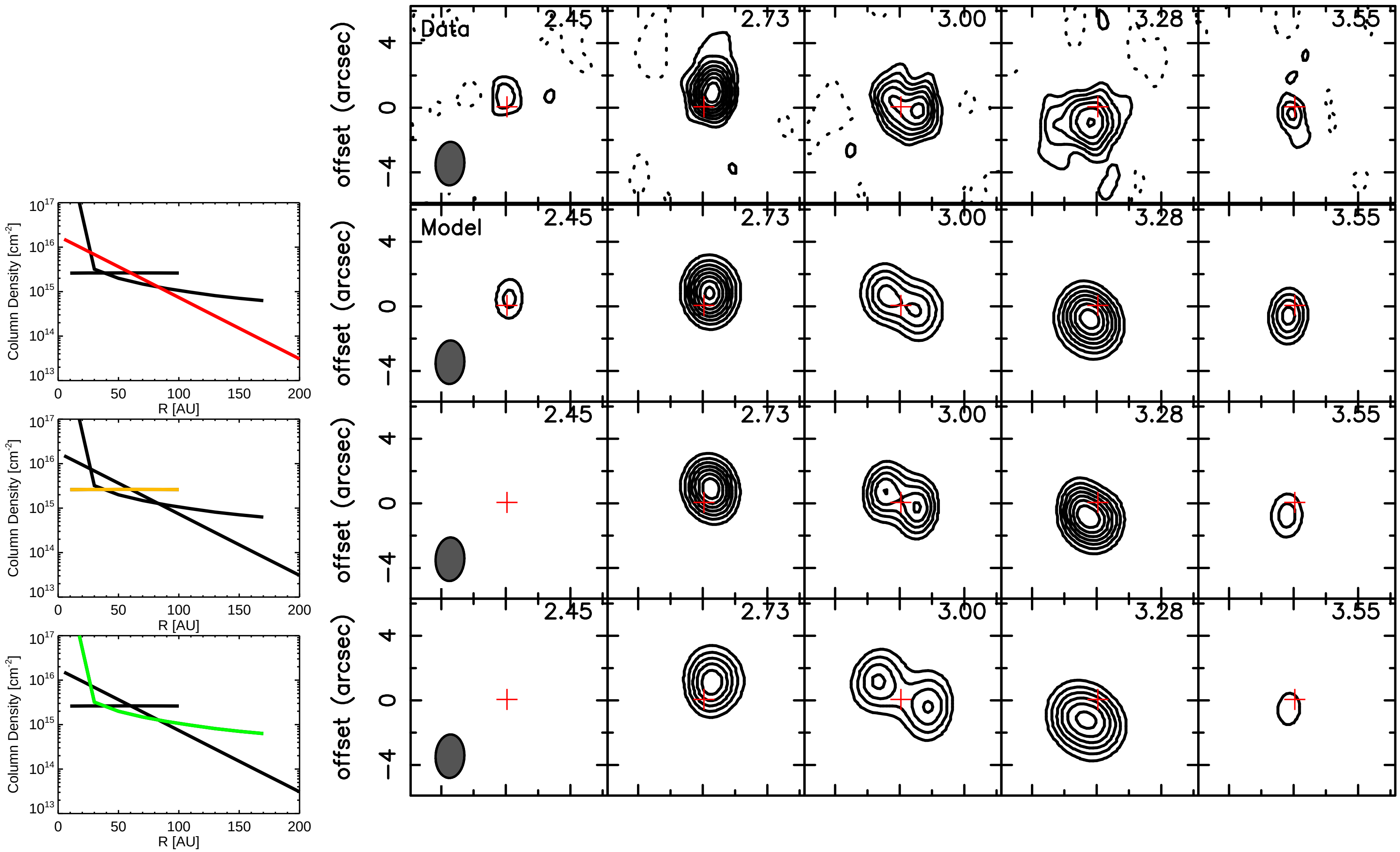


- Assuming ^{13}CO and CO share the same distribution including R_{out} .
- $CO/^{13}CO = 40 \pm 5$

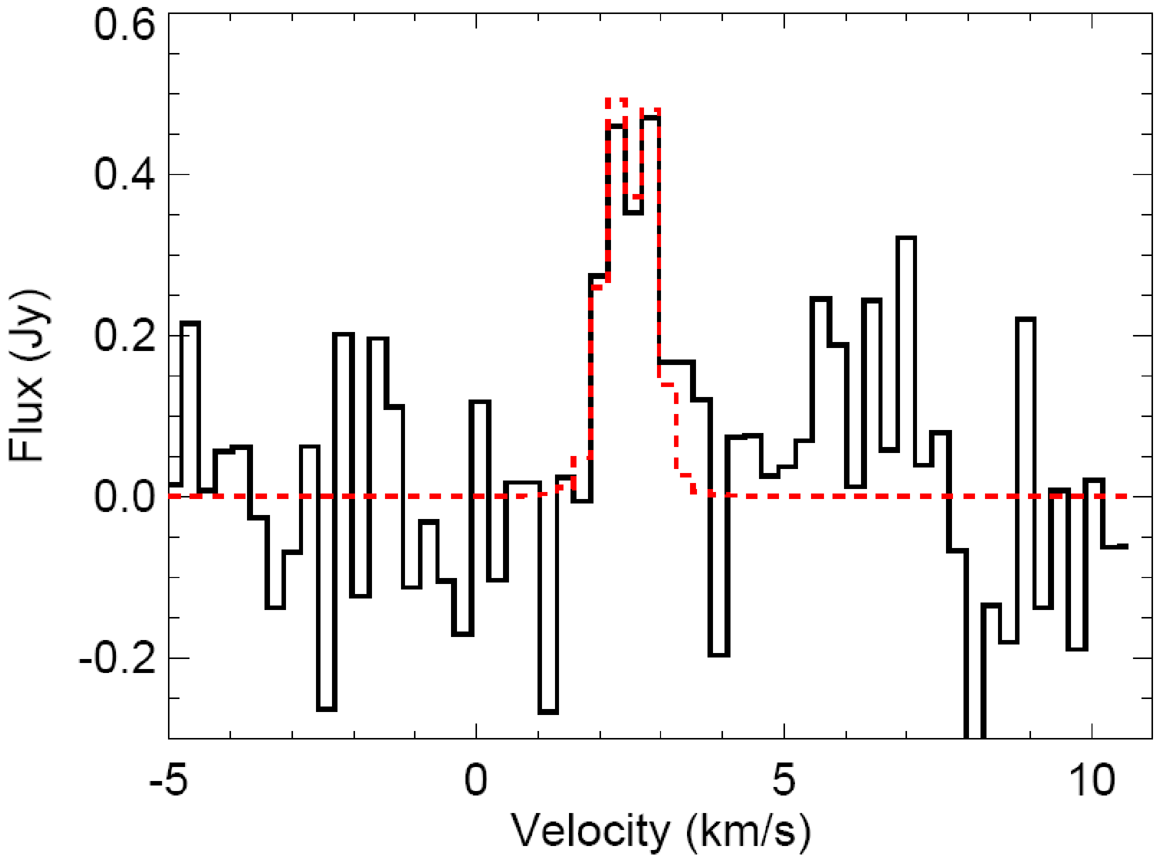
Models with different column density radial distributions (^{13}CO)



Data vs Models with different column density radial distributions (^{13}CO)

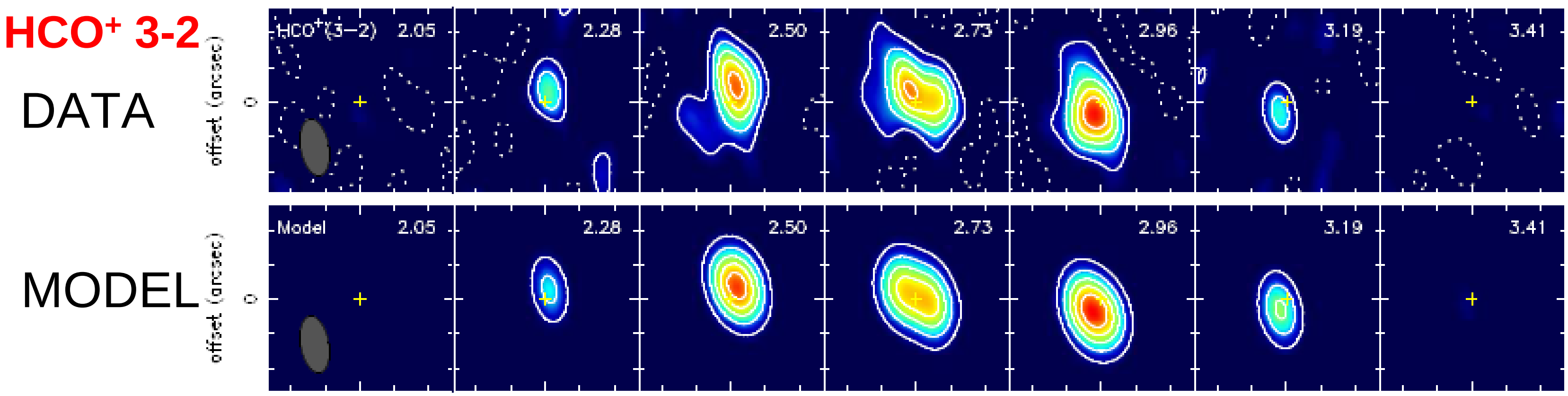


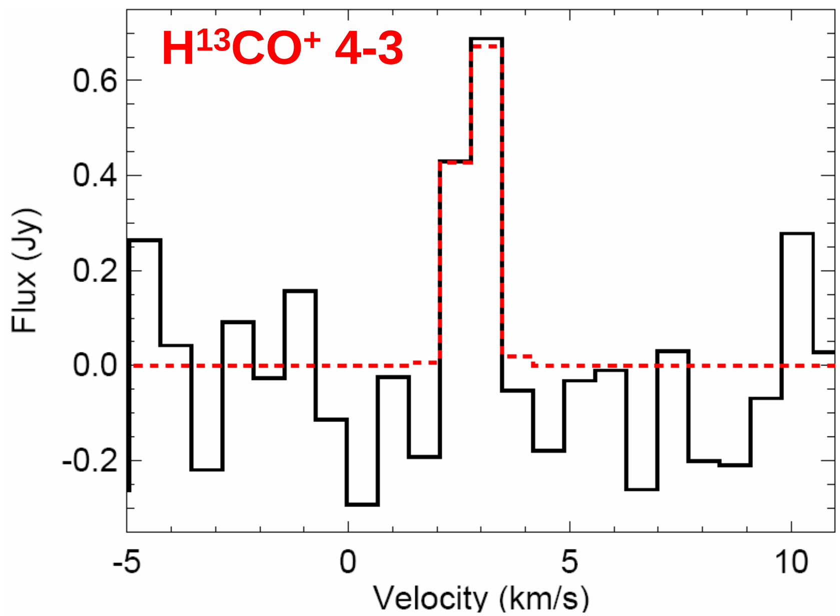
TW Hya $C^{18}O$ 2-1



- $CO/C^{18}O = 200 \pm 50$

TW Hya HCO^+ 3-2 and $H^{13}CO^+$ 4-3



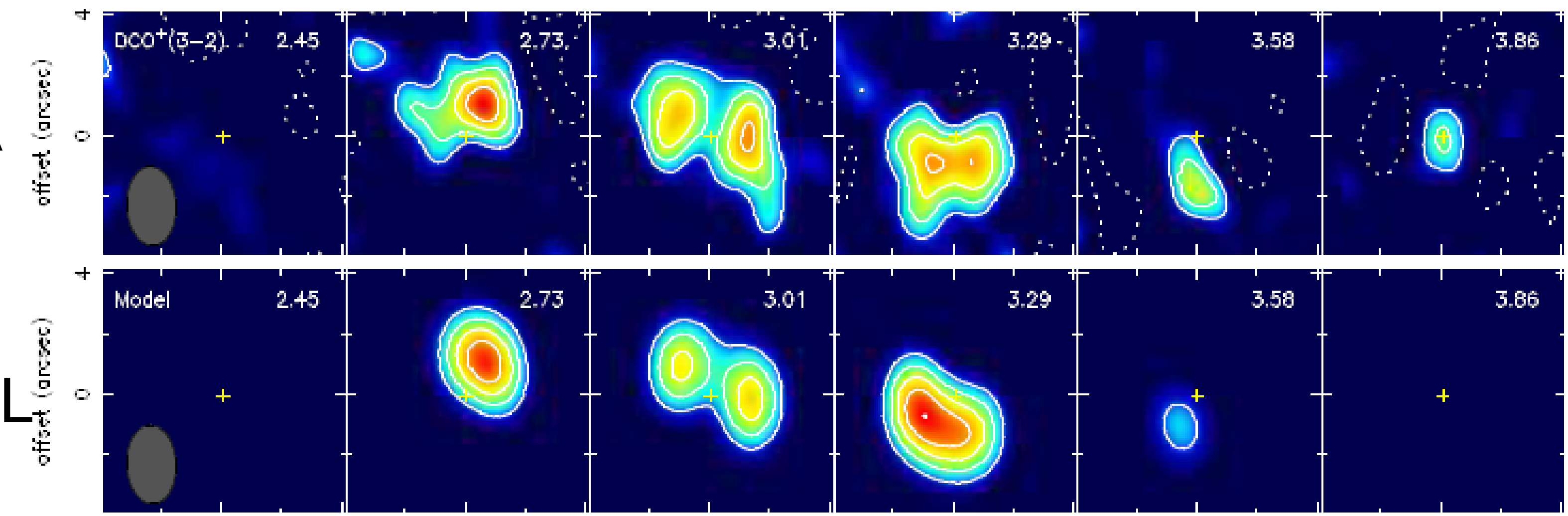


$HCO^+/H^{13}CO^+ = 50\pm10$

TW Hya DCO^+ 3-2

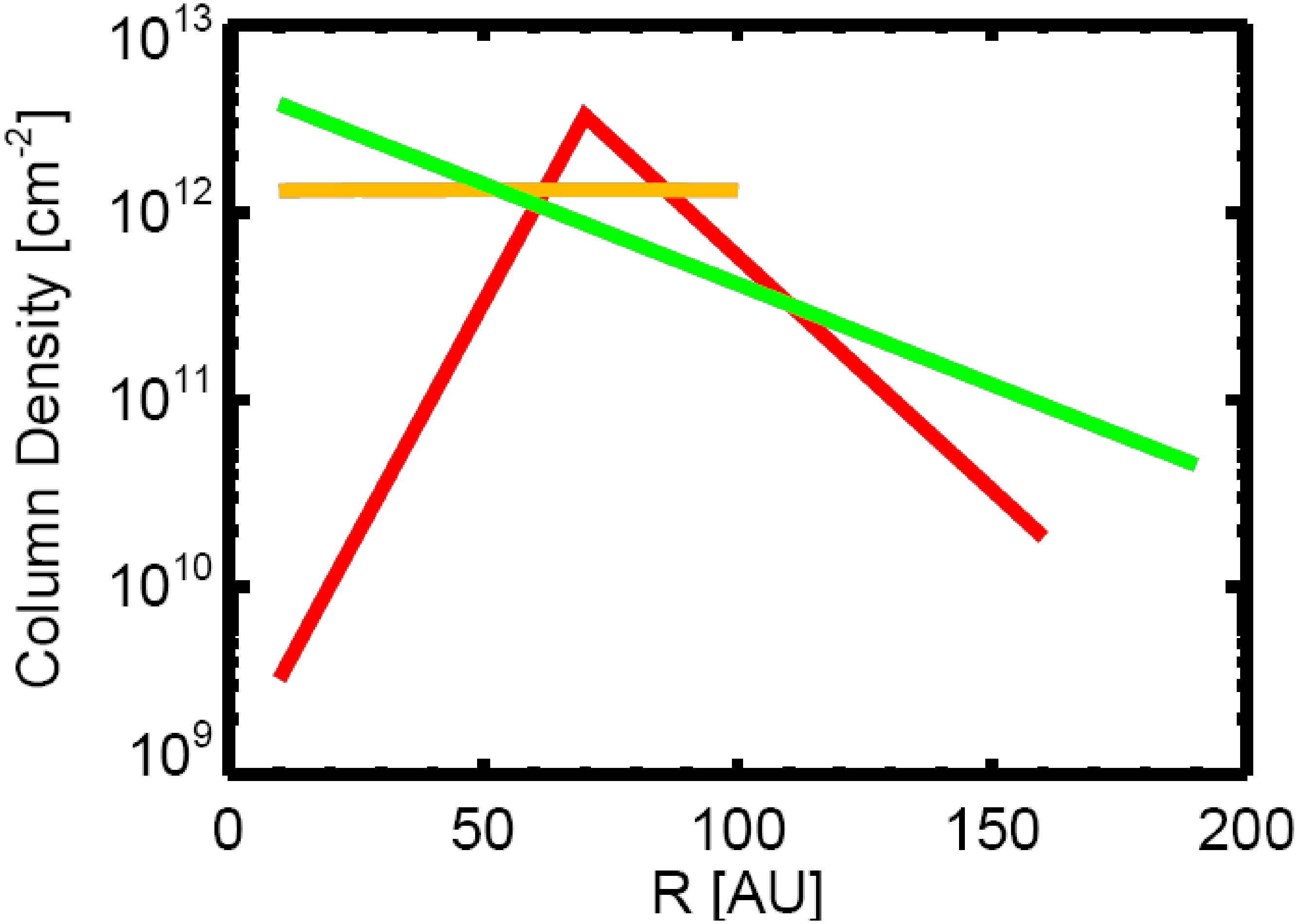
DATA

MODEL

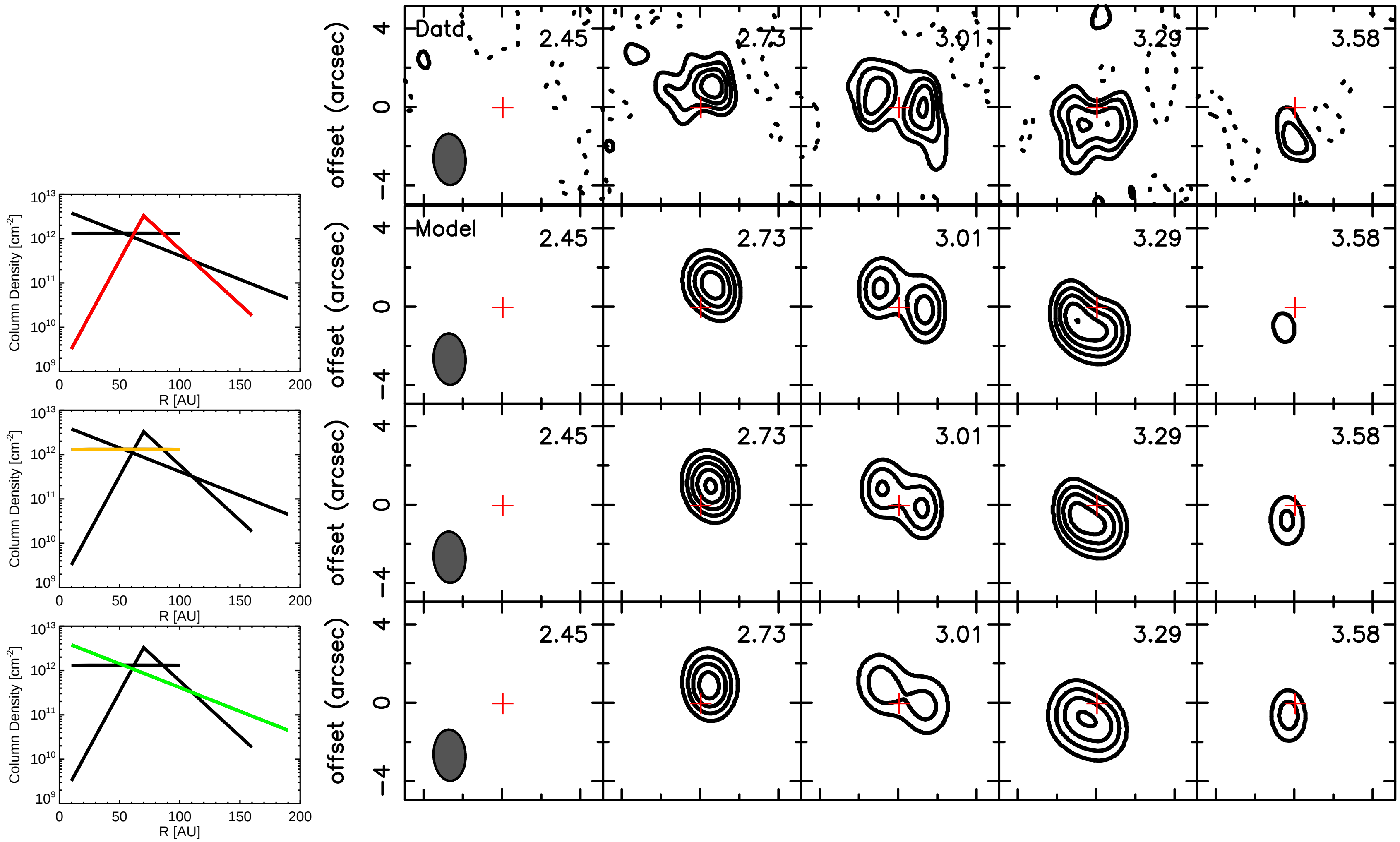


- The abundance of DCO^+ is found to increase with increasing radius till 70 AU.
- The distribution of DCO^+ clearly doesn’t follow that of HCO^+.

Models with different vertical column density distributions (DCO^+)



Data vs Models with different vertical column density distributions (DCO^+)

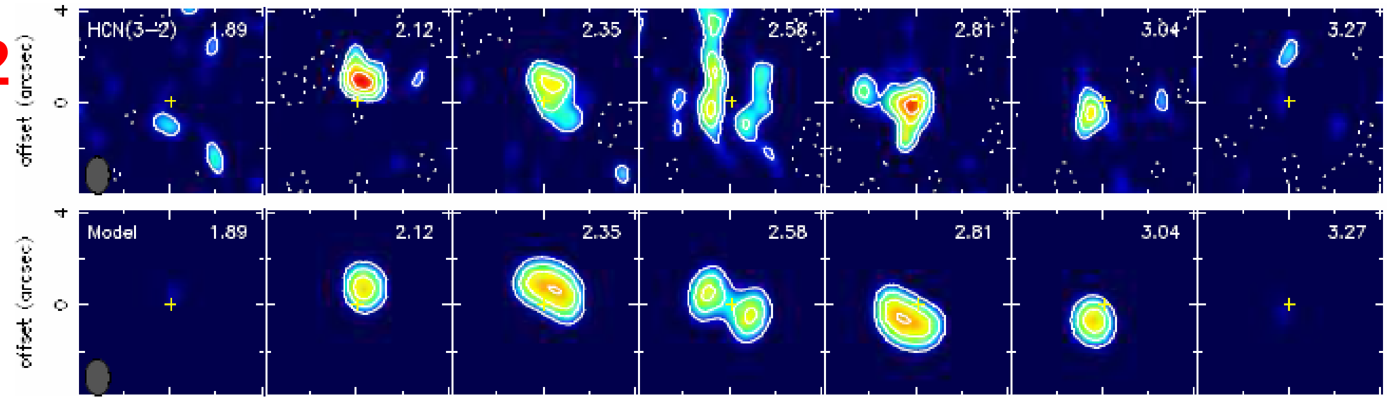


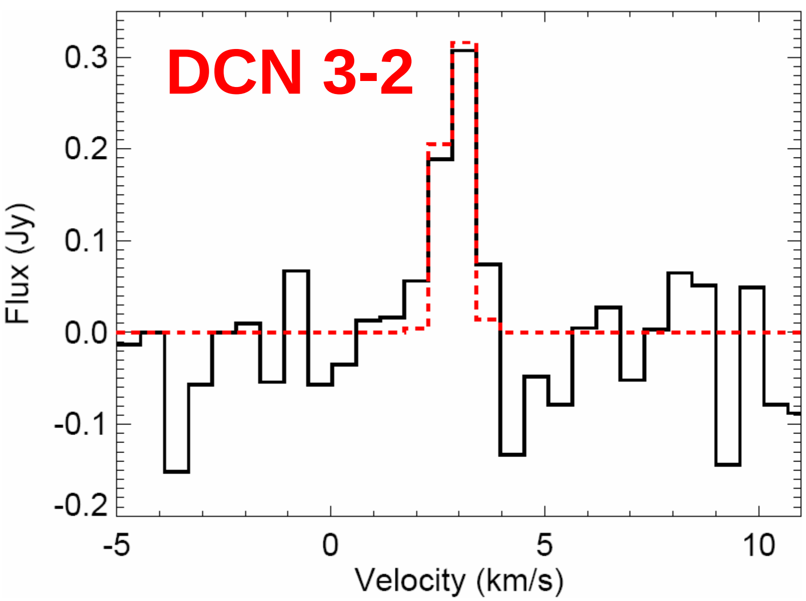
TW Hya HCN/DCN 3-2

HCN 3-2

DATA

MODEL



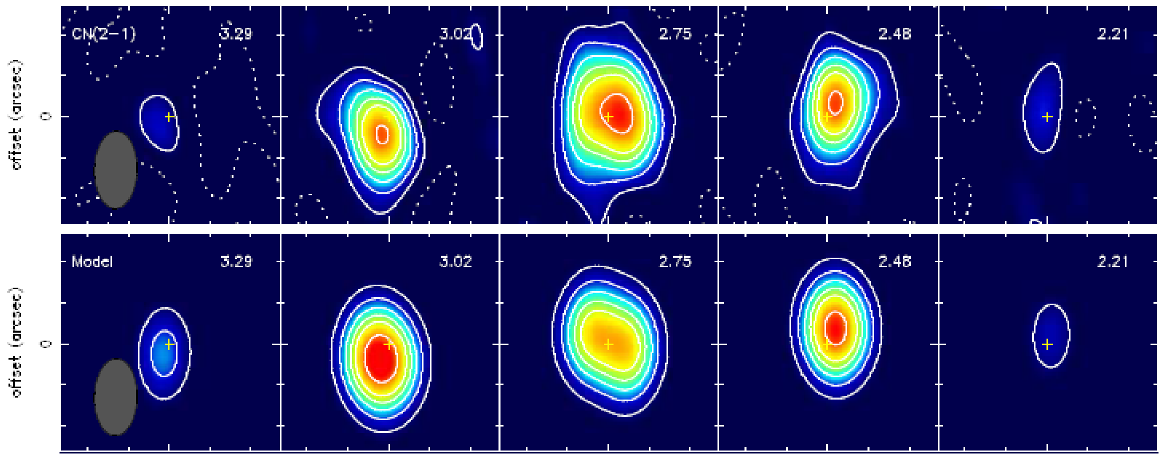


- First detection of DCN in disks.
- DCN/HCN=2×10^{-3}
  — Consistent with the observation of comets.

TW Hya CN 2-1

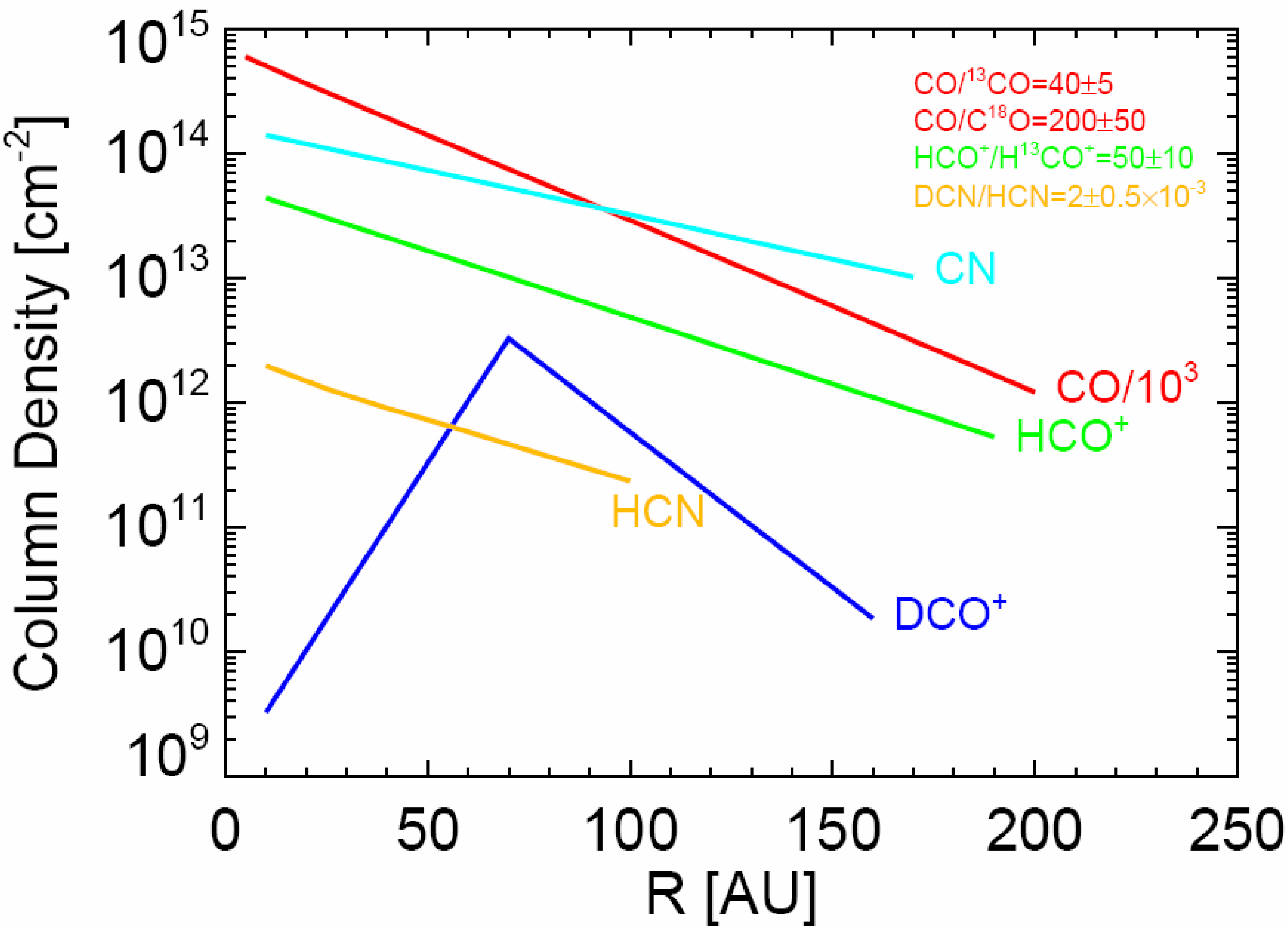
DATA

MODEL



- 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 α emission, while CN cannot.

Radial Distribution of Molecular Column Densities in the Disk of TW Hya (Best Fit Model)



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 $^{13}CO/C^{18}O$ 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 Lyα emission, while CN cannot.

Concluding Remarks II

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

END