

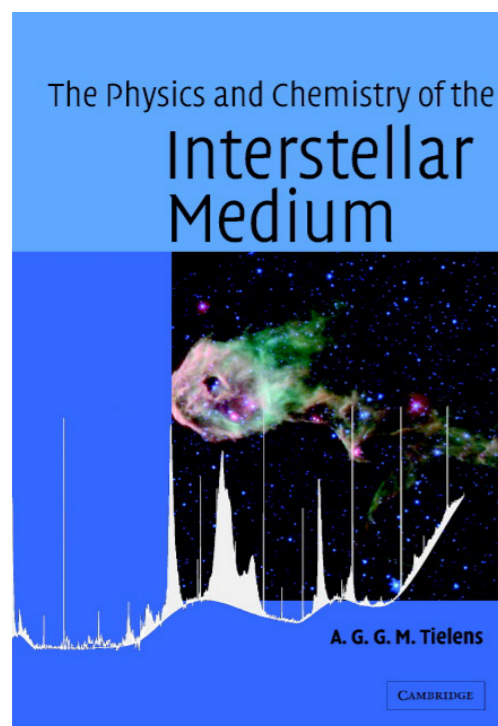
# Gas in protoplanetary disks

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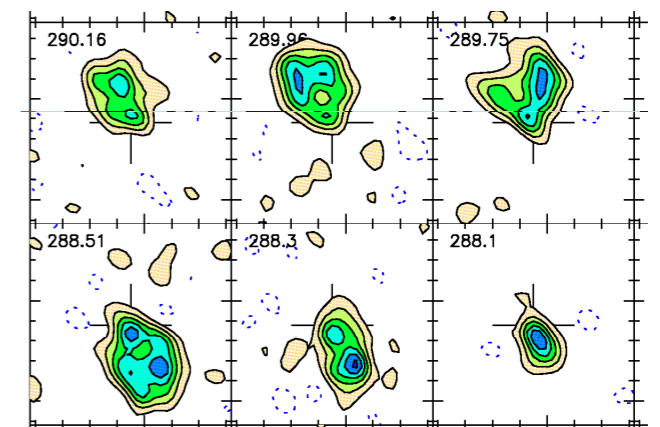
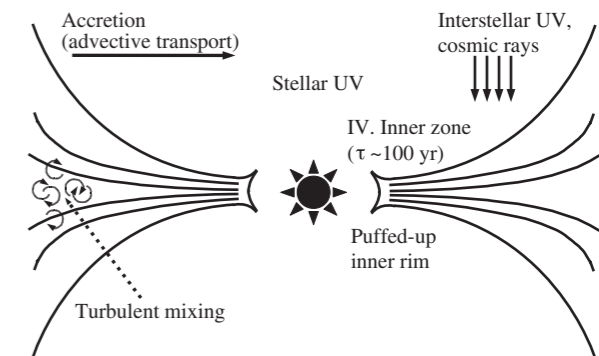
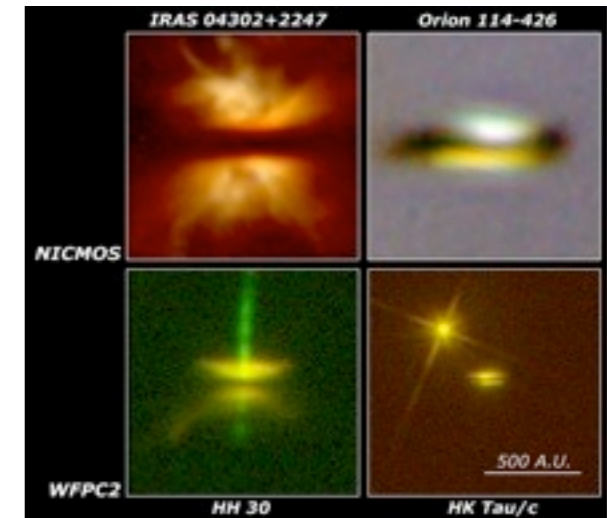
# Suggested literature

- 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.
- D. Semenov, "Chemistry in protoplanetary disks", Encyclopedia of Astrobiology, Springer Ver. ISBN: 978-3-642-11279-9



# Outline

- Formation of molecular lines
- Molecules as disk probes
- Disk chemical structure
- Observations of molecules in disks
- Modeling disk chemical evolution with dynamics
- Predictions for ALMA



# Advantages of millimeter observations

- Optically thin dust emission (outer disk)
- Rotational transitions of many molecules
- High frequency resolution:  $\sim 10^6$  ( $\sim 0.05$  km/s)
- Sensitive to cold regions:  $T \sim 10$  K
- Interferometers: sub-arcsec resolution
- Many spectral lines within a bandwidth
- Day-time observations

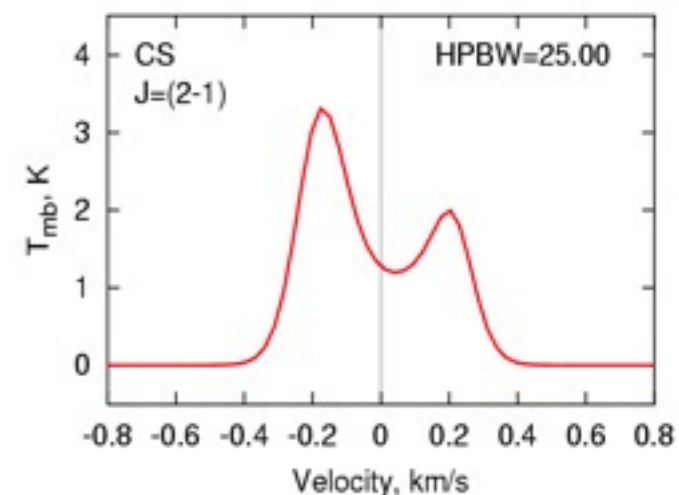
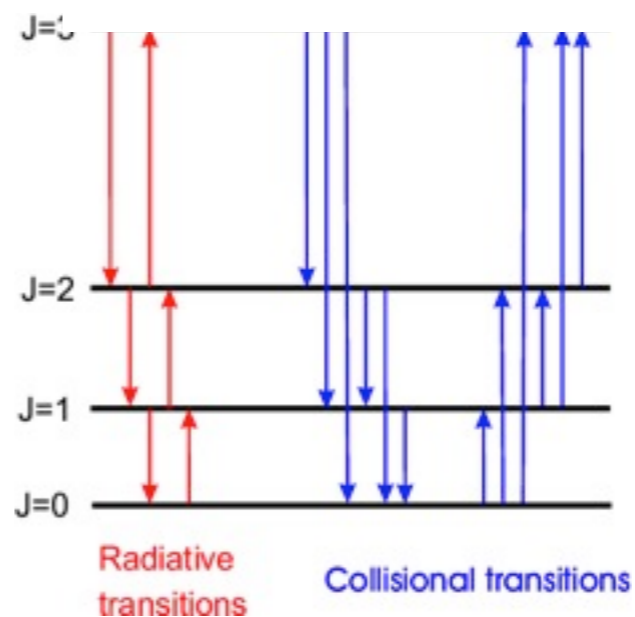
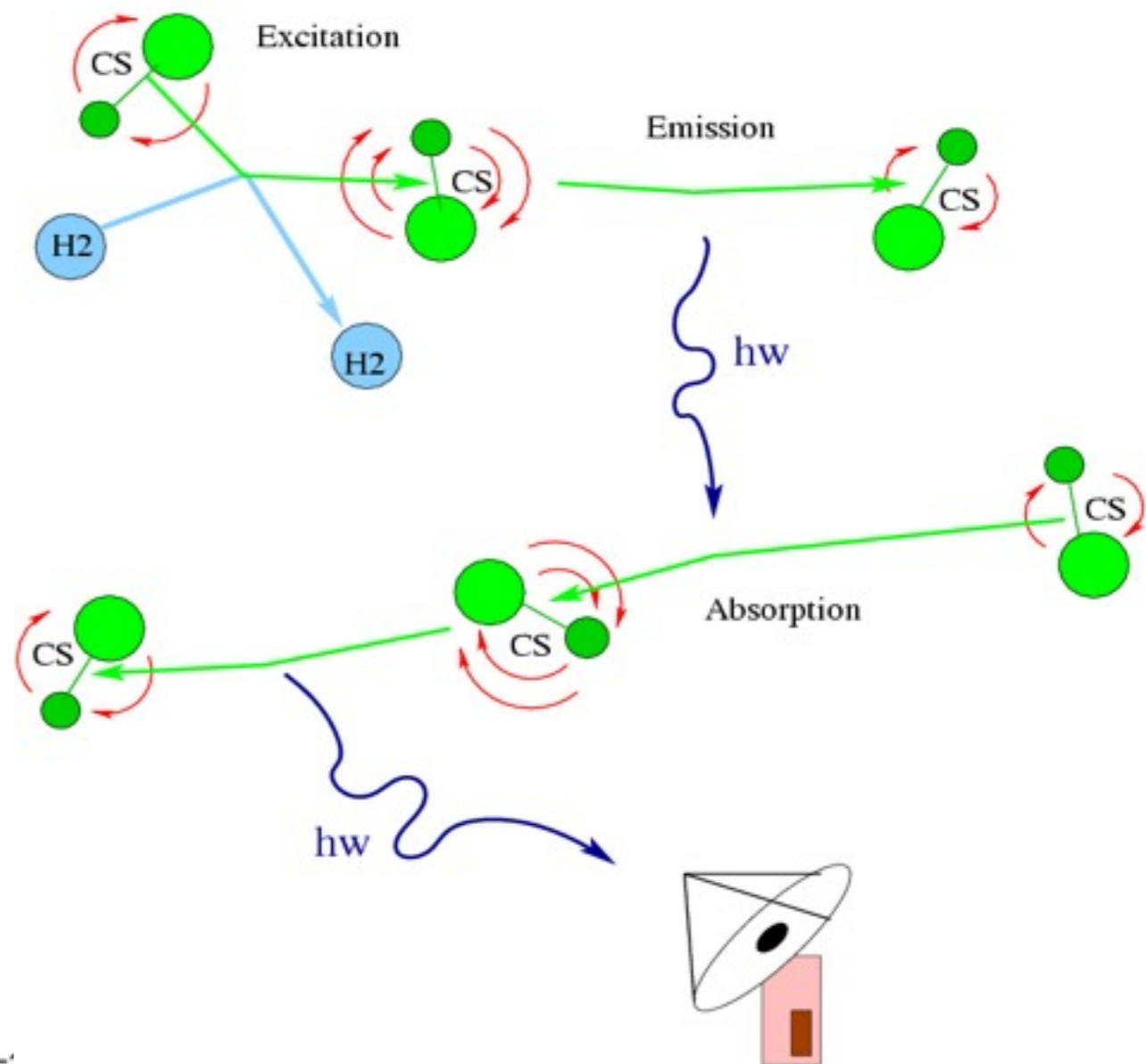


- Plateau de Bure interferometer, Submillimeter Array, Very Large Array, CARMA, ATCA
- IRAM 30-m, Apex 12-m, Effelsberg 100-m, Aresibo 100-m, JCMT 15m, Nobeyama 45-m

# **I. Basics of line excitation and line analysis**

# Analysis of emission line data

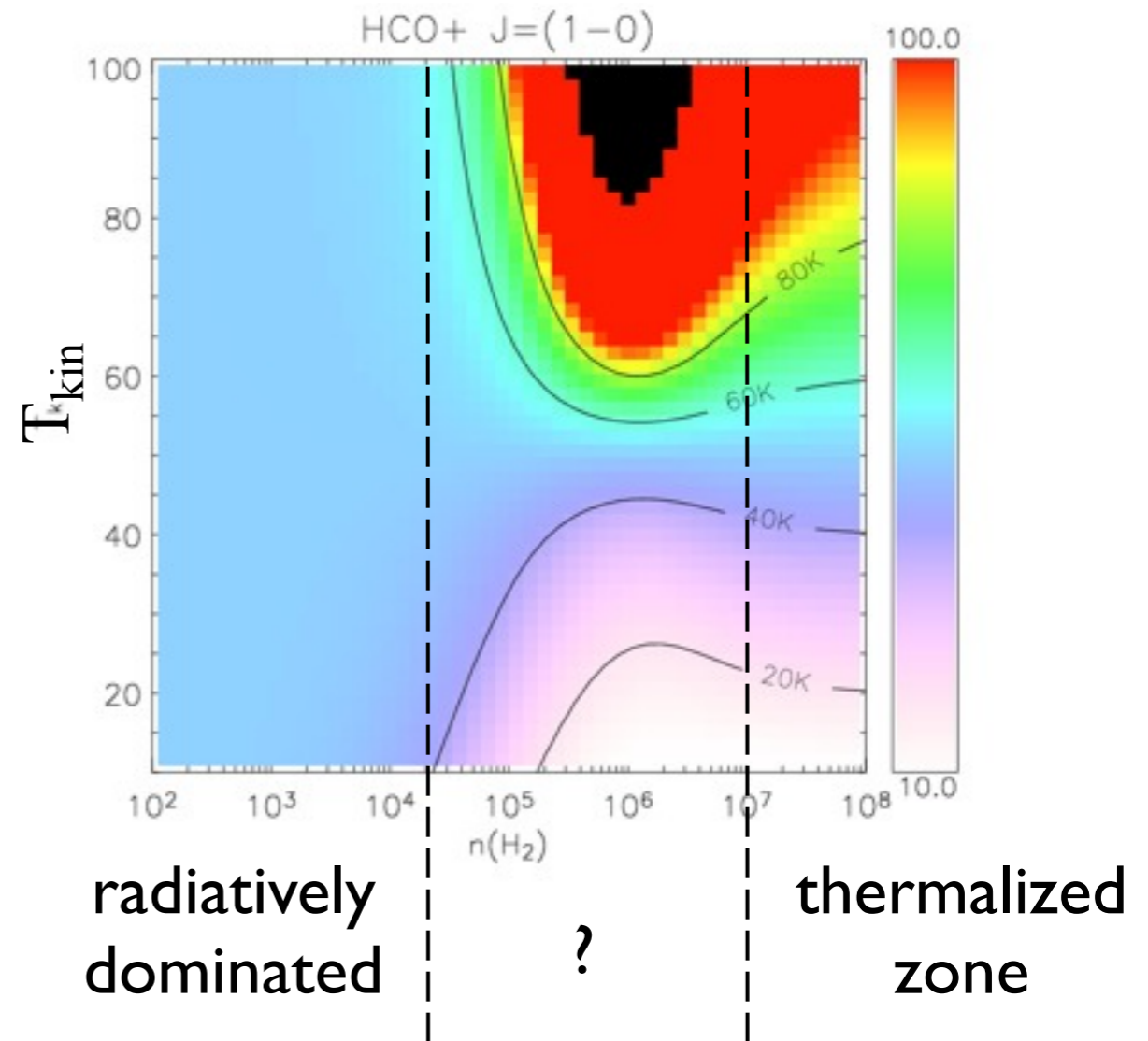
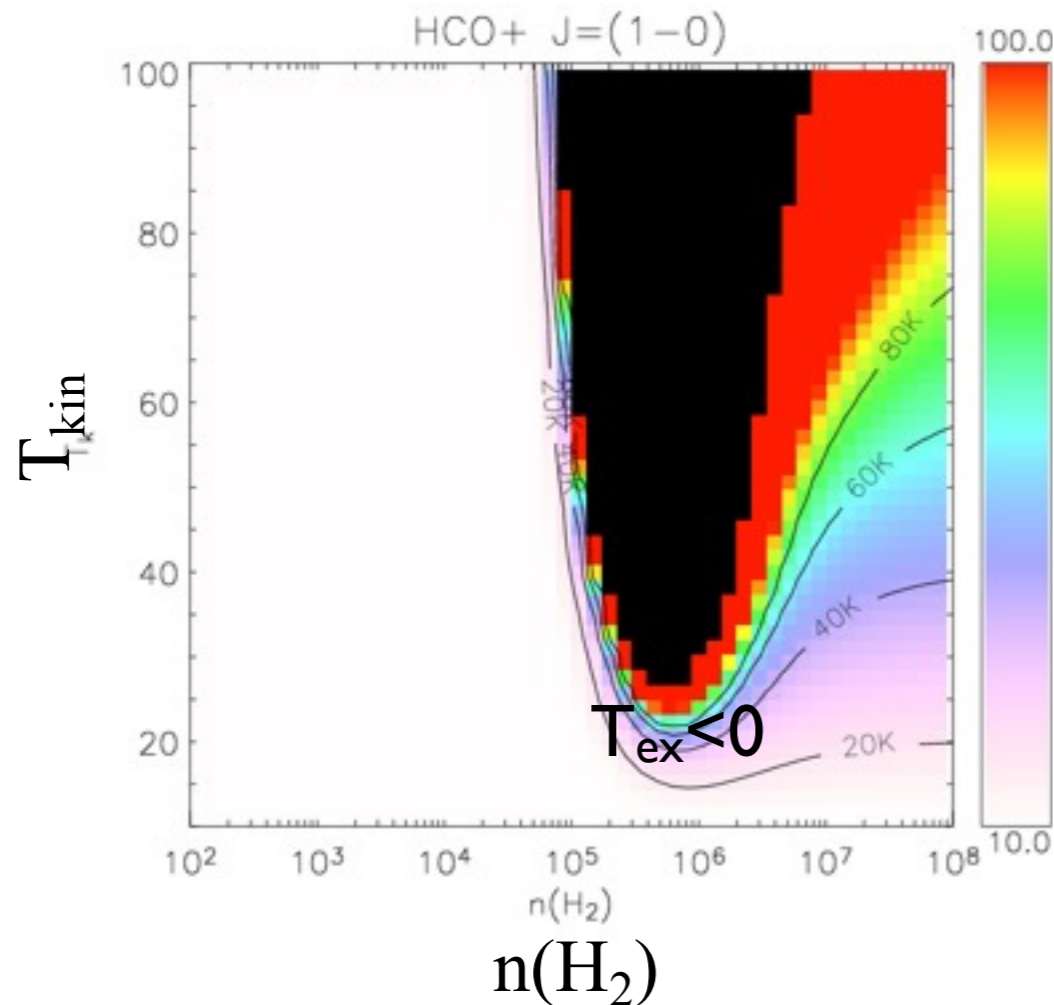
- $n, T$  + chemistry + excitation + kinematics + radiative transfer: line
- Excitation: radiation & collisions
- Excitation & RT: non-local problem
- 6D: 3D  $n, T$  + 1D  $v$  + 2D sky plane
- Incomplete coverage of  $(u, v)$  plane
- Optically thick lines: Intensity  $\sim T_{\text{exc}}$  ( $^{12}\text{CO}$ ,  $\text{H}_2\text{O}$ )
- Optically thin lines: Intensity  $\sim \tau^* T_{\text{exc}}$



# Excitation temperatures: HCO<sup>+</sup>(1-0)

$$T_{bg} = 2.73 \text{ K}$$

$$T_{bg} = 50 \text{ K}$$



$$\frac{n_u}{n_l} = \frac{g_u}{g_l} \exp\left(-\frac{\Delta E}{kT_{ex}}\right),$$

$$T_{exc} = T_{bg}$$

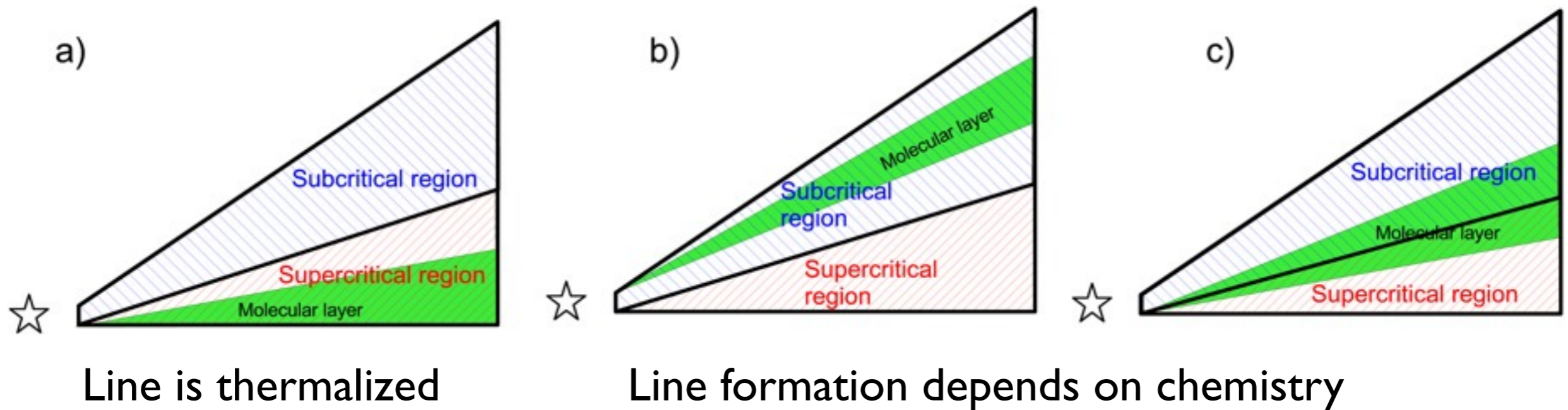
Non-LTE

$$T_{exc} = T_{kin}$$

LTE

# Excitation conditions in PPDs

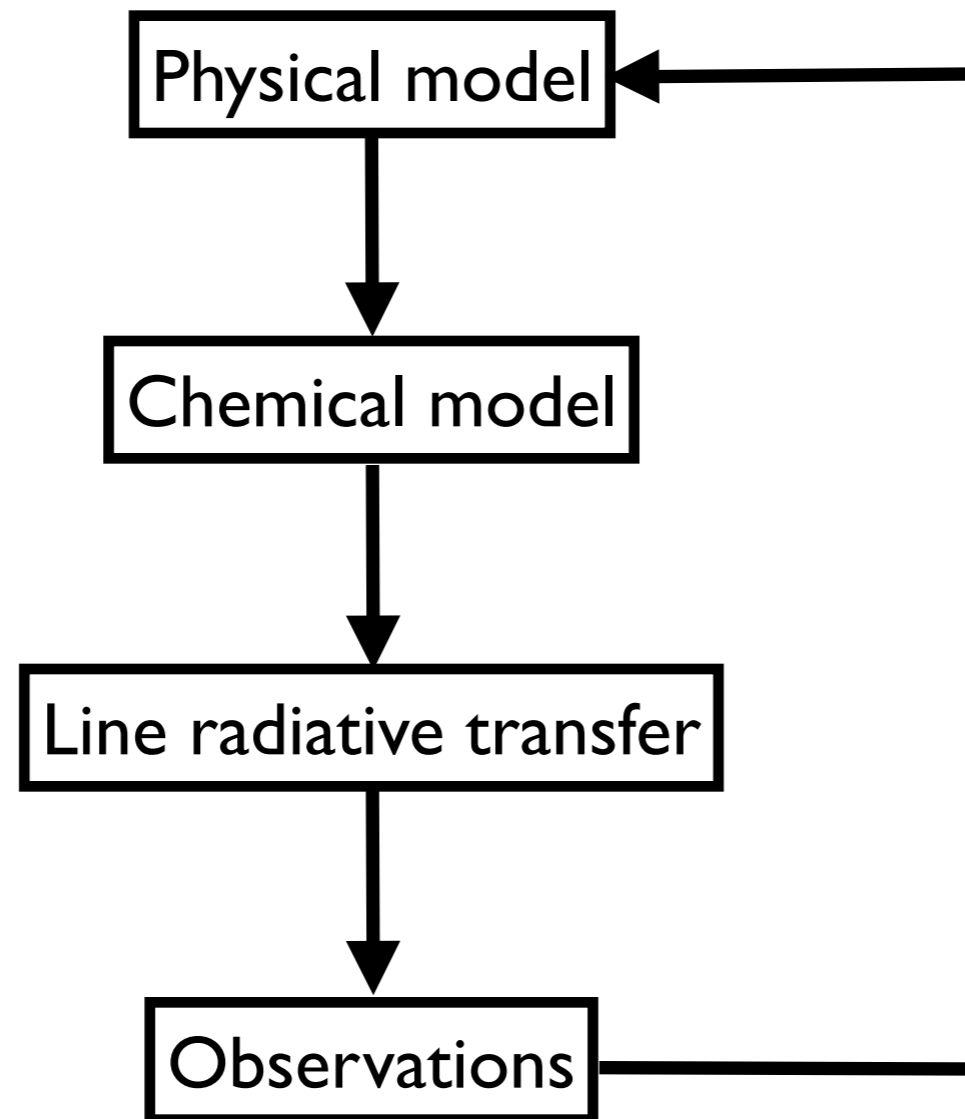
Rotational transition: thermally, sub-thermally, or super-thermally excited



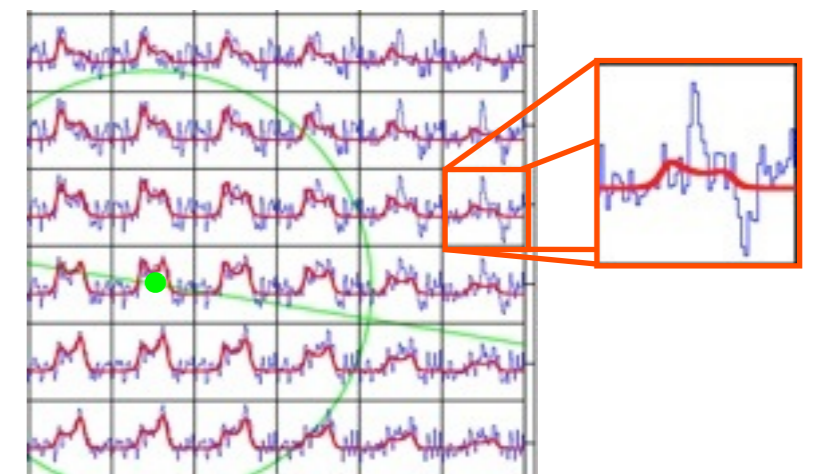
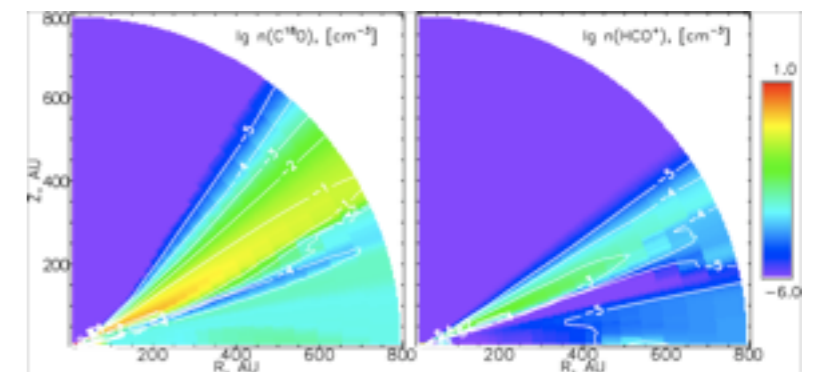
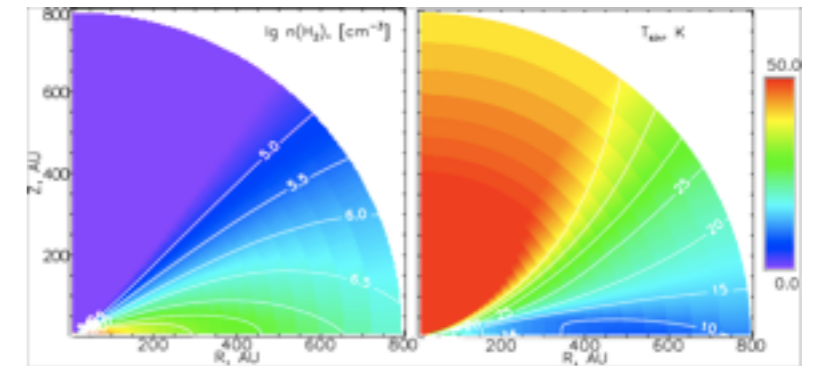
- Molecules in disks populate dense regions:  $n_{\text{H}} > 10^5 - 10^6 \text{ cm}^{-3}$
- Thermalized: low-lying transitions of observed molecules
- Asymmetric molecules have perplex level structure:  $\text{H}_2\text{O}$
- High-lying transitions: LTE or non-LTE?



# Analysis of emission line data



Iterative fitting



- LTE assumption
- $T_{\text{kin}}$  is often fixed
- Chemistry is often ignored: fixed abundances
- Optical thin approx./LVG/escape probability

# LRT tools & databases:

- 1/2/3D Line Radiative Transfer codes:
  - RADEX/RATRAN (F. van der Tak, M. Hogerheijde)
  - URANIA (Ya. Pavlyuchenkov)
  - RADLITE (K. Pontoppidan)
  - RADMC-3D (C. Dullemond)
  - LIME (C. Brich & M. Hogerheijde)
  - Photon-Dominated Region (PDR) code (F. Le Petit)
- Collisional rates: Leiden Atomic & Molecular Database:  
<http://www.strw.leidenuniv.nl/~moldata/>
- Line frequencies:
  - Cologne Database for Molecular Spectroscopy: <http://www.astro.uni-koeln.de/cdms/>
  - NIST, JPL, ...

# I. LRT basics: Summary

- Formation of emission in molecular lines is a tricky problem
- LTE/non-LTE
- Observed molecules:  $T_{\text{exc}} \sim T_{\text{kin}}$
- High-lying lines may reach  $\tau > 1$
- Complex molecules:  $T_{\text{exc}} = ?$
- LRT codes & databases (limited)
- Full modeling cycle to fit interferometric data

# **II. Molecules as probes**

# Molecules in space (~170)

Number of Atoms										
2	3	4	5	6	7	8	9	10	11	13
H <sub>2</sub>	C <sub>3</sub>	c-C <sub>3</sub> H	C <sub>5</sub>	C <sub>5</sub> H	C <sub>6</sub> H	CH <sub>3</sub> C <sub>3</sub> N	CH <sub>3</sub> C <sub>4</sub> H	CH <sub>3</sub> C <sub>5</sub> N?	HC <sub>9</sub> N	HC <sub>11</sub> N
AlF	C <sub>2</sub> H	l-C <sub>3</sub> H	C <sub>4</sub> H	l-H <sub>2</sub> C <sub>4</sub>	CH <sub>2</sub> CHCN	HCOOCH <sub>3</sub>	CH <sub>3</sub> CH <sub>2</sub> CN	(CH <sub>3</sub> ) <sub>2</sub> CO		
AlCl	C <sub>2</sub> O	C <sub>3</sub> N	C <sub>4</sub> Si	C <sub>2</sub> H <sub>4</sub>	CH <sub>3</sub> C <sub>2</sub> H	CH <sub>3</sub> COOH?	(CH <sub>3</sub> ) <sub>2</sub> O	NH <sub>2</sub> CH <sub>2</sub> COOH?		
C <sub>2</sub>	C <sub>2</sub> S	C <sub>3</sub> O	l-C <sub>3</sub> H <sub>2</sub>	CH <sub>3</sub> CN	HC <sub>5</sub> N	C <sub>7</sub> H	CH <sub>3</sub> CH <sub>2</sub> OH			
CH	CH <sub>2</sub>	C <sub>3</sub> S	c-C <sub>3</sub> H <sub>2</sub>	CH <sub>3</sub> NC	HCOCH <sub>3</sub>	H <sub>2</sub> C <sub>6</sub>	HC <sub>7</sub> N			
CH <sup>+</sup>	HCN	C <sub>2</sub> H <sub>2</sub>	CH <sub>2</sub> CN	CH <sub>3</sub> OH	NH <sub>2</sub> CH <sub>3</sub>		C <sub>8</sub> H			
CN	HCO	CH <sub>2</sub> D <sup>+</sup> ?	CH <sub>4</sub>	CH <sub>3</sub> SH	c-C <sub>2</sub> H <sub>4</sub> O					
CO	HCO <sup>+</sup>	HCCN	HC <sub>3</sub> N	HC <sub>3</sub> NH <sup>+</sup>						
CO <sup>+</sup>	HCS <sup>+</sup>	HCNH <sup>+</sup>	HC <sub>2</sub> NC	HC <sub>2</sub> CHO						
CP	HOC <sup>+</sup>	HNCO	HCOOH	NH <sub>2</sub> CHO						
CSi	H <sub>2</sub> O	HNCS	H <sub>2</sub> CHN	C <sub>5</sub> N						
HCl	H <sub>2</sub> S	HOCO <sup>+</sup>	H <sub>2</sub> C <sub>2</sub> O							
KCl	HNC	H <sub>2</sub> CO	H <sub>2</sub> NCN							
NH	HNO	H <sub>2</sub> CN	HNC <sub>3</sub>							
NO	MgCN	H <sub>2</sub> CS	SiH <sub>4</sub>							
NS	MgNC	H <sub>3</sub> O <sup>+</sup>	H <sub>2</sub> COH <sup>+</sup>							
NaCl	N <sub>2</sub> H <sup>+</sup>	NH <sub>3</sub>								
OH	N <sub>2</sub> O	SiC <sub>3</sub>								
PN	NaCN									
SO	OCS									
SO <sup>+</sup>	SO <sub>2</sub>									
SiN	c-SiC <sub>2</sub>									
SiO	CO <sub>2</sub>									
SiS	NH <sub>2</sub>									
CS	H <sub>3</sub> <sup>+</sup>									
HF										

[http://www.astrochymist.org/astrochymist\\_mole.html](http://www.astrochymist.org/astrochymist_mole.html)

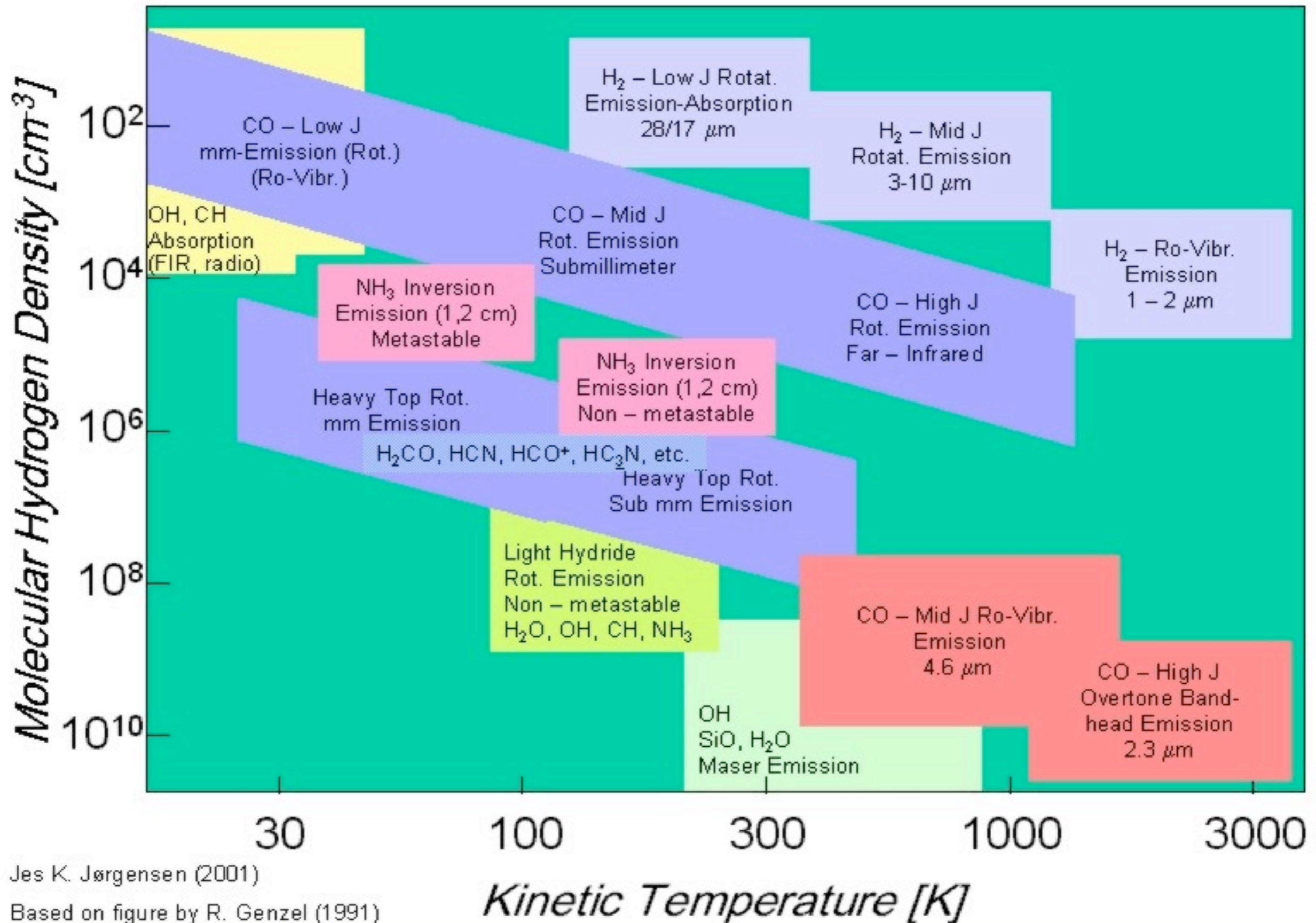
<http://www.astro.uni-koeln.de/cdms/molecules>

Note that observations suggest the presence of large PAHs and fullerenes in the interstellar gas (Tielens et al 1999, Foing & Ehrenfreund 1997).

Detected in disks: CO, HCO<sup>+</sup>, DCO<sup>+</sup>, CN, HCN, DCN, HNC, N<sub>2</sub>H<sup>+</sup>,

H<sub>2</sub>CO, CS, HDO, C<sub>2</sub>H<sub>2</sub>, CO<sub>2</sub>, OH, H<sub>2</sub>O, Ne, Fe, Si, H<sub>2</sub>

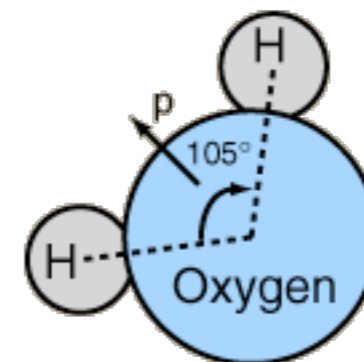
# Molecules as probes of T and n<sub>H</sub>



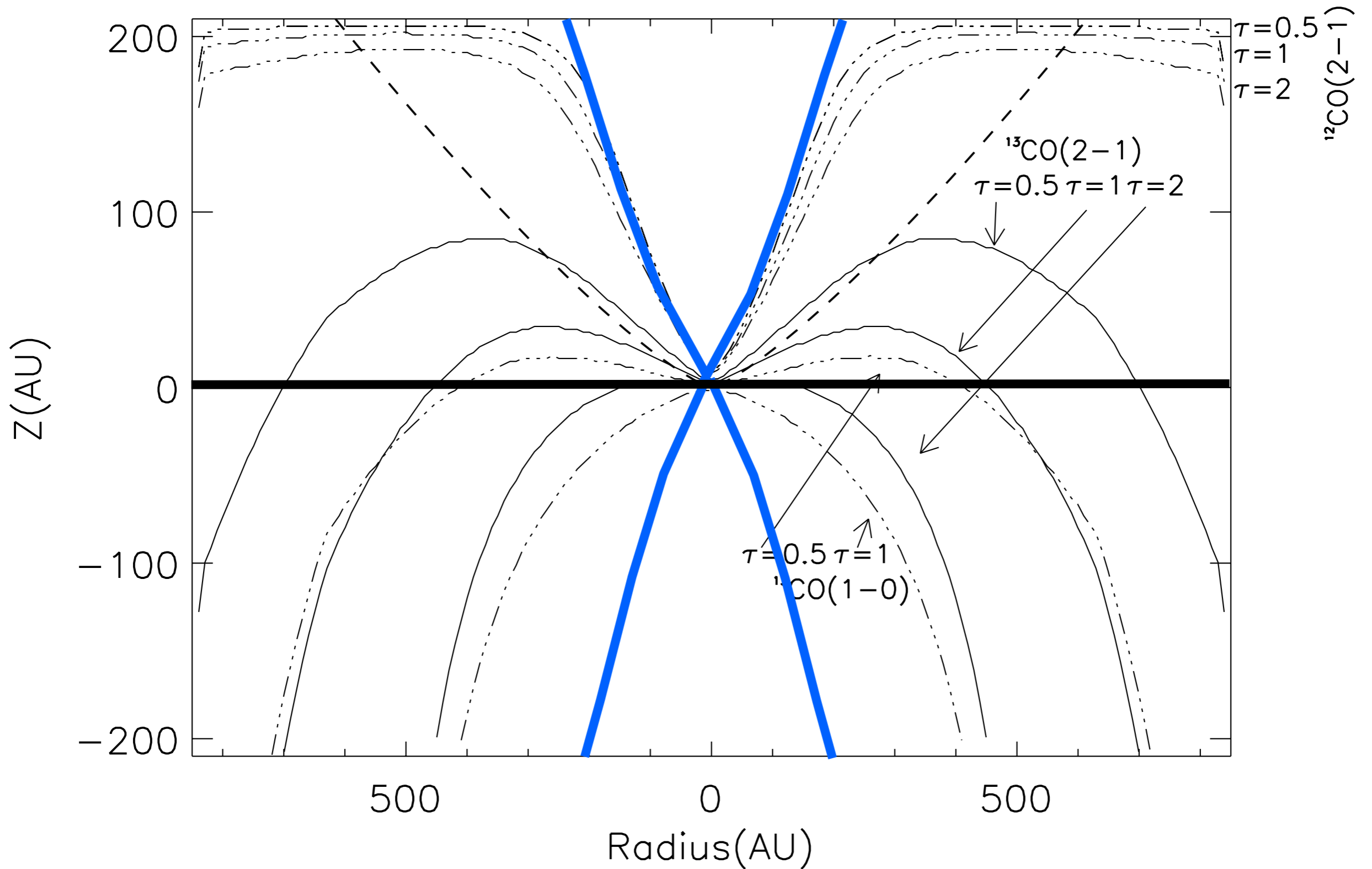
# Other molecular tracers

Tracer	Quantity
$^{12}\text{CO}$ , $^{13}\text{CO}$	Temperature
$\text{H}_2$	—
$\text{NH}_3$	—
$\text{CS}$ , $\text{H}_2\text{CO}$	Density
$\text{CCH}$ , $\text{HCN}$ , $\text{CN}$	Photochemistry
$\text{HCO}^+$	Ionization
$\text{N}_2\text{H}^+$ , $\text{H}_2\text{D}^+$	—
$\text{C}^+$	—
Metal ions	—
Complex organics	Surface processes
$\text{DCO}^+$ , $\text{DCN}$ , $\text{H}_2\text{D}^+$	Deuterium fractionation

- Large-dipole moment molecules: density
- Optically-thick lines: temperature
- Ions: ionization
- Radicals: FUV/X-ray radiation
- Complex molecules: surface chemistry/transport processes
- Isotopes: fractionation & thermal history



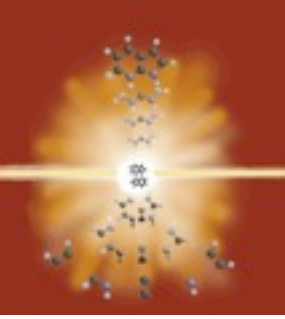
# CO isotopologues in disks: $T_{\text{kin}}(z)$



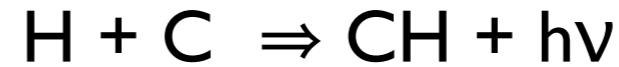




# Reactions in disks



Radiative association:



Surface reactions:



Neutral-neutral:



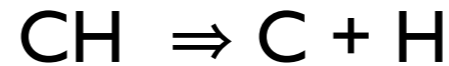
Ion-molecule:



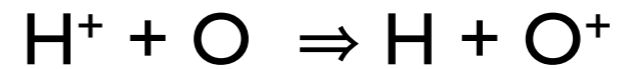
Ionization:



Photodissociation:



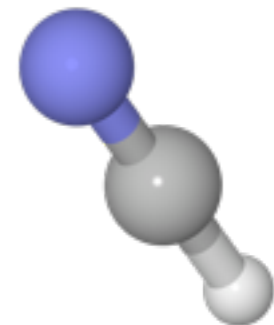
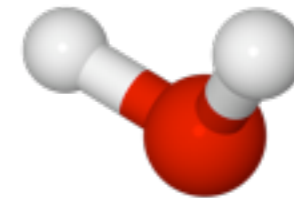
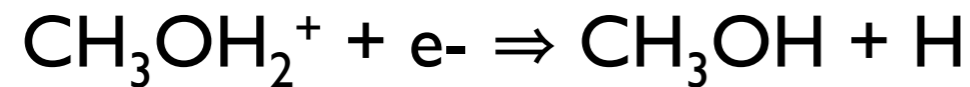
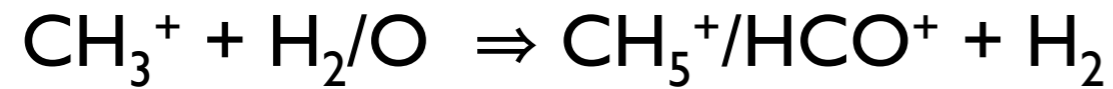
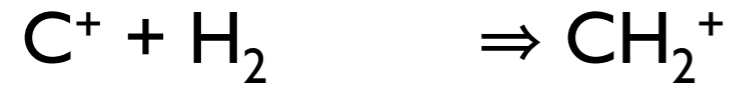
Charge exchange:



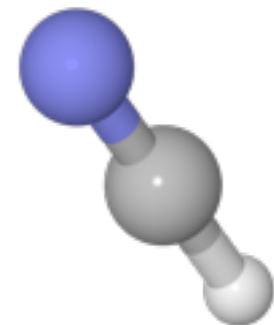
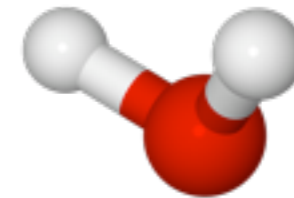
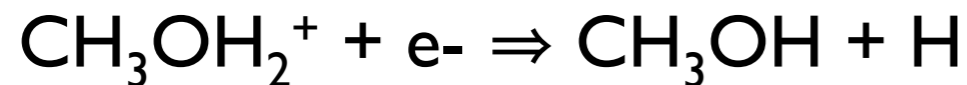
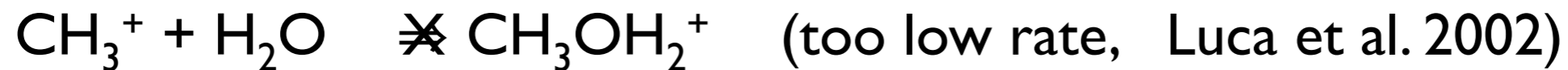
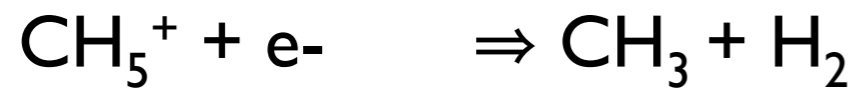
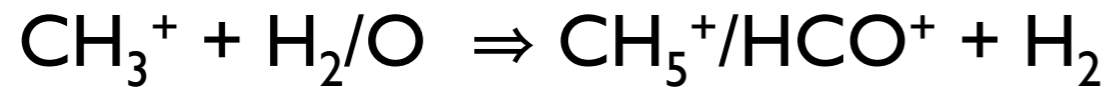
Dissociative recombination:  $\text{H}_3\text{O}^+ + \text{e}^- \Rightarrow \text{H}_2\text{O} + \text{H}$

- ~600 species & ~6000 reactions (no isotopes)
- Only ~10-20% of accurate rates
- Uncertainty in abundances: ~0.5 dex

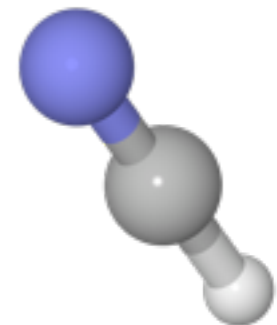
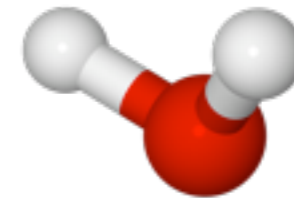
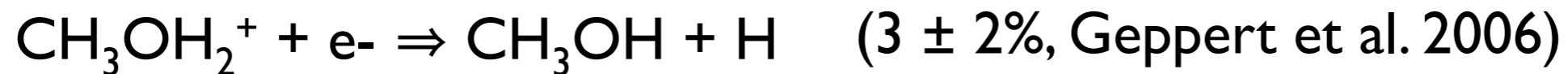
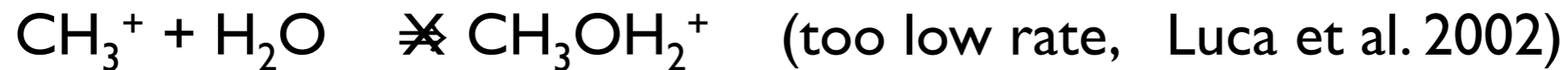
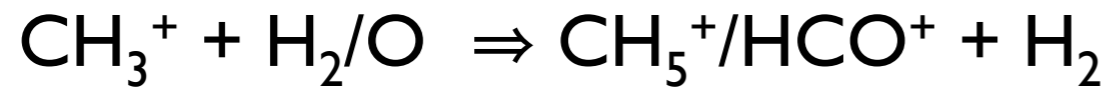
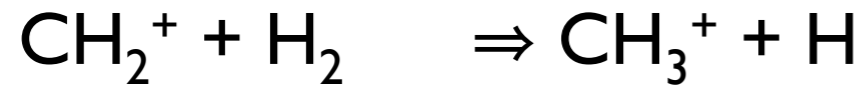
# Gas-phase formation of complex molecules



# Gas-phase formation of complex molecules



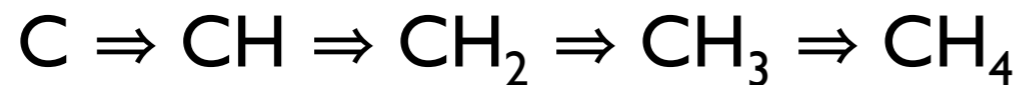
# Gas-phase formation of complex molecules



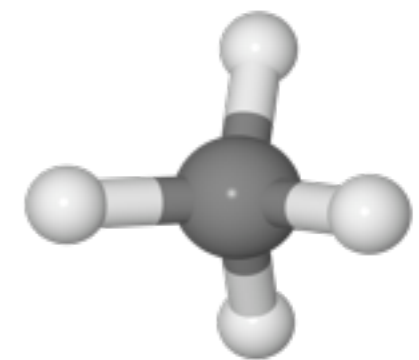
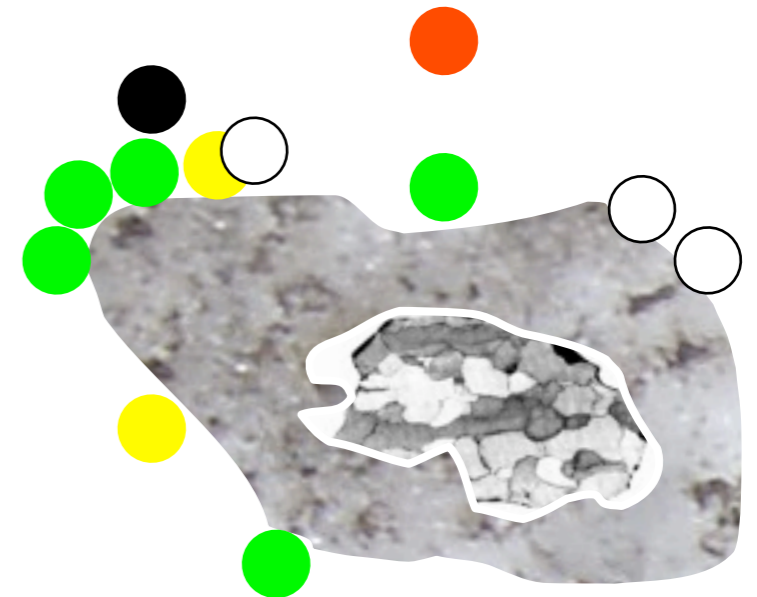
# Surface formation of complex molecules

- Accretion
- Surface synthesis
- Photoprocessing of ices
- Desorption: T, UV, CRPs

Surface chemistry:



C + C, CO + OH, etc. in warm regions

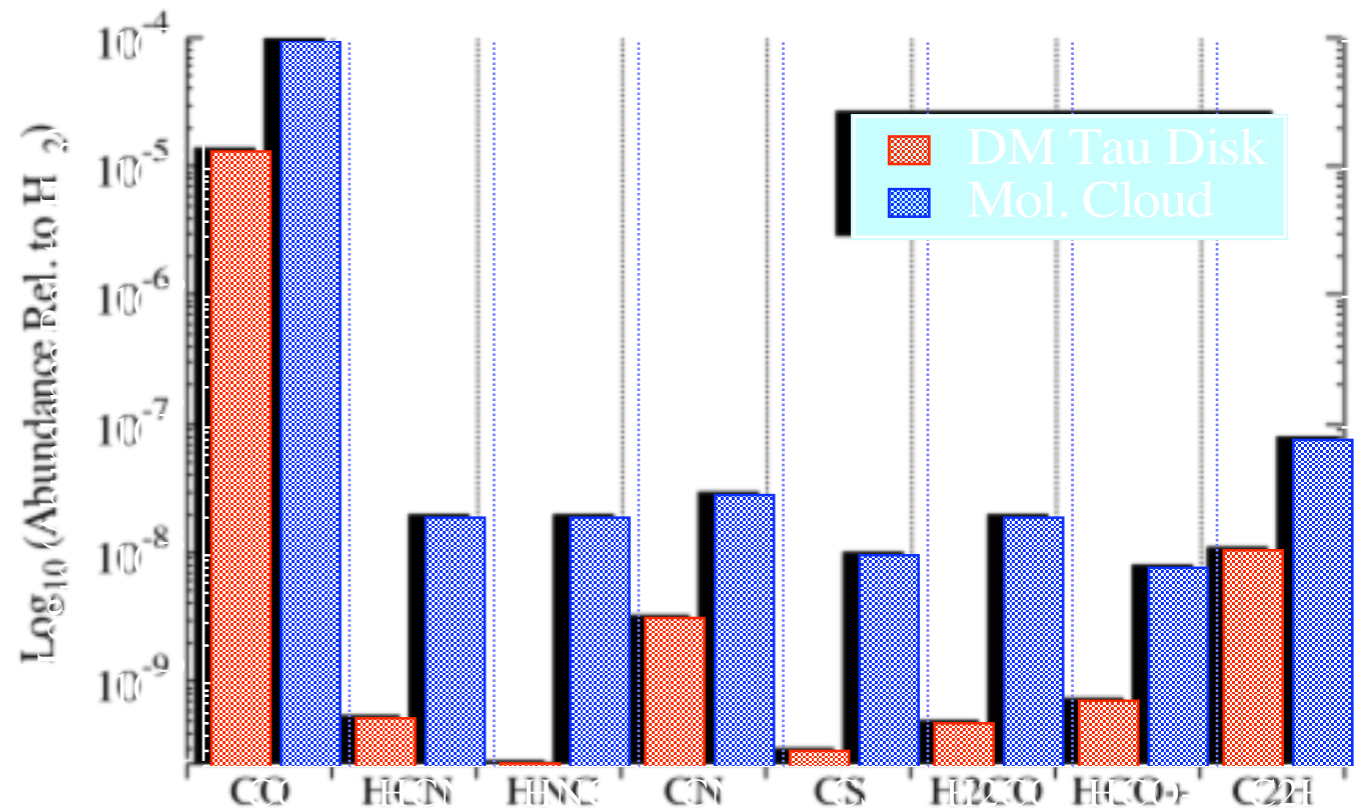


# III. Observations of molecules in PPDs

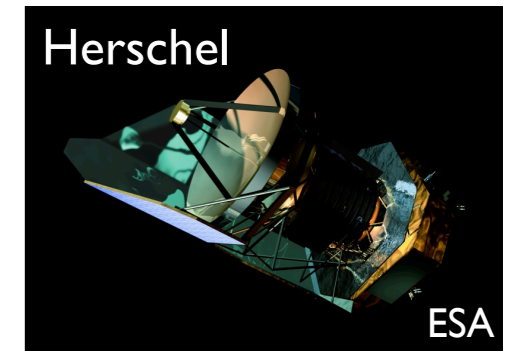
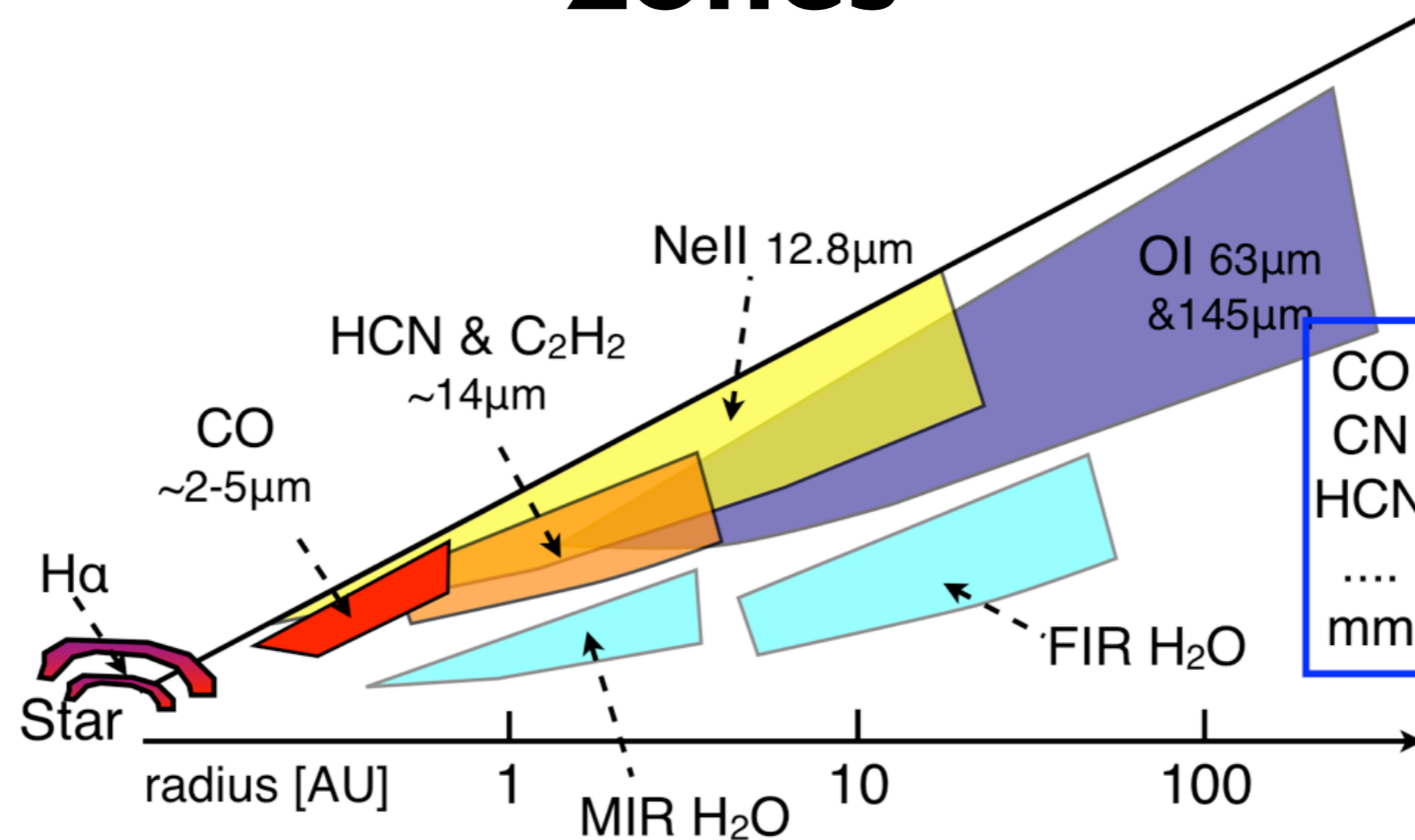
- IR (space) spectroscopy:
  - inner regions: <20 AU
  - rotational/vibrational lines
  - absorption/emission
  - Boltzmann diagrams, LTE,  $T_{\text{kin}}$
- (Sub-)millimeter observations:
  - outer regions: >50–100 AU
  - rotational/vibrational lines
  - emission lines
  - antennas: no spatial information, surveys
  - interferometers: resolved structures, restricted disk sample

# Observational findings: outer disks

- Gas: depletion of molecules
- Ices:  $\text{H}_2\text{O}$ ,  $\text{NH}_3$ ,  $\text{CH}_4$ ,  $\text{H}_2\text{CO}$ ,  $\text{CH}_3\text{OH}$
- Vertical gradients of T
- Photo-dominated chemistry
- Cold CO, CCH, HCN
- "Dry" interiors: where is water?
- Keplerian rotation
- Non-thermal line broadening



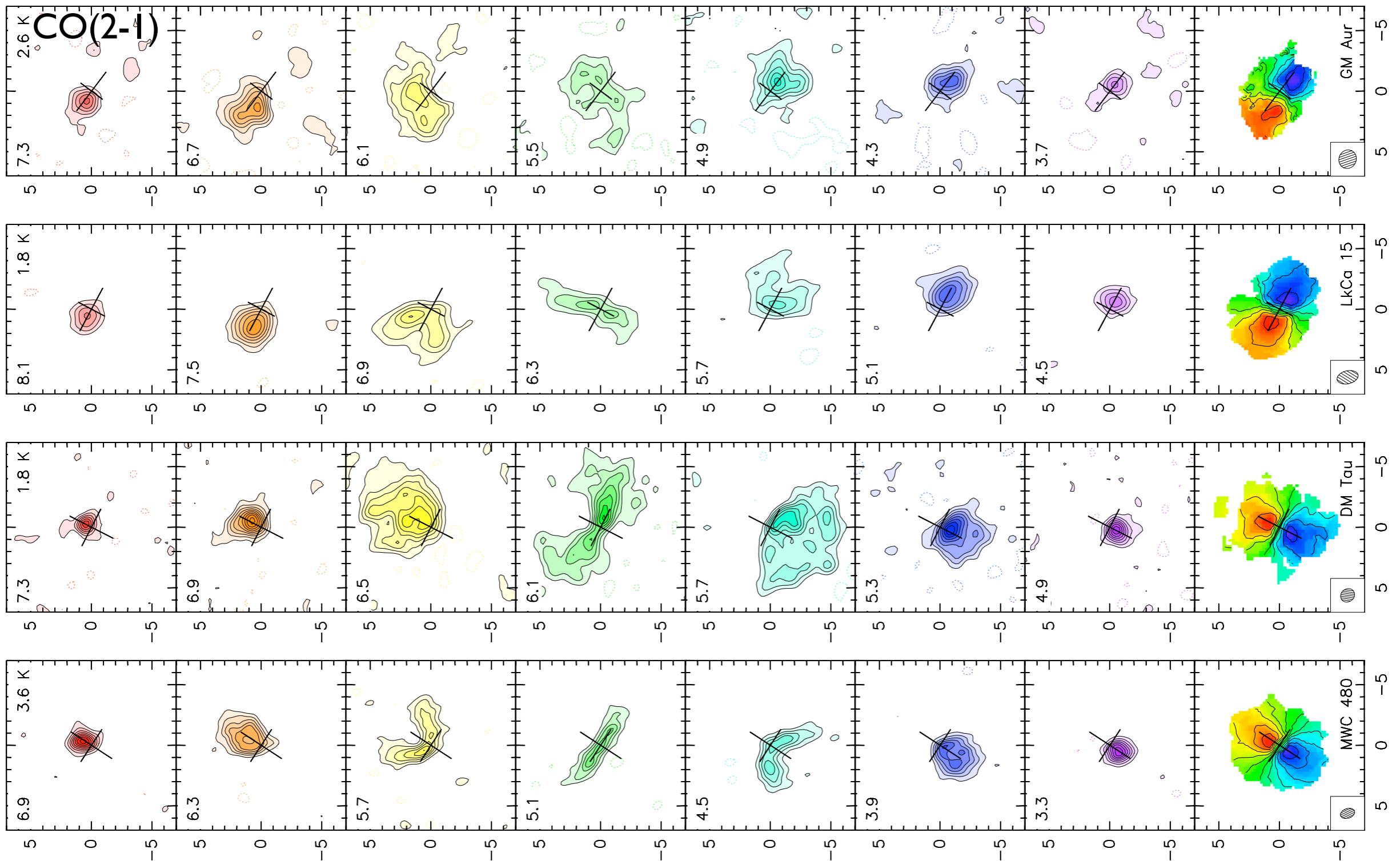
# IR revolution: molecules in planet-forming zones



- Nell, Fell, 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



# Kinematics: weighting stars



- $M_*$  from high SNR measurements of  $\Omega_K$ : evolutionary track models

# Chemistry in T Tau and Herbig Ae disks

- Large programs: "Chemistry in Disks" (CID), Europe
- CID strategy: observations + modeling
- "Disk Imaging Survey of Chemistry with SMA" (DISCS), USA
- DISCS strategy: observations

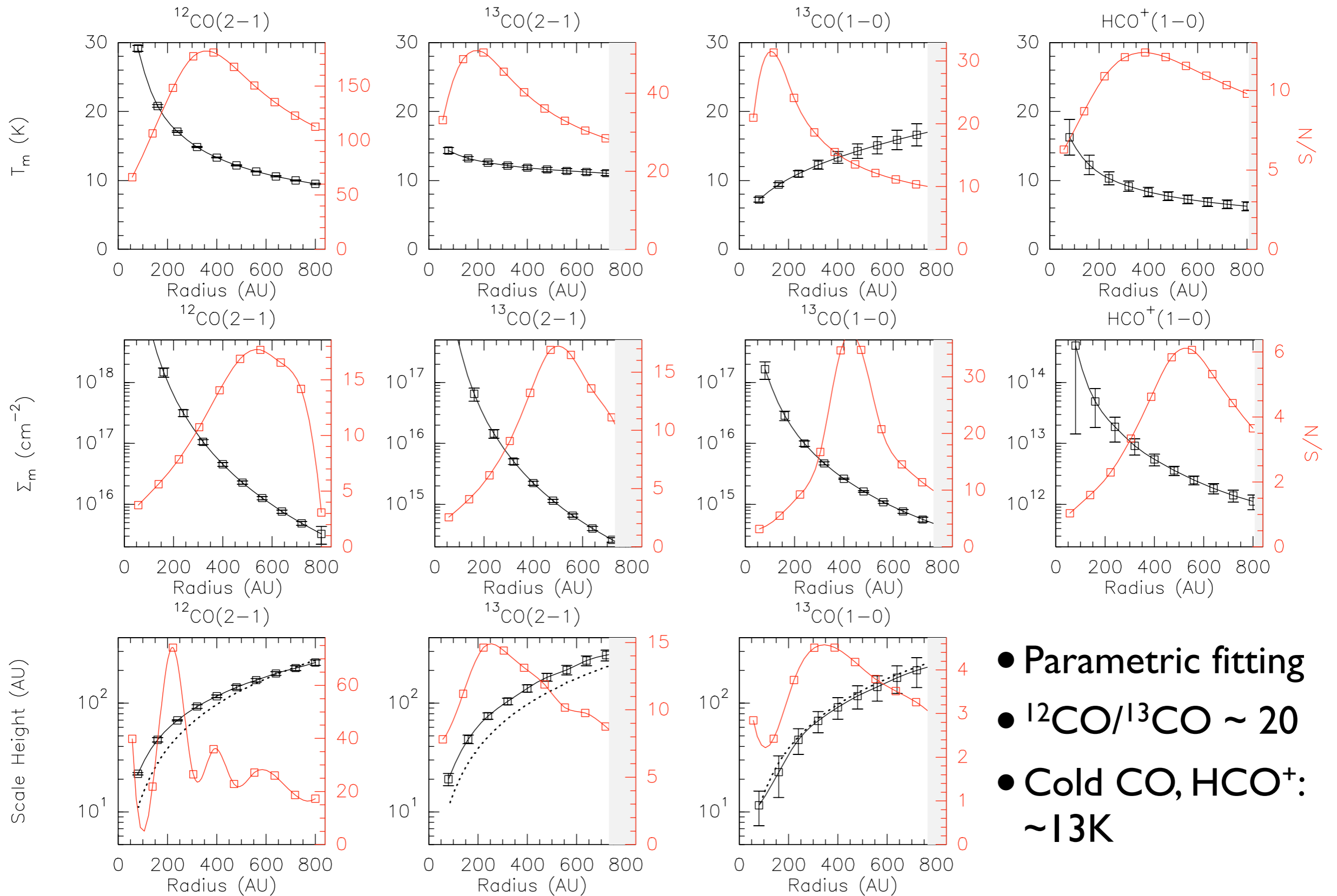


- Limited sample: large, face-on disks (~6)
- Lines are weak: ~0.3–3K (0.1–1Jy)
- 1 line: ~1–10 hours



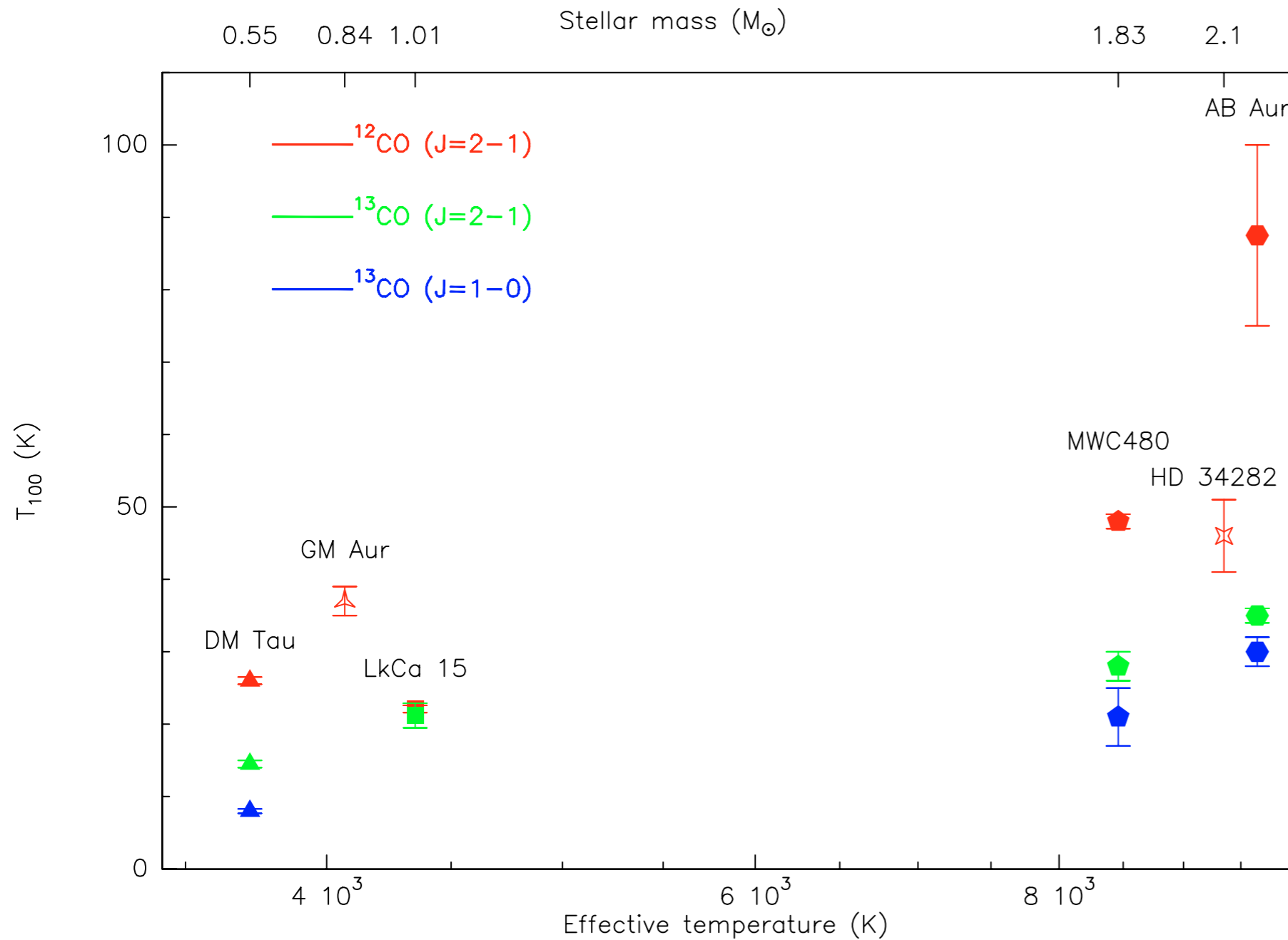
- Herbig Ae: CO, HCO<sup>+</sup>, CN, HCN
- T Tau: CO, HCO<sup>+</sup>, HCN, N<sub>2</sub>H<sup>+</sup>, CCH, CS, H<sub>2</sub>CO, DCO<sup>+</sup>, DCN

# Resolved surface density & T: DM Tau



- Parametric fitting
- $^{12}\text{CO}/^{13}\text{CO} \sim 20$
- Cold CO,  $\text{HCO}^+$ :  $\sim 13\text{K}$

# Temperature in T Tau and Herbig Ae disks



- "Warm" Herbig Ae disks:  
 $T_{\text{kin}} > 20\text{--}100\text{K}$

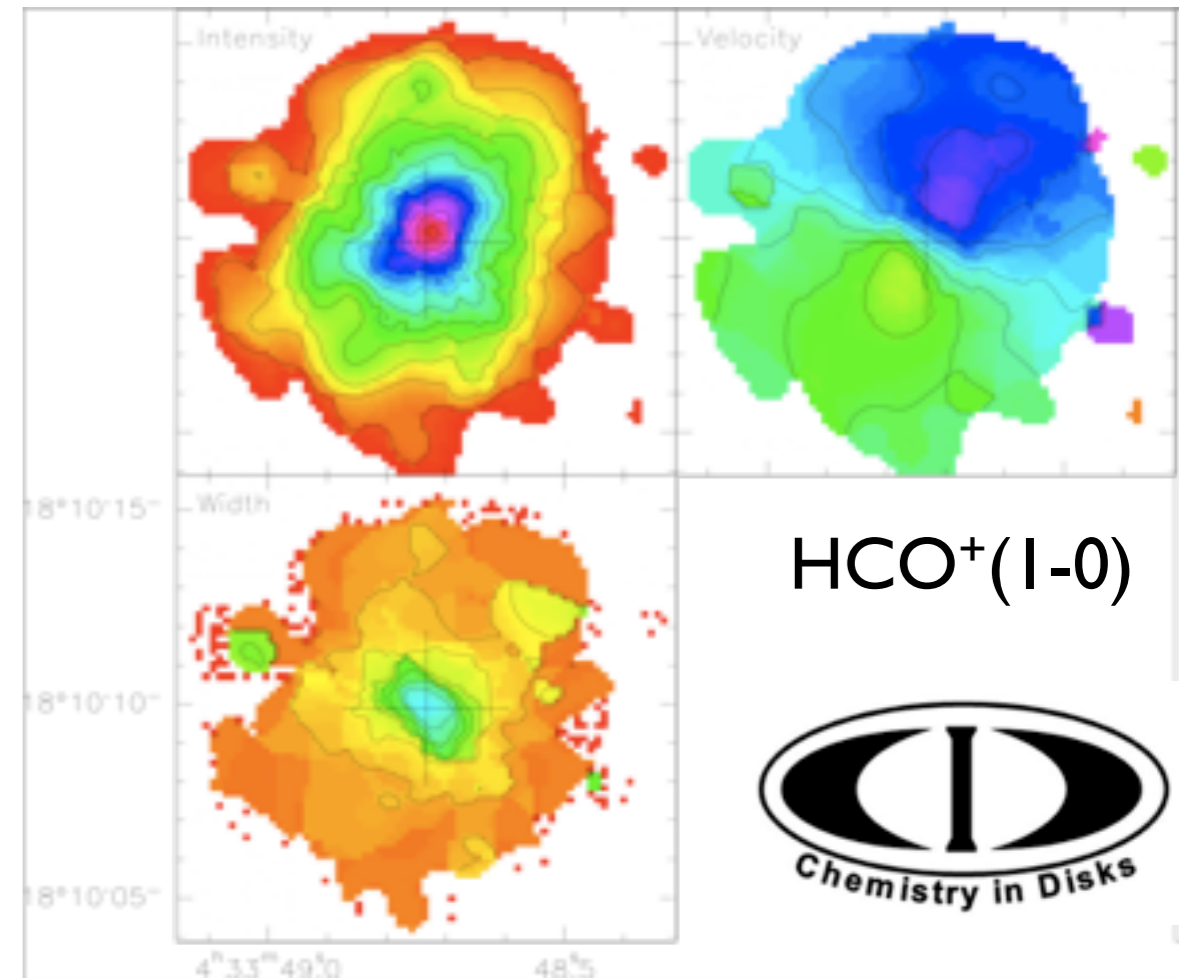
- "Cool" T Tauri disks:  
 $T_{\text{kin}} \sim 10\text{--}30\text{K}$

- No gradient in LkCa 15:  
inner hole of  $\sim 45\text{ AU}$

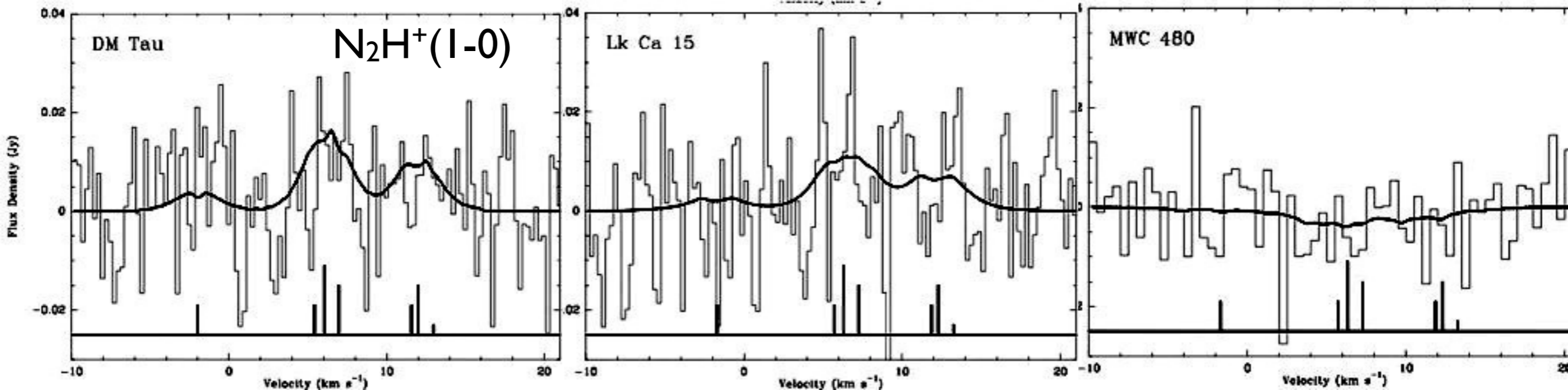
- Are transitional disks peculiar?

# Ionization: $\text{HCO}^+$ and $\text{N}_2\text{H}^+$

- LkCa 15 (K5), DM Tau (M1) and MWC480 (A4)
- $J=1-0, 2-1$
- Two  $5\sigma$  detections:  $\text{N}_2\text{H}^+$  in LkCa 15 & DM Tau
- Upper limit: MWC480



Dutrey et al. (2007)



# Ionization: $\text{HCO}^+$ and $\text{N}_2\text{H}^+$

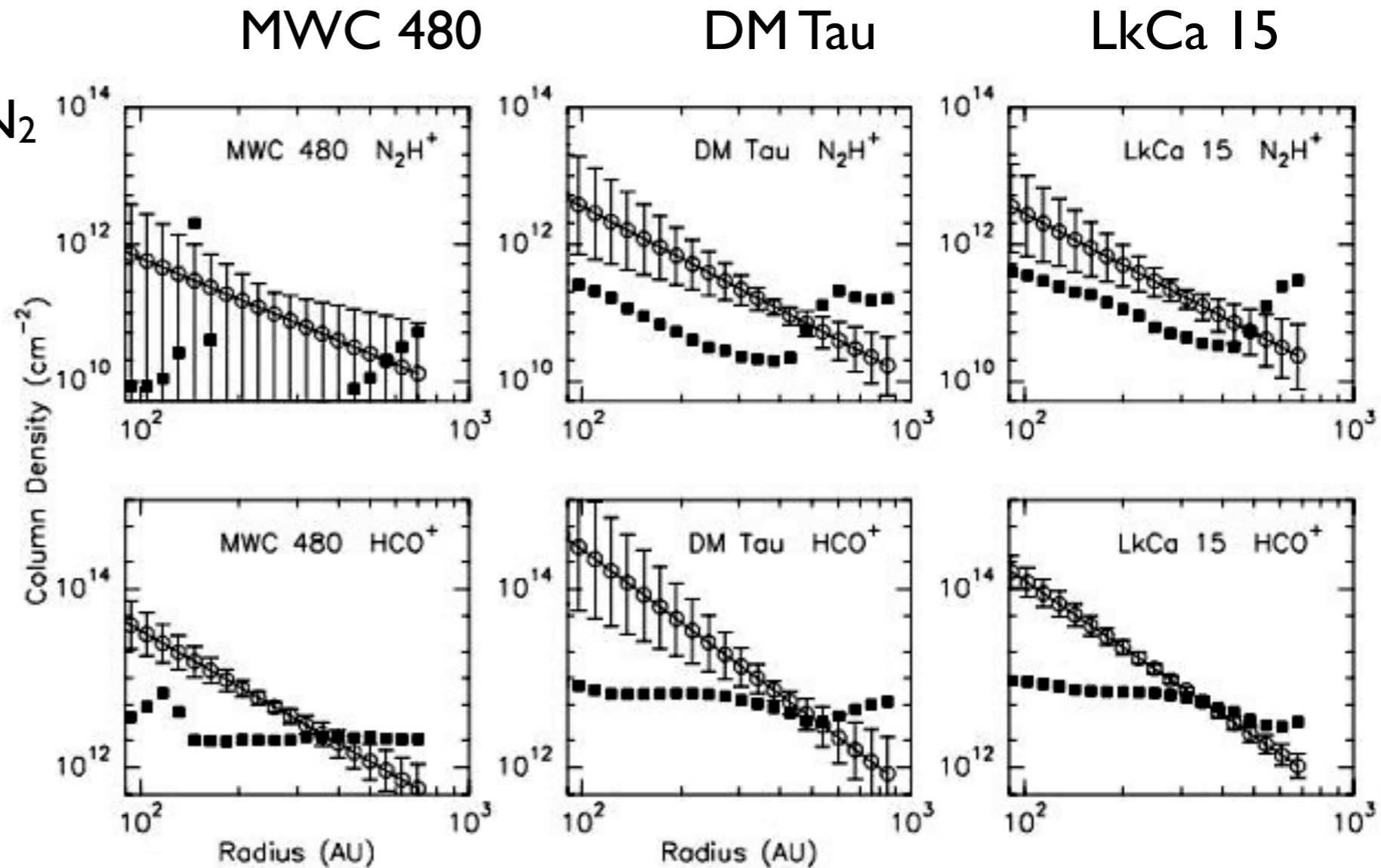
- $\text{HCO}^+$  is dominant ion:  
 $\text{N}_2\text{H}^+ + \text{CO} \Rightarrow \text{HCO}^+ + \text{N}_2$

- $[\text{N}_2\text{H}^+]/[\text{HCO}^+] \sim 2\text{--}5\%$

- $X(e) > \sim 10^{-10}$

- Radial profiles are poorly reproduced

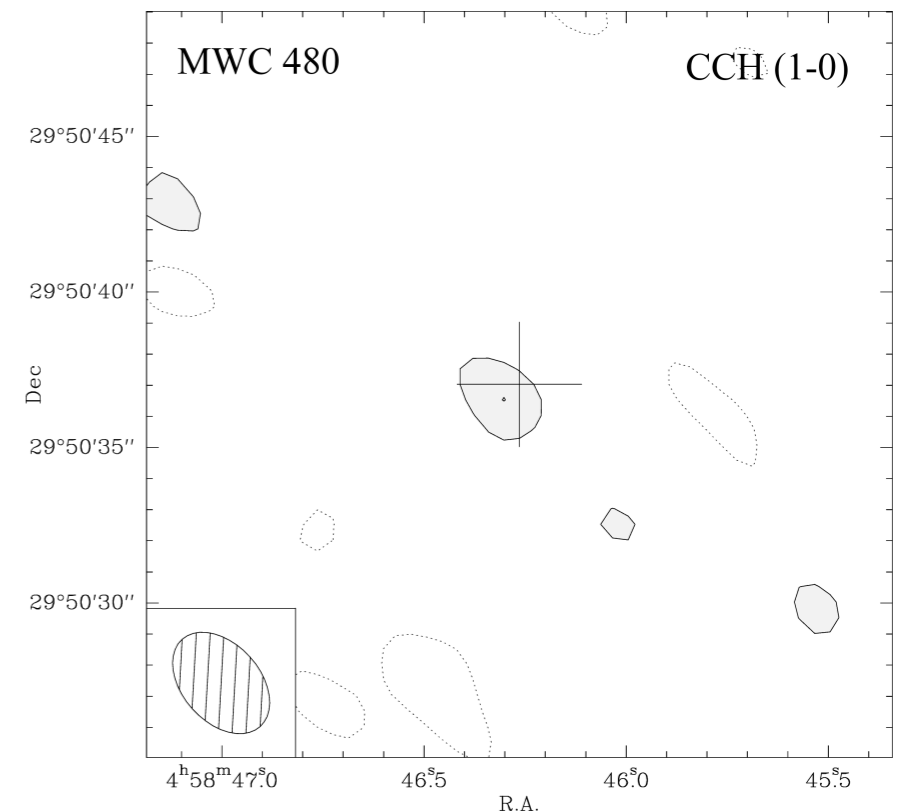
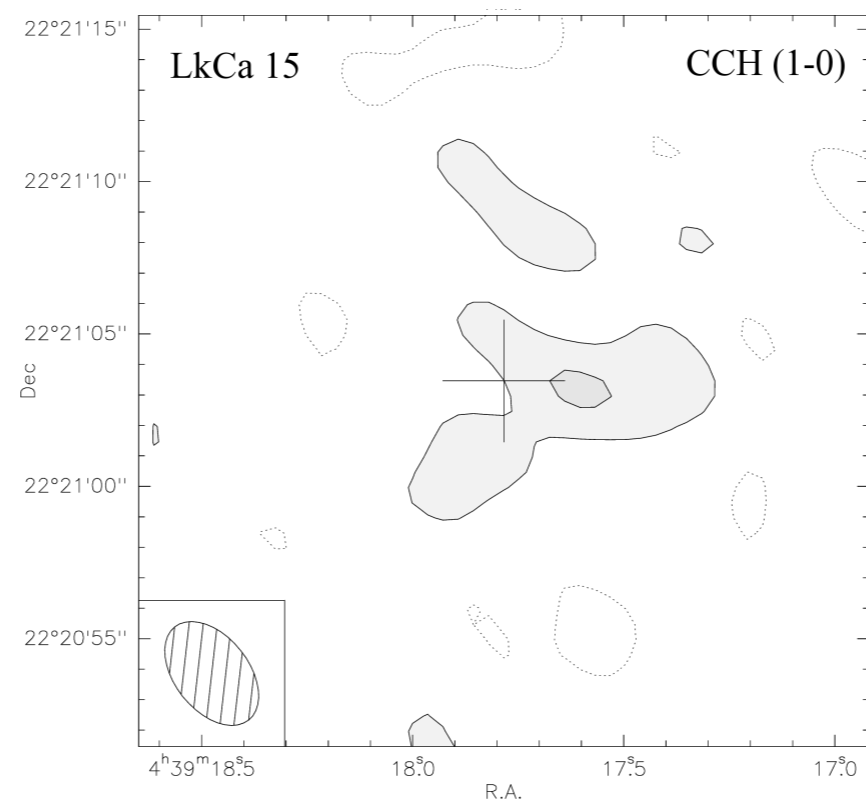
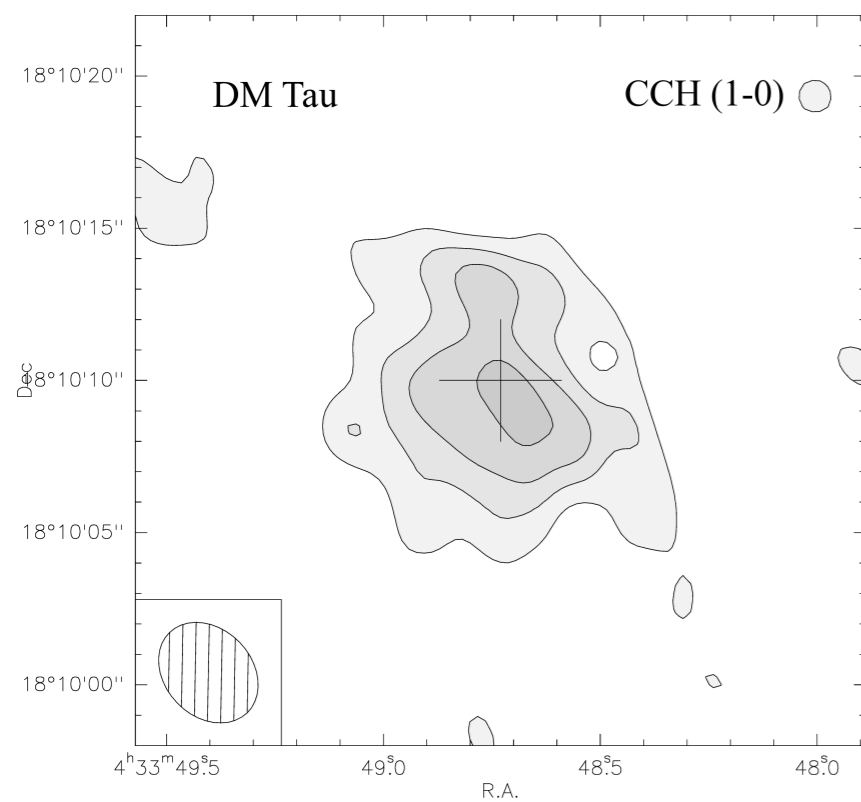
- Absolute values are in qualitative agreement



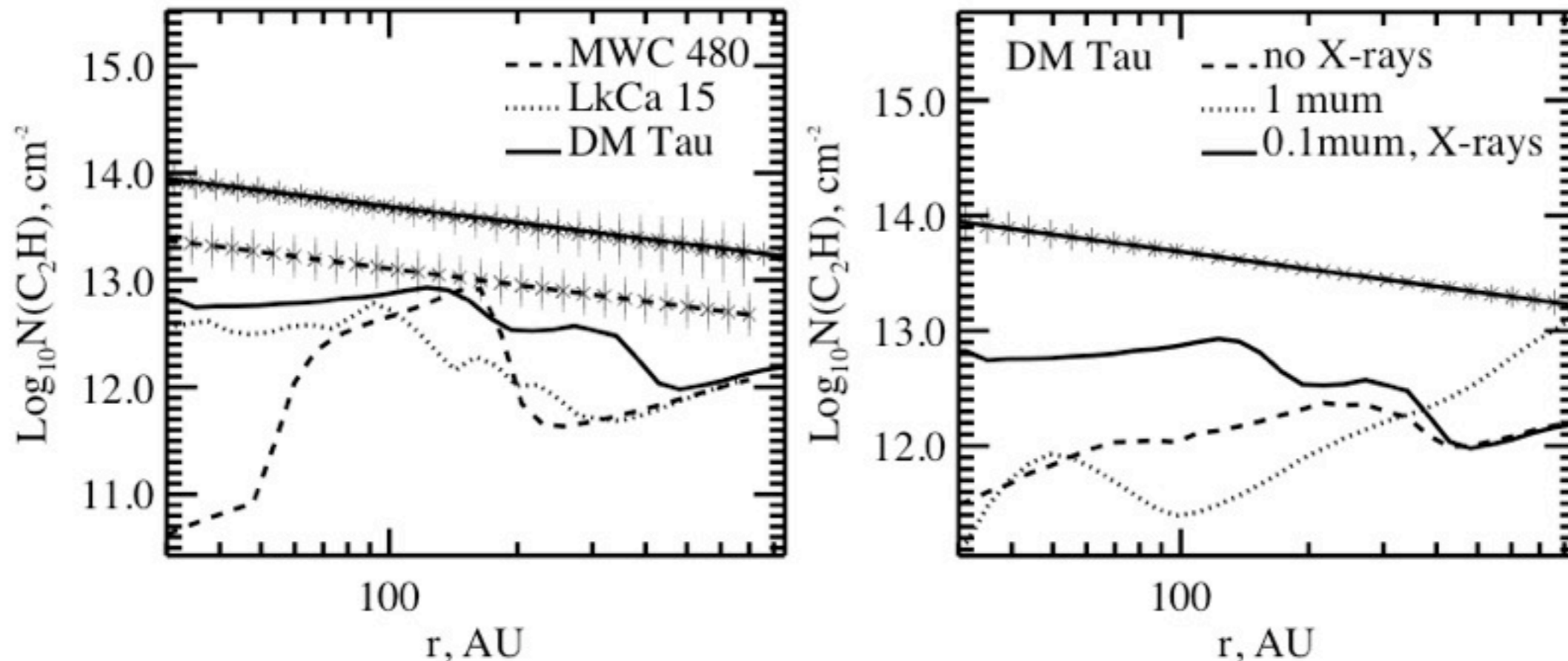
# X-ray-driven chemistry in disks



- DM Tau (M1), LkCa 15 (K5), MWC 480 (A4)
- CCH (1-0) & (2-1)
- Hard to photodissociate
- Chemistry is known



# X-ray-driven chemistry in disks



- $T_{\text{exc}}$ :  $\sim 6$  K
- Large-scale mixing or sub-thermal excitation?
- Less CCH in MWC 480
- Strong photodissociation by the Herbig Ae star?
- Low  $L_X$  in MWC 480: less efficient ion-molecule chemistry?

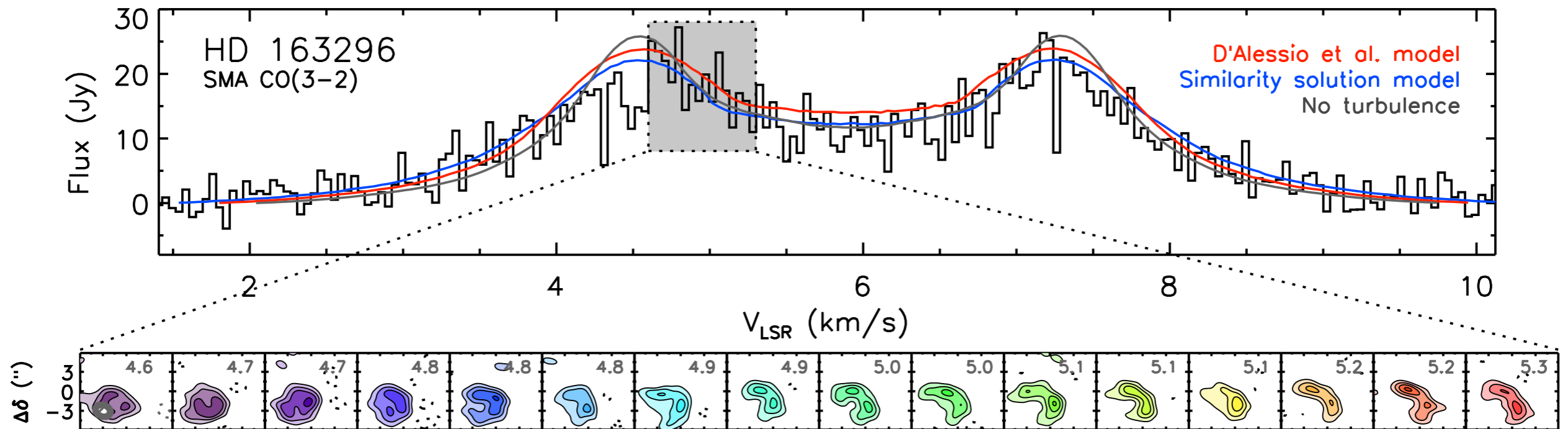


# Chemistry in T Tau and Herbig Ae disks

Molecule	$\chi^2$ -minimization method			Chemical model		DM Tau
	N [cm <sup>-2</sup> ]	1 $\sigma$ error	N/N( <sup>13</sup> CO) <sup>(1*)</sup>	N [cm <sup>-2</sup> ]	N/N( <sup>13</sup> CO) <sup>(2*)</sup>	N/N( <sup>13</sup> CO) <sup>(1*)</sup>
H <sub>2</sub>	6 10 <sup>22</sup>	1 10 <sup>22</sup>	1.5 10 <sup>6</sup>	5 10 <sup>22</sup>	1.3 10 <sup>6</sup>	1 10 <sup>7</sup>
<sup>13</sup> CO <sup>(*3)</sup>	4 10 <sup>16</sup>	5 10 <sup>15</sup>	1	4 10 <sup>16</sup>	1	1
HCO <sup>+</sup>	6 10 <sup>12</sup>	3 10 <sup>11</sup>	1.5 10 <sup>-4</sup>	1.5 10 <sup>13</sup>	4 10 <sup>-4</sup>	2 10 <sup>-3</sup>
HCN	5 10 <sup>11</sup>	3 10 <sup>11</sup>	1.3 10 <sup>-5</sup>	4 10 <sup>11</sup>	10 <sup>-5</sup>	7 10 <sup>-4</sup>
CS	3 10 <sup>12</sup>	3 10 <sup>12</sup>	< 8 10 <sup>-5</sup>	2 10 <sup>11</sup>	5 10 <sup>-6</sup>	3 10 <sup>-4</sup>
C <sub>2</sub> H	2 10 <sup>13</sup>	2 10 <sup>13</sup>	< 5 10 <sup>-4</sup>	10 <sup>10</sup>	2.5 10 <sup>-7</sup>	10 <sup>-3</sup>
CH <sub>3</sub> OH	0	7 10 <sup>15</sup>	< 2 10 <sup>-1</sup>	0	0	0

- AB Aur: less amount of complex molecules per CO
- Are Herbig Ae disks "deserts" for complex molecules?
- No CO freeze-out in Herbig Ae disks: no surface chemistry
- Lower L<sub>X</sub>: less efficient ion-molecule chemistry
- CO + He<sup>+</sup> ⇒ C<sup>+</sup> + O + He<sup>+</sup>

# Turbulence in disks



- Temperature from CO lines
- Keplerian velocity:  $M_*$ ,  $r$
- Subsonic components:  $\sim 0.1\text{--}0.4$  km/s
- Comparable with MHD models

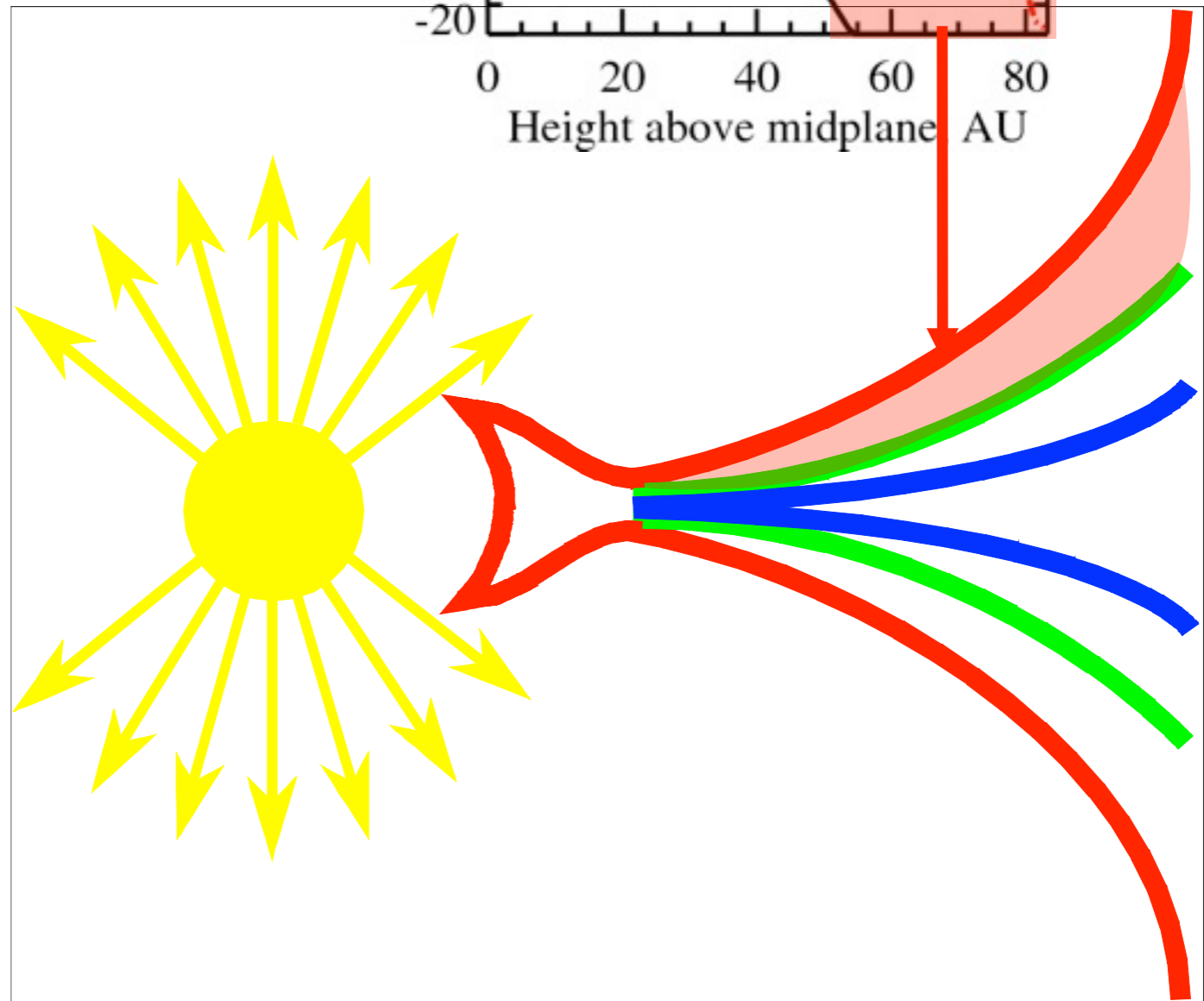
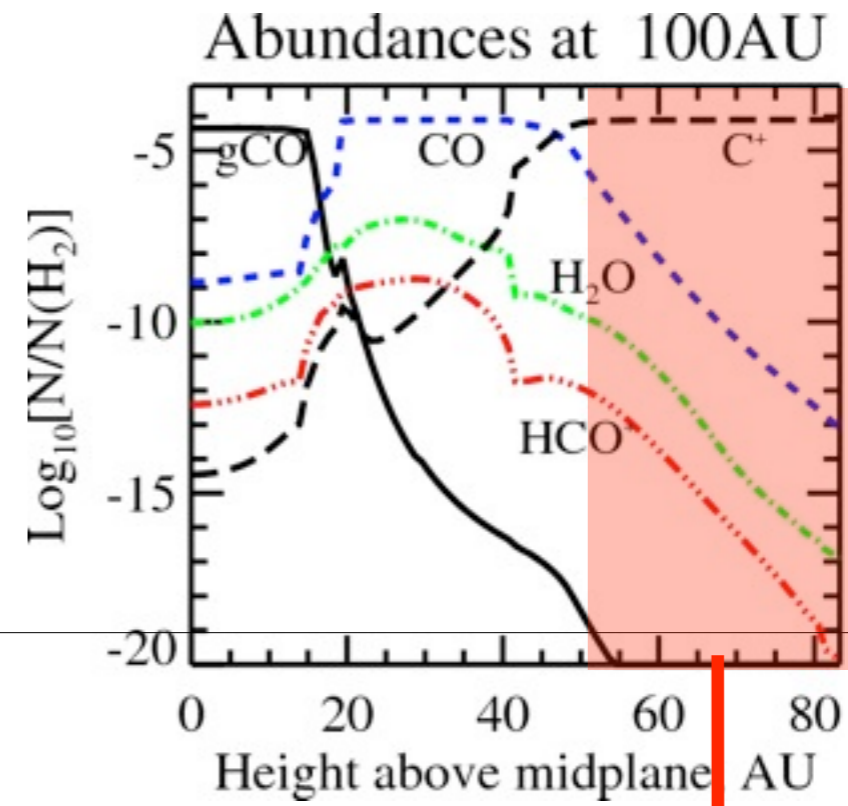
# III. Observations of molecules in PPDs: Summary

- Probes of disk structure
- Analysis techniques are available
- Vertical gradients of T
- CO freeze-out in "cold" T Tauri disks
- "Warm" Herbig Ae disks are less rich in molecules
- High-energy stellar radiation
- Models are in "qualitative" agreement
- Turbulent line broadening
- Rich inner disk chemistry

# **IV. Disk chemical structure from modeler's perspective**

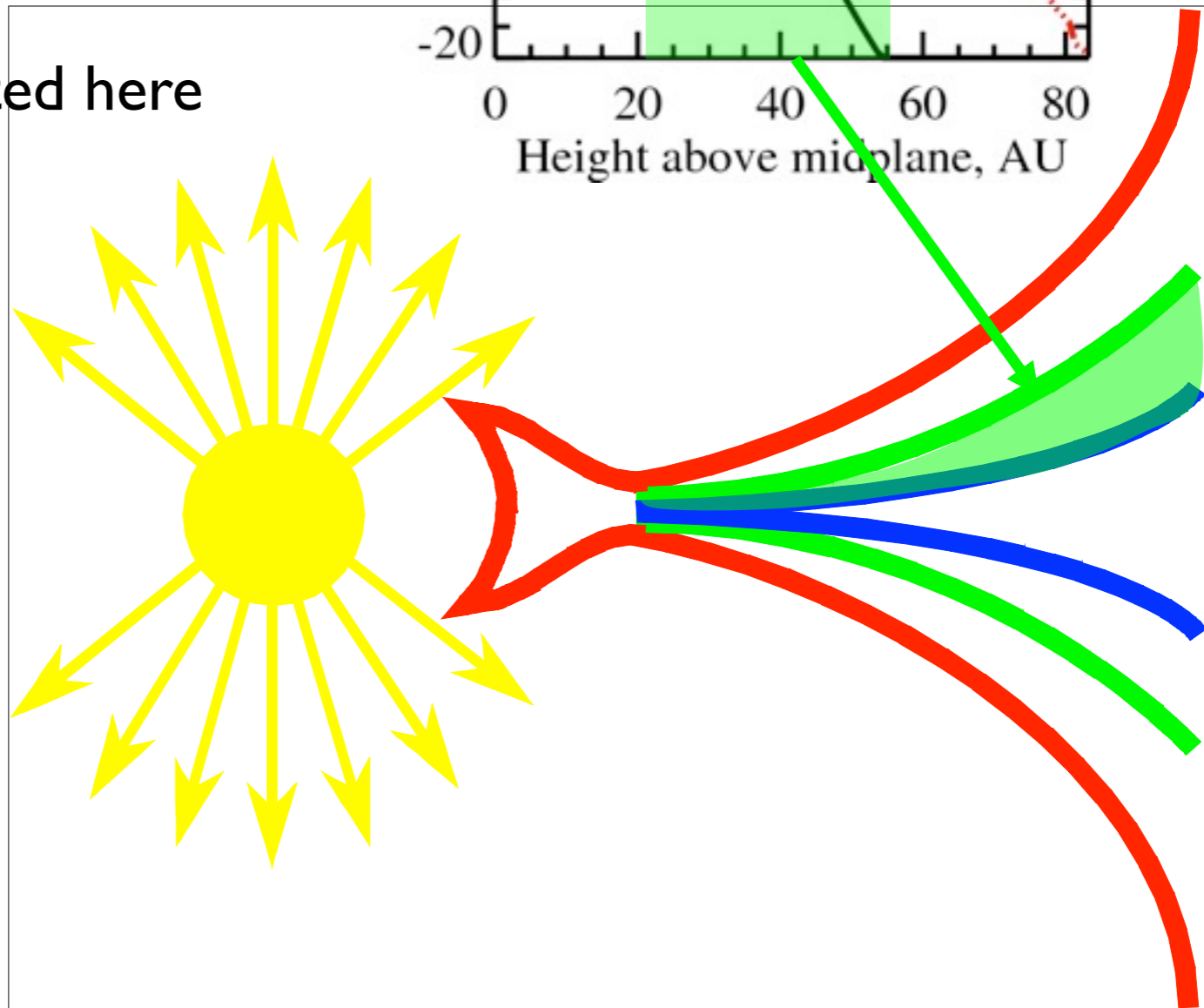
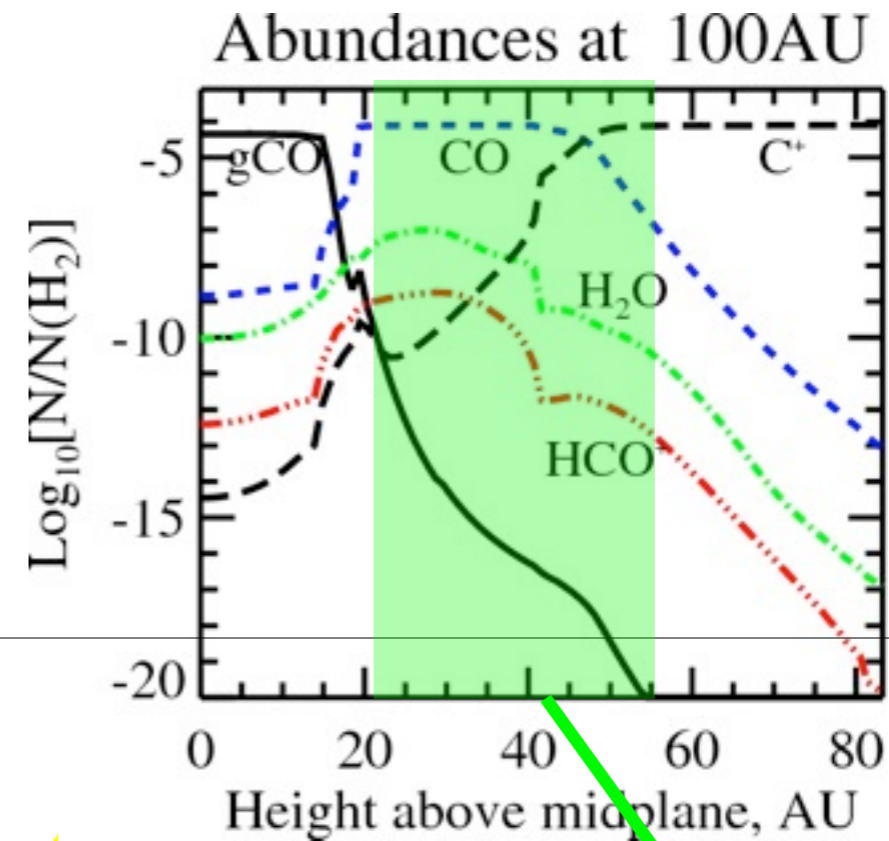
# Zone of ions and radicals (atmosphere)

- Intense UV and X-rays
- Low densities
- High temperatures
- High ionization degree
- Limited gas-phase chemistry



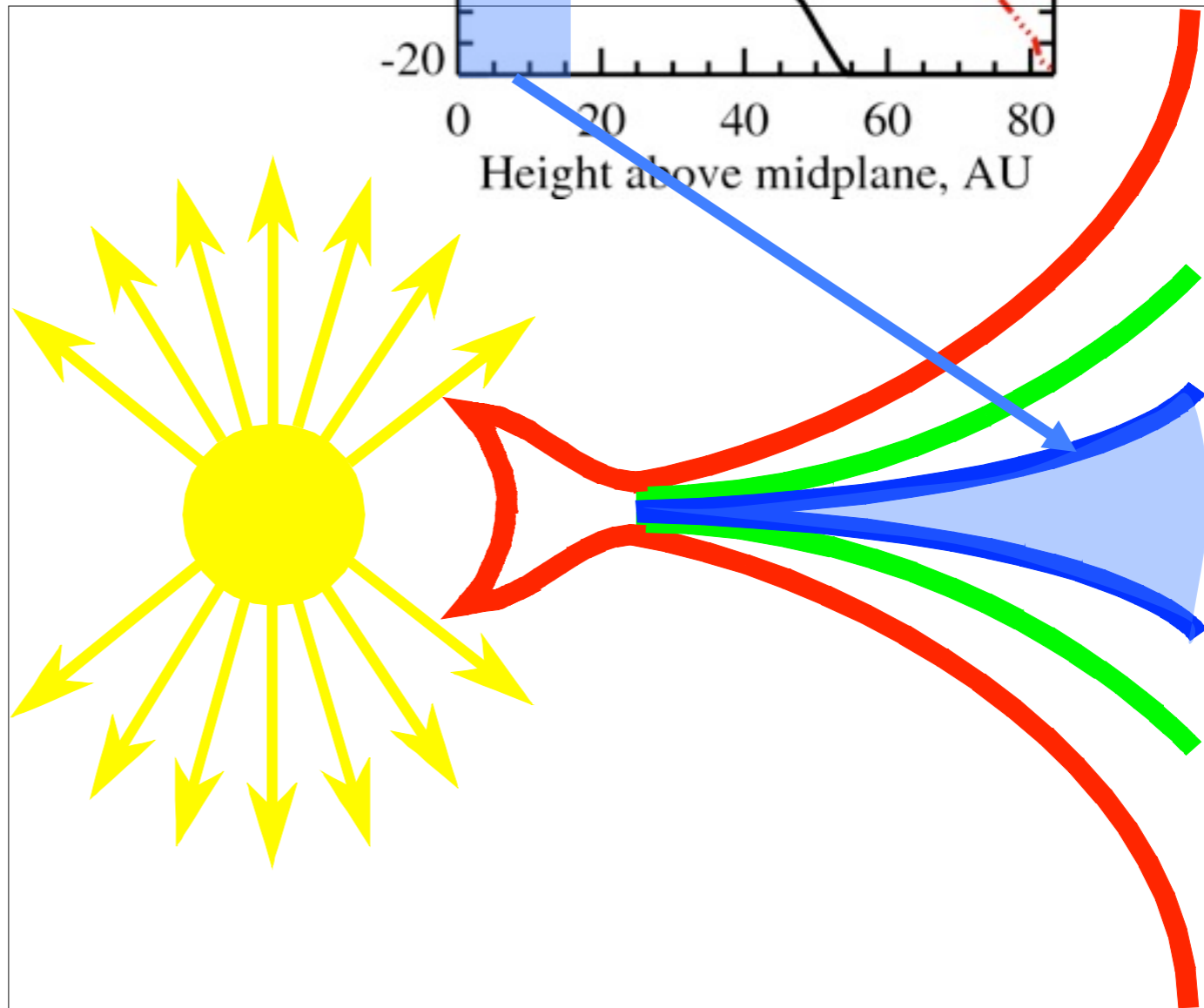
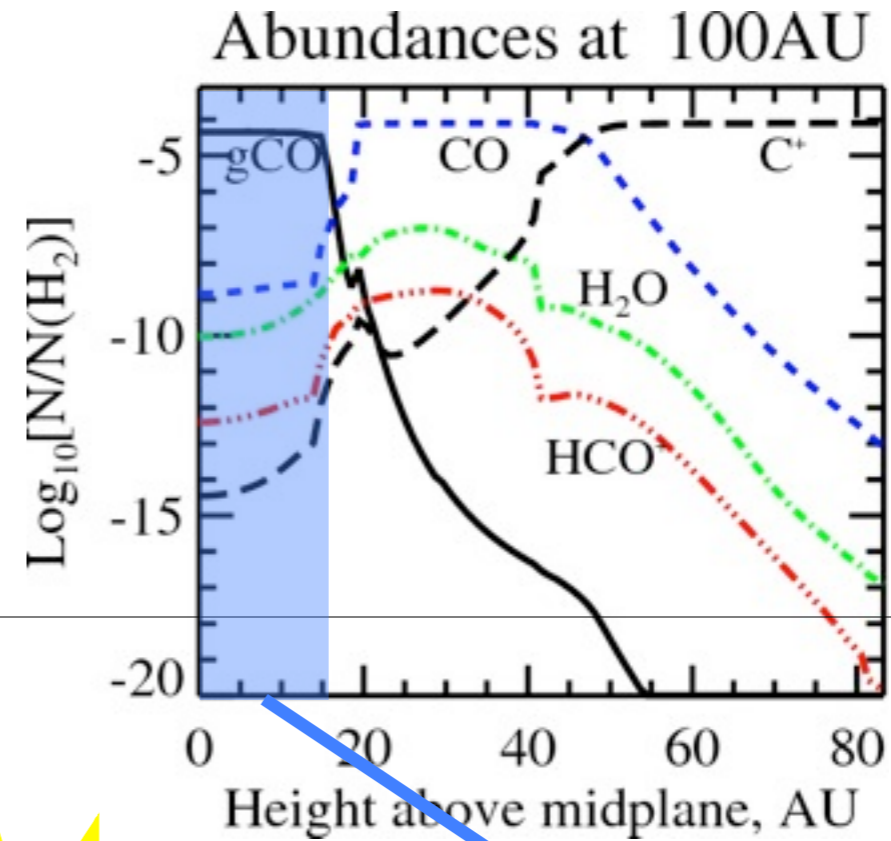
# Zone of molecules (intermediate layer)

- 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



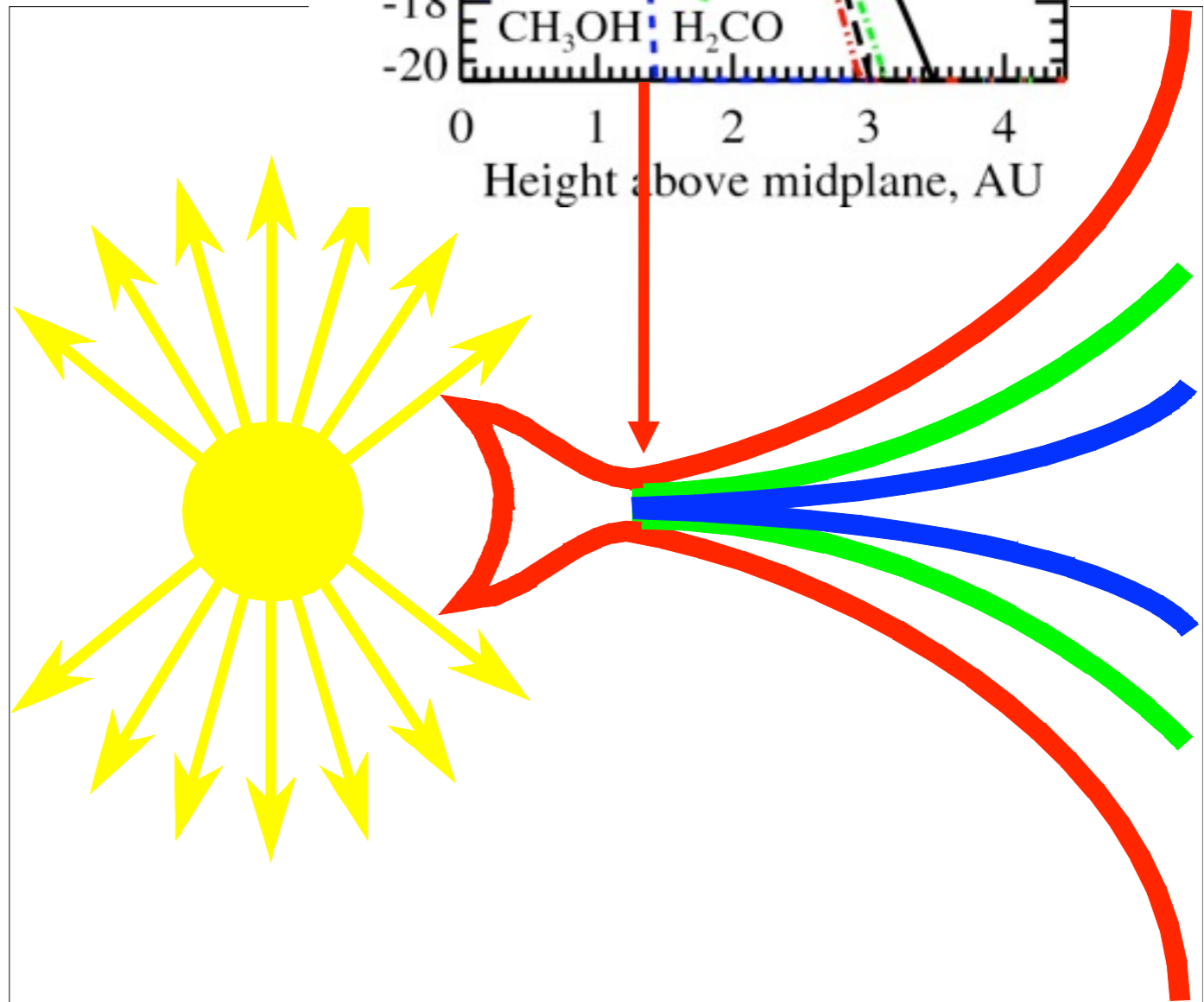
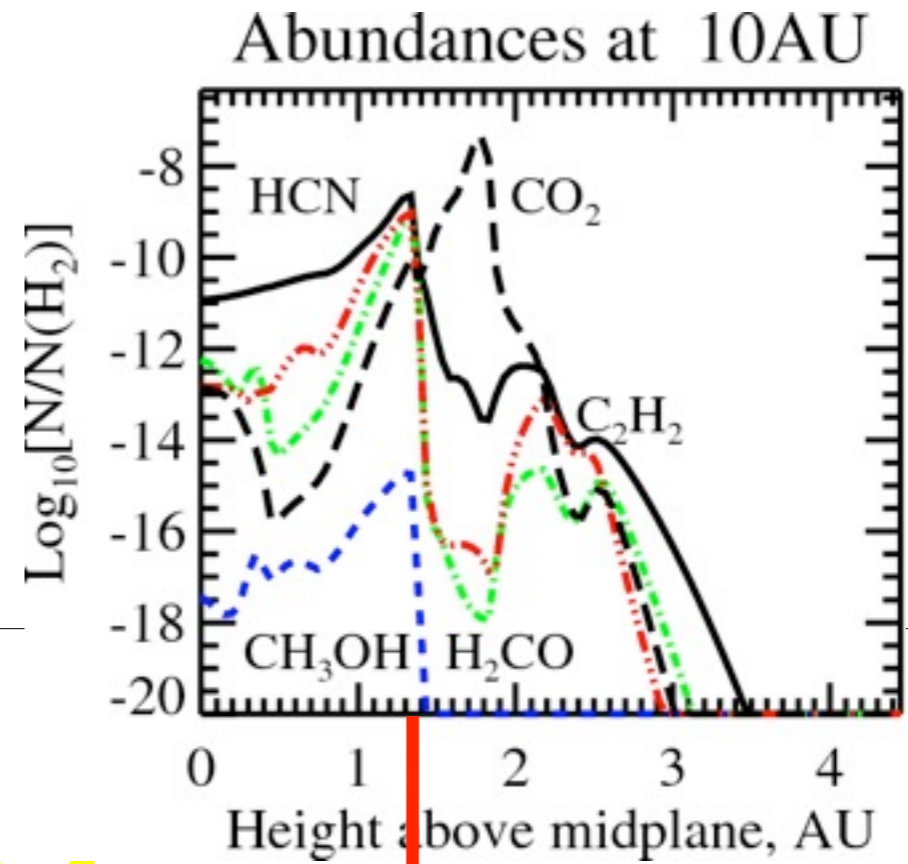
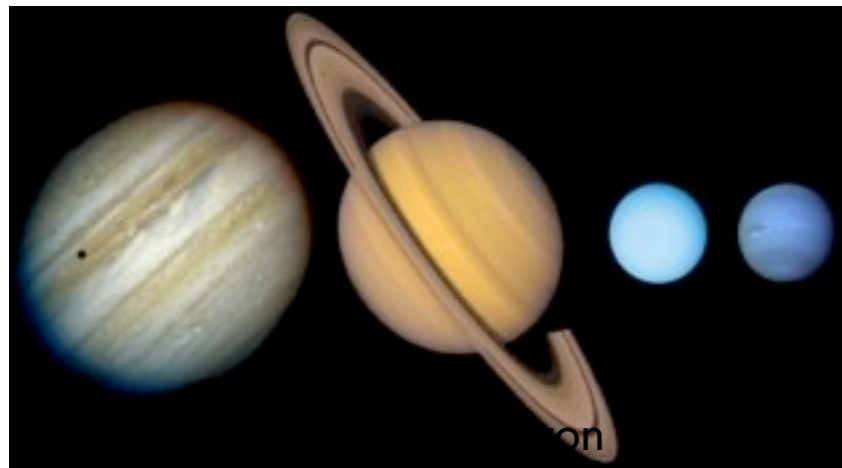
# Zone of ices (midplane)

- Only cosmic rays can penetrate
- High densities
- Low temperatures
- Molecules are frozen out
- Rich chemistry on dust surfaces



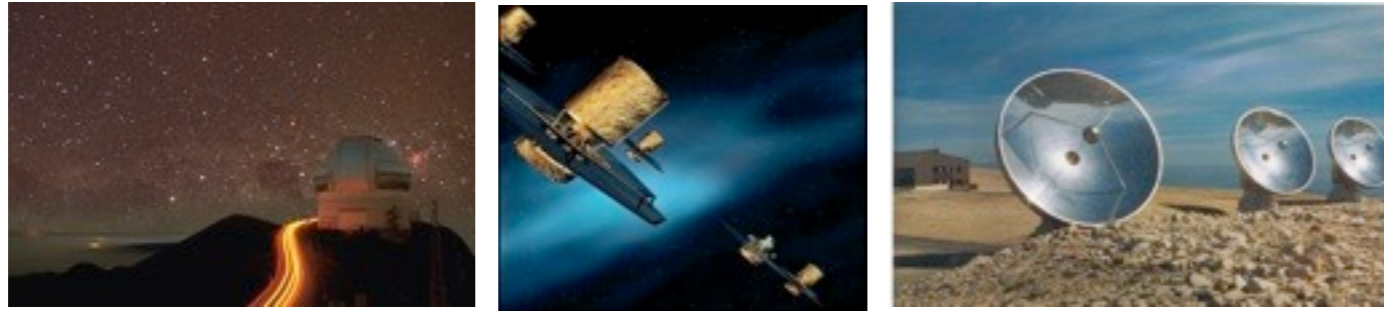
# Inner, planet-forming zone

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



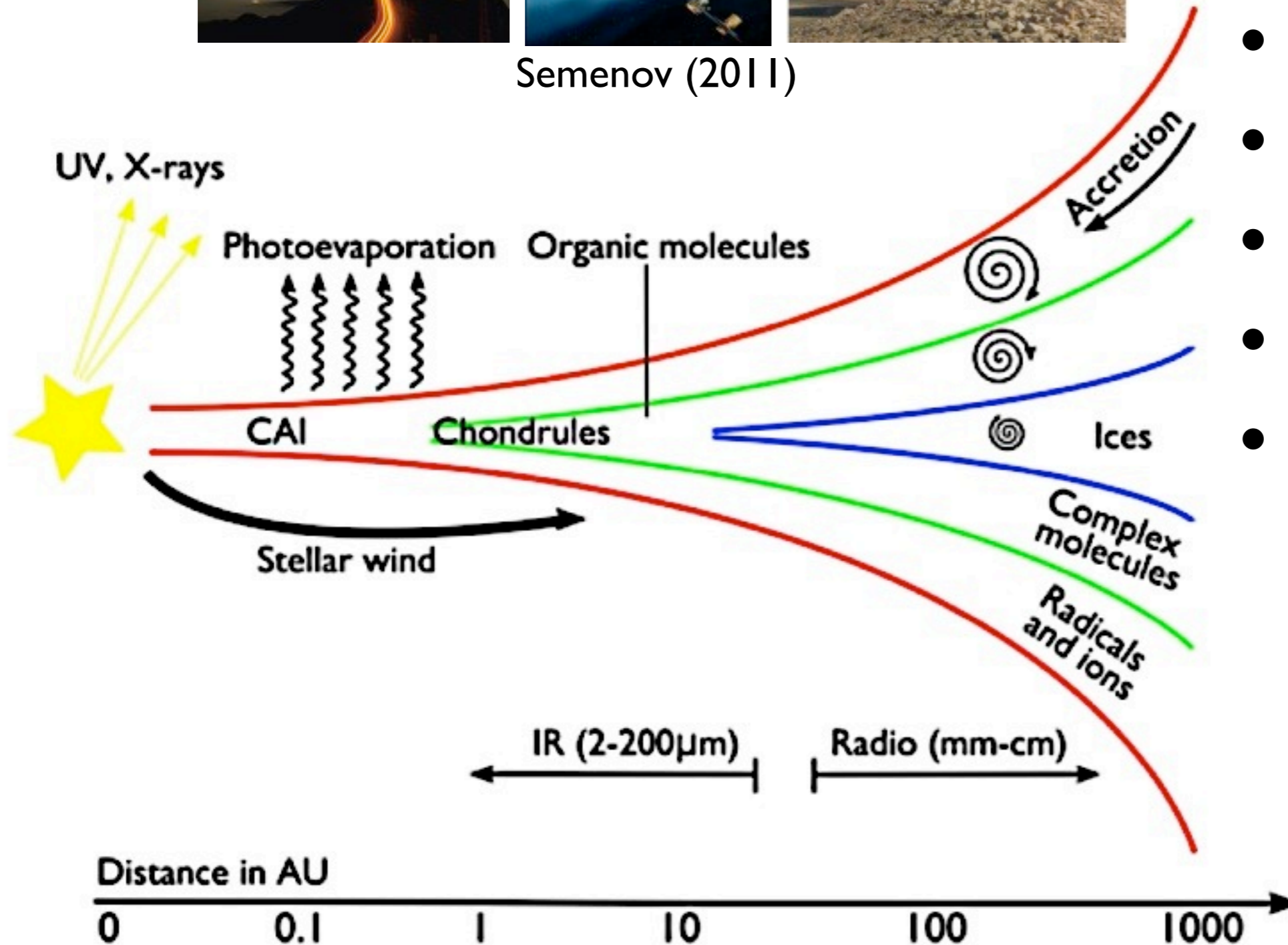


# A scheme of disk structure



Semenov (2011)

- Wide range of  $T$  &  $n_H$
- FUV, X-rays, cosmic rays
- Dynamical evolution
- Photoevaporation
- Grain evolution
- No equilibrium



# IV. Disk chemical structure from modeler's perspective: Summary

- "Sandwich"-like chemical structure
- Cold midplane: freeze-out, thick ices, surface chemistry
- Hot atmosphere: dissociation/ionization, ions/radicals, gas-phase chemistry
- Warm molecular layer: oasis of molecules, UV-assisted gas-phase & gas-grain chemistry
- Dense planet-forming zone: endothermic neutral-neutral chemistry, X-ray-assisted ion-molecule chemistry

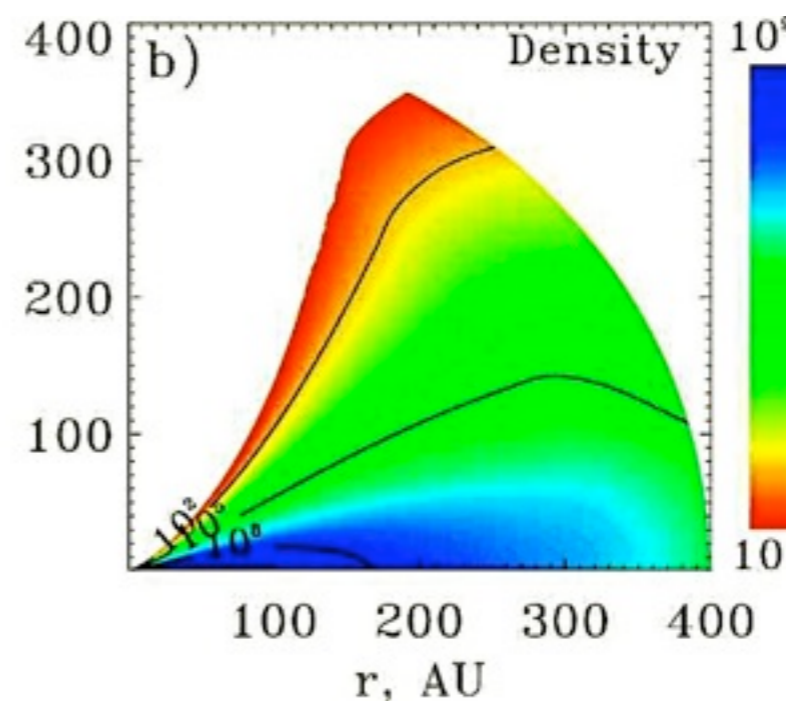
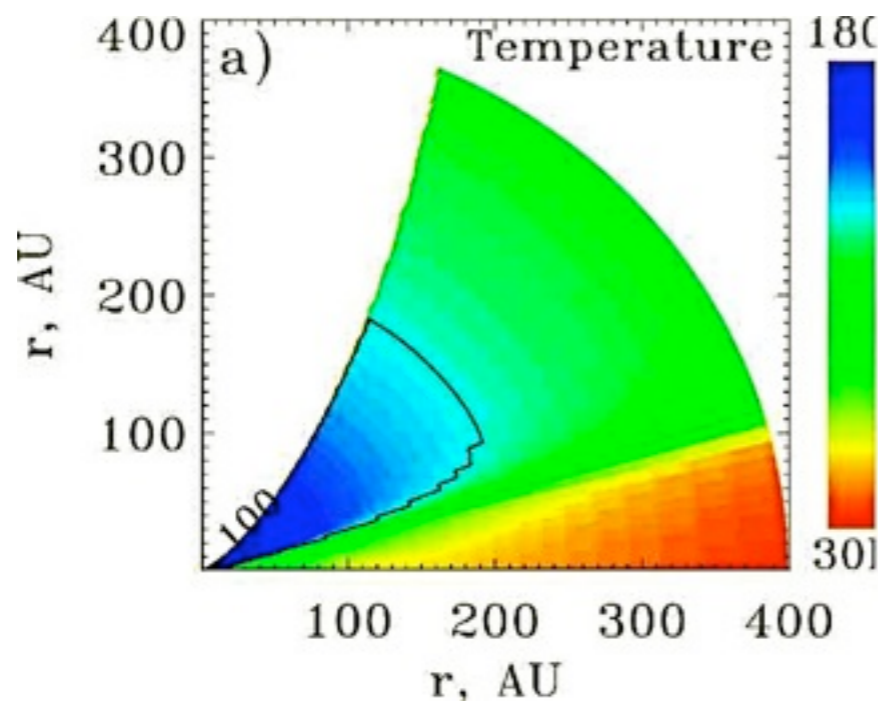
# **V. Modeling disk chemistry**

# Chemical kinetics equations

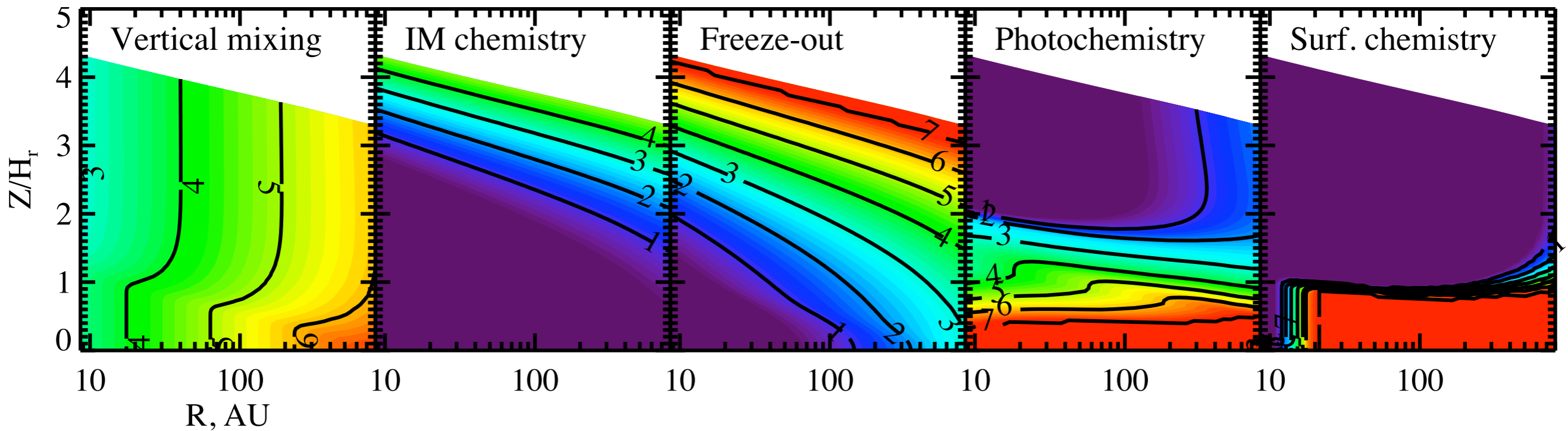
$$\frac{\partial n_i}{\partial t} = \sum_{j,k \neq i} k_{jk} n_j n_k - n_i \sum_l k_{li} n_l + \nabla D n_H \nabla n_i / n_H - \nabla U n_i$$

Evolution = Formation - Destruction + Diffusion + Advection  
[ Chemistry ] [ Dynamics ]

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



# Timescales in disks: chemistry vs dynamics

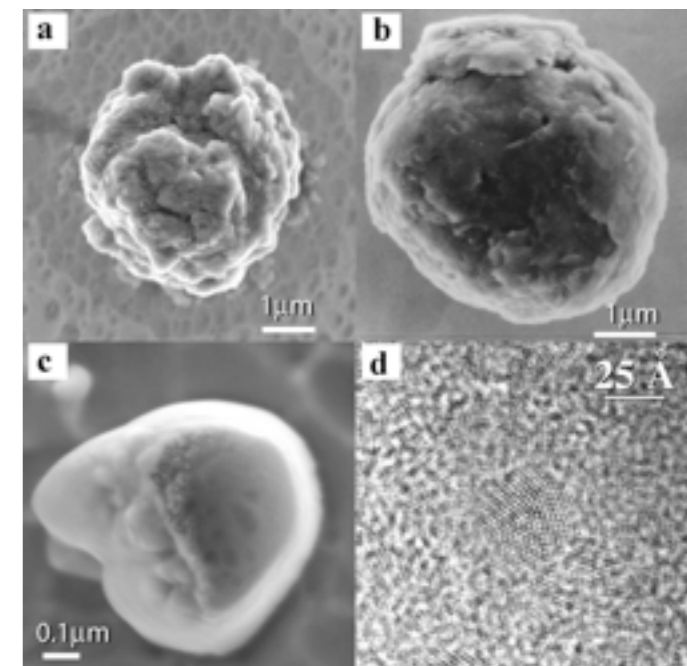
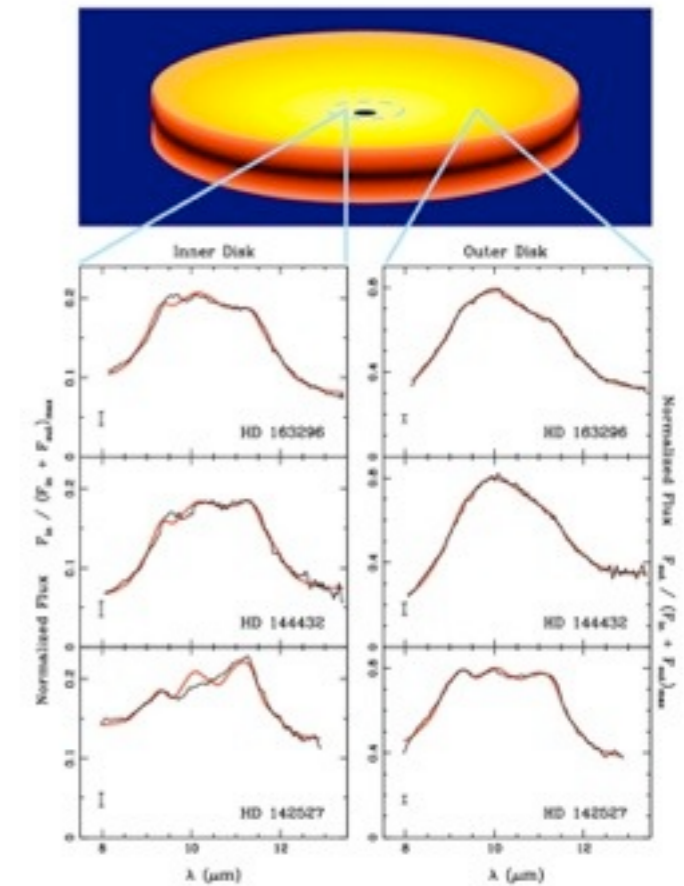


Characteristic Timescales: Outer Disk (250 AU)

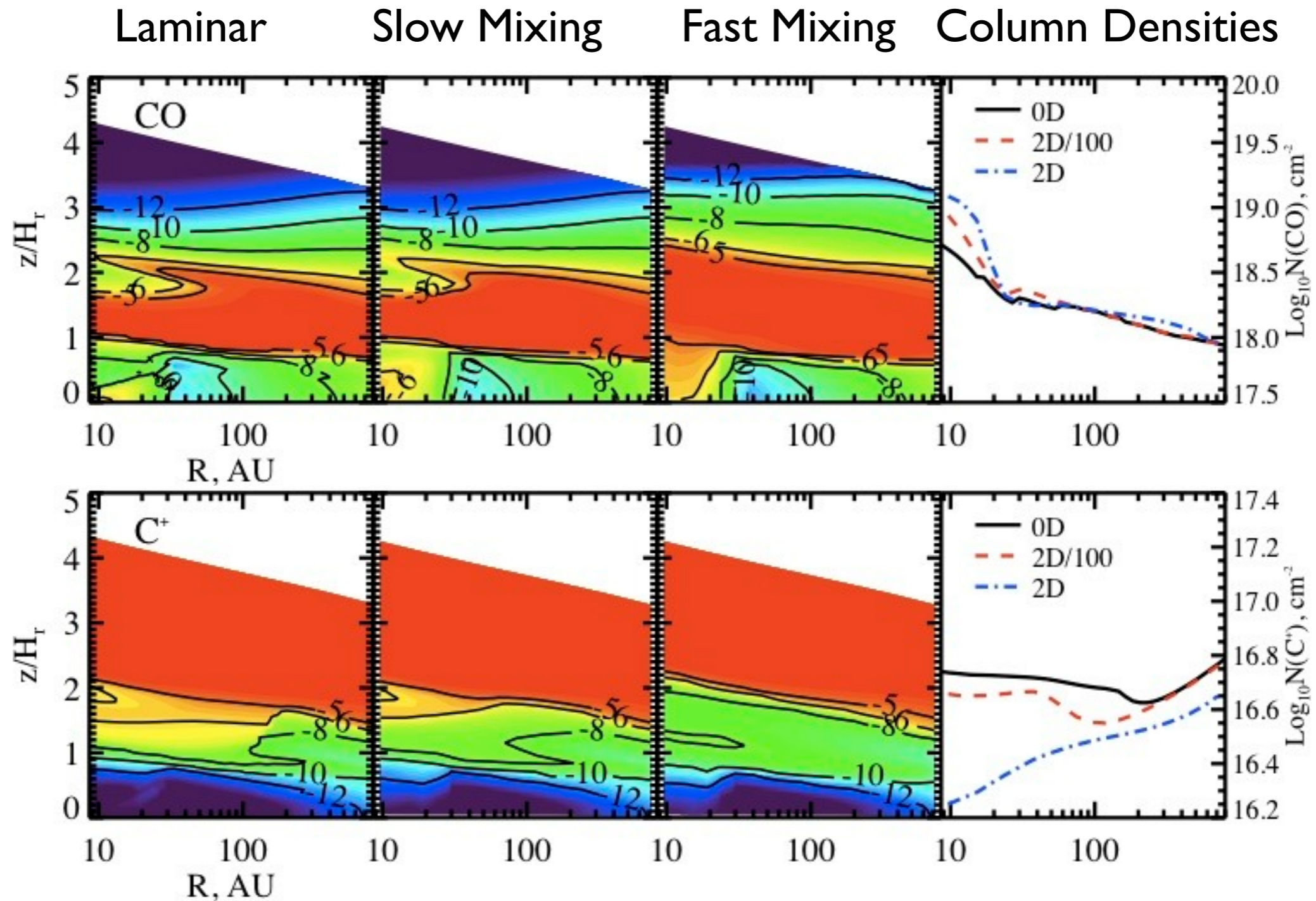
Processes	Midplane [yr]	Warm layer* [yr]	Atmosphere* [yr]
Mixing	1.0 (6)	2.5 (5)	1.4 (5)
Gas-phase	2.0 (-2)	1.8 (-1)	2.9 (0)
UV	>1.0 (7)	1.2 (6)	3.1 (1)
Accretion	2.7 (1)	1.8 (2)	2.3 (3)
Desorption	1.0 (6)	4.3 (0)	<1.0 (-7)
Surface*	>1.0 (7)	>1.0 (7)	1.4 (5)

# Chemistry with dynamics

- Turbulence & accretion
- Isotopic homogeneity of the Solar Nebula
- Crystalline silicates in comets and outer disk regions
- Extended gas-grain chemistry
- 1D/2D turbulent mixing
- "ALCHEMIC" code
- "Qualification" fit to observations
- Reduced and oxidized ices in comets

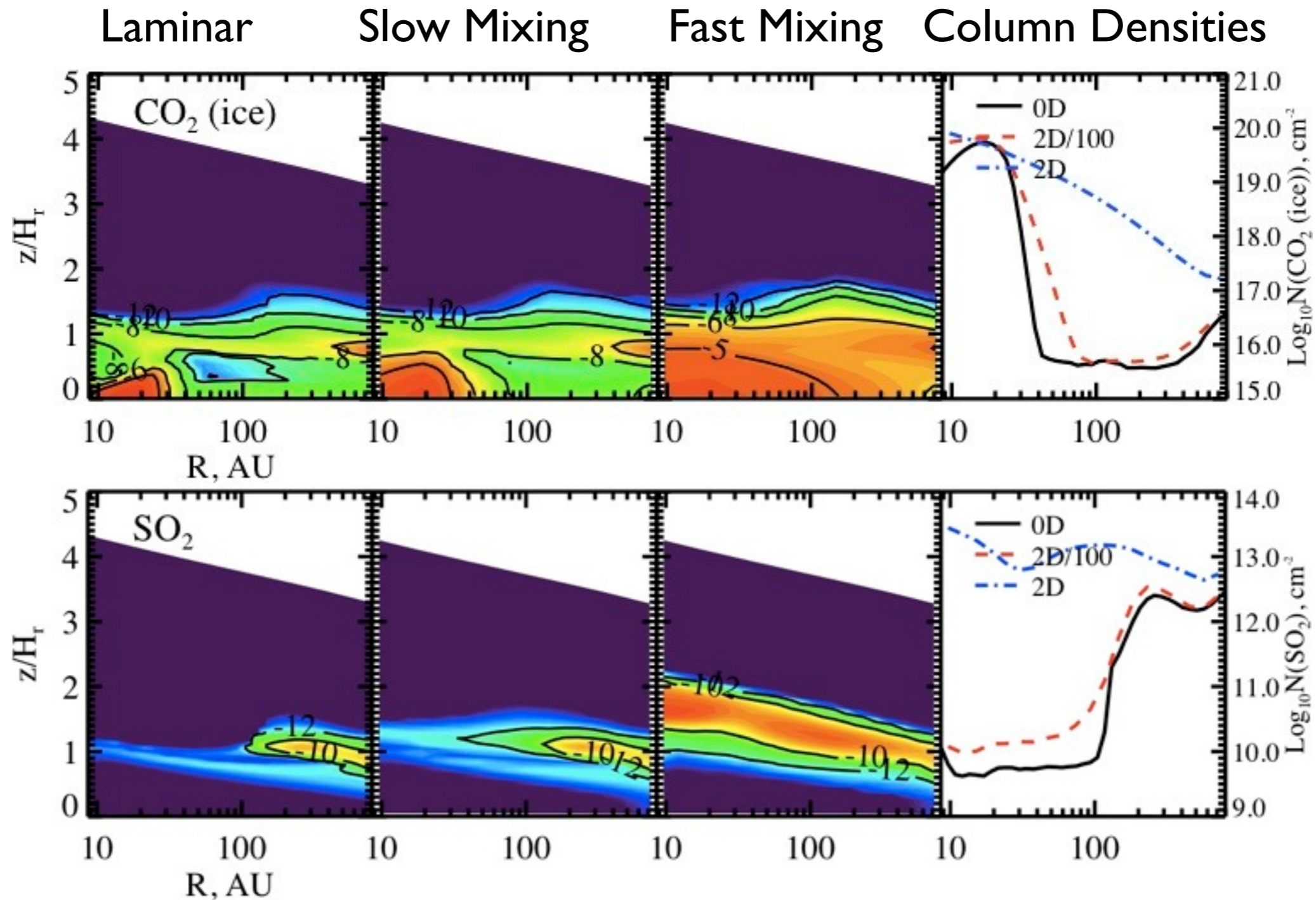


# Turbulence: Steadfast species



- Fast gas-phase formation and destruction
- $t$ : Gas-phase chemistry < Dynamics
- Example: CO, OH, H<sub>2</sub>O ice, CCH, C<sup>+</sup>, CN, HCN

# Turbulence: Sensitive species



- Slow surface formation & desorption
- $\tau$ : Surface chemistry  $>$  Dynamics
- Hydrocarbons ( $\text{C}_2\text{H}_2$ ), organics ( $\text{HCOOH}$ ),  $\text{SO}$ ,  $\text{SO}_2$ ,  $\text{C}_2\text{S}$ ,  $\text{C}_3\text{S}$



# VI. The Brave New World: ALMA

- Atacama Large Millimeter Array (2013)
- 50 x 12m + 12x7m + 4x12m
- Spatial resolution: 0.005''
- Spectral resolution: <math><0.05\text{ km/s}</math>
- 8 GHz bandwidth for continuum
- 86 – 950 GHz (250  $\mu\text{m}$  – 1 mm)
- x100 resolution
- x20 sensitivity

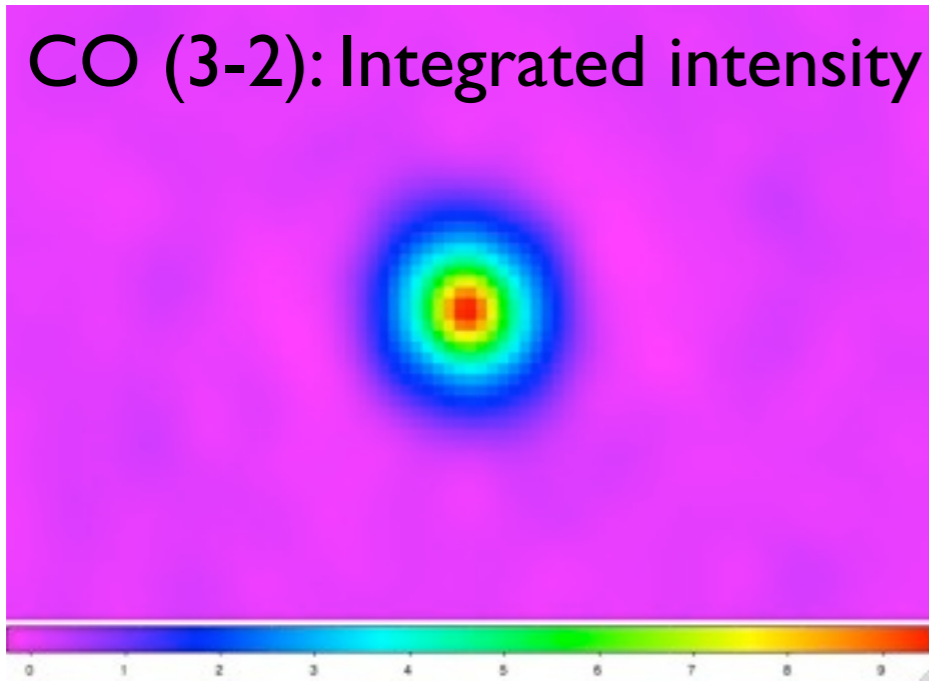


# ALMA imaging of gas in PPDs:

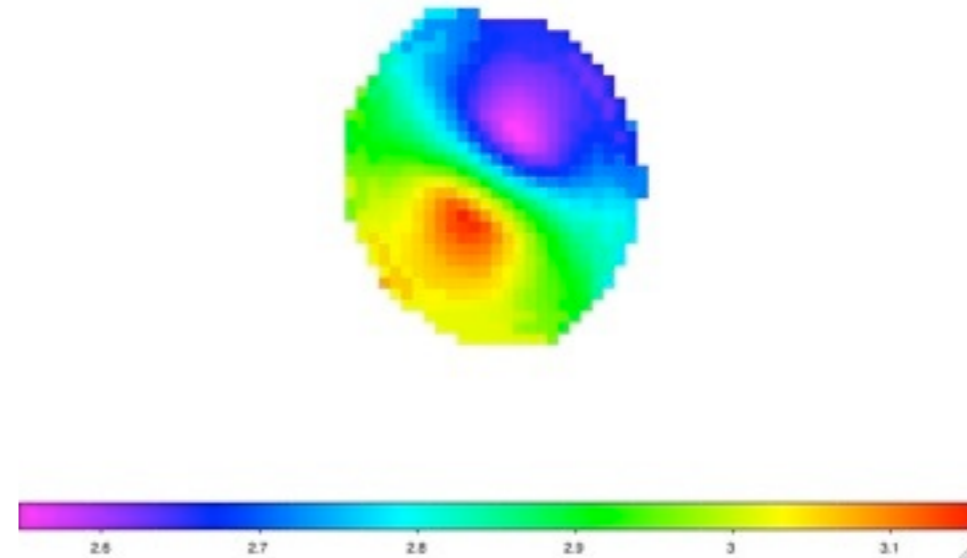
- "Hot core/corinos"-like complex molecules:  $>\text{CH}_3\text{OH}$ ,  $\text{C}_n\text{H}_m$
- Molecules with S, P, Si, Cl, ...
- Anions:  $\text{C}_8\text{H}^-$
- Isotopologues:  $^{15}\text{N}$ ,  $^{34}\text{S}$ ,  $^{17,18}\text{O}$ , D,  $^{13}\text{C}$
- Ionization structure
- Planet-forming inner regions
- Molecular layers
- Large- and small-scale dynamics
- Large surveys
- Unknown unknowns!

# ALMA is working: TW Hya

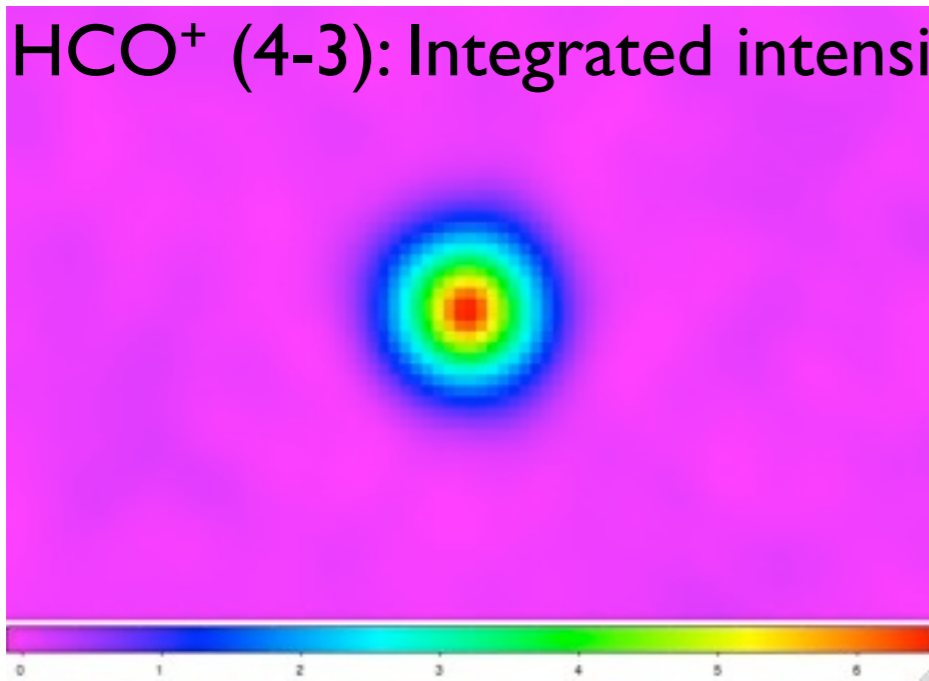
CO (3-2): Integrated intensity



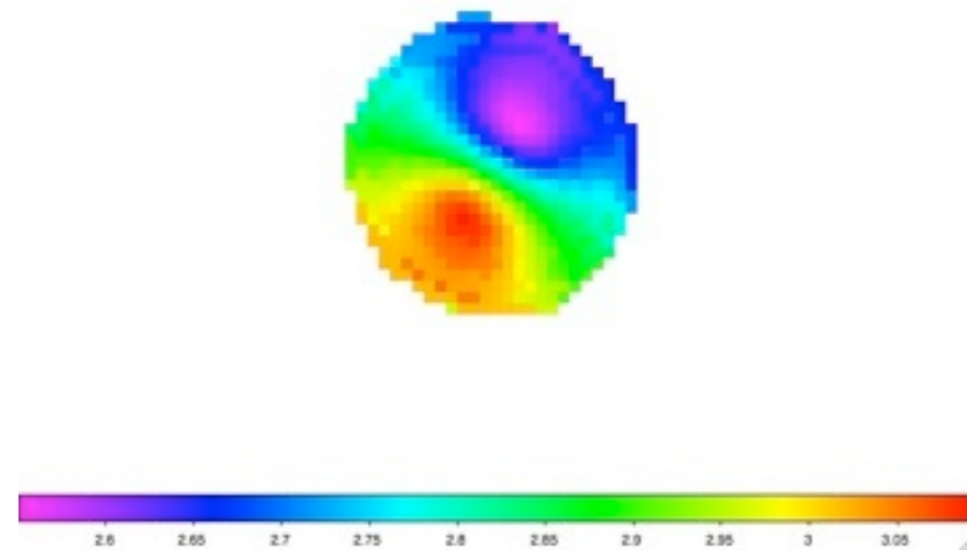
CO (3-2): Rotation



HCO<sup>+</sup> (4-3): Integrated intensity



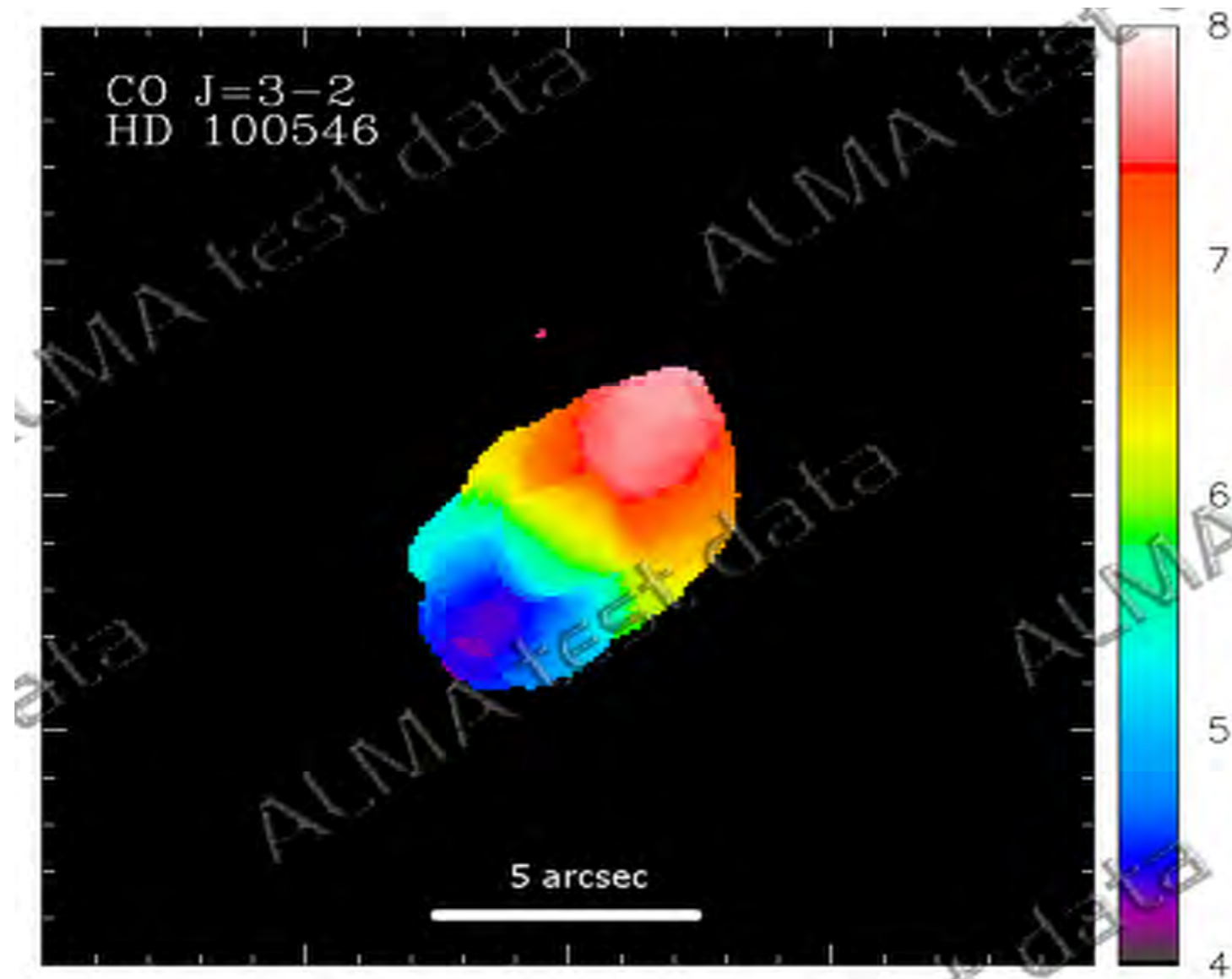
HCO<sup>+</sup> (4-3): Rotation



Science Verification observations of TW Hya at 345 GHz

# ALMA is working: HD 100546

CO (3-2): Rotation

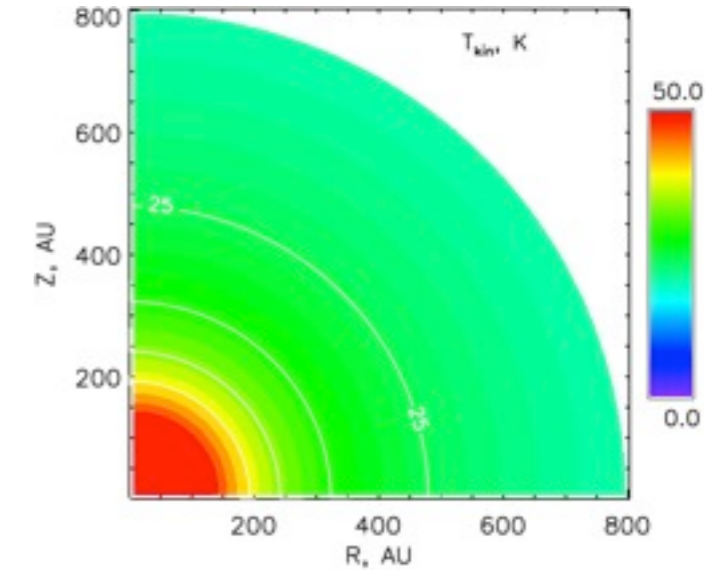
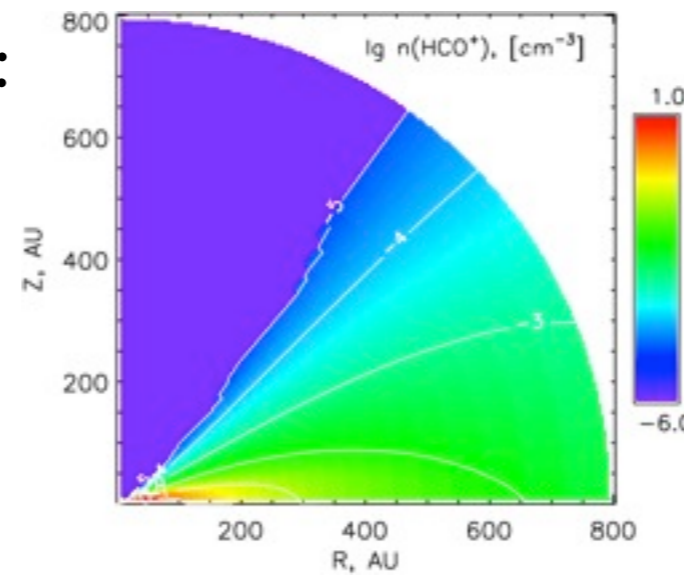


ALMA commissioning

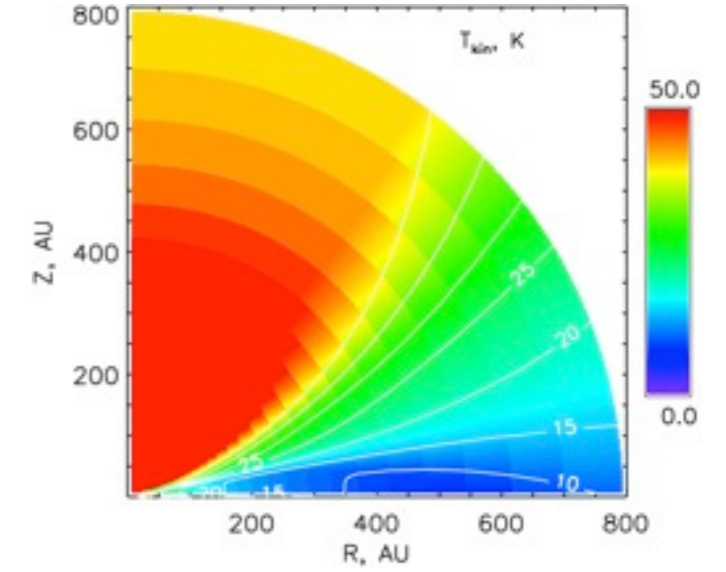
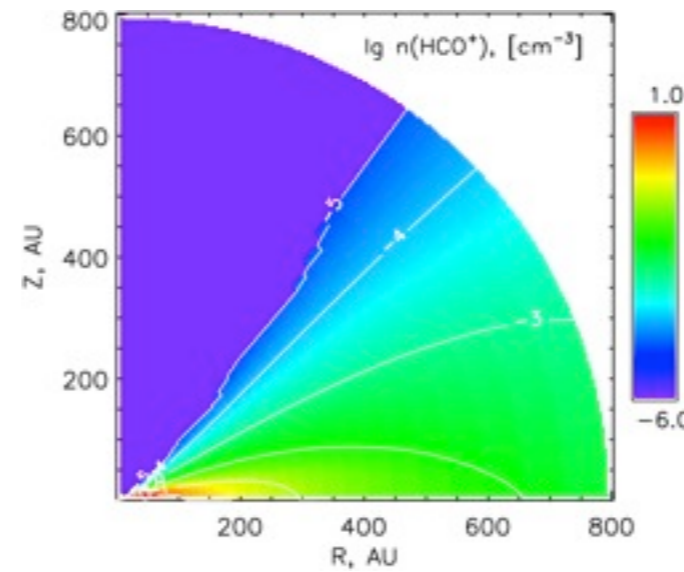
# Disk models for ALMA: HCO<sup>+</sup> (4-3)

2D Monte-Carlo LRT calculations:

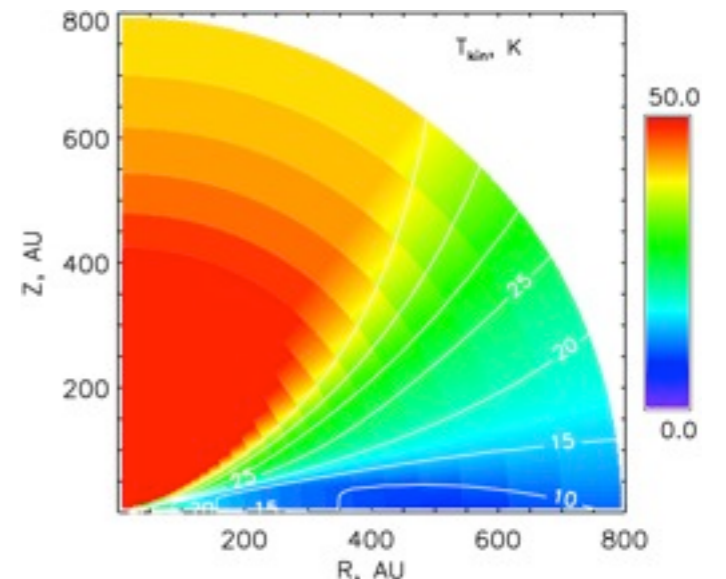
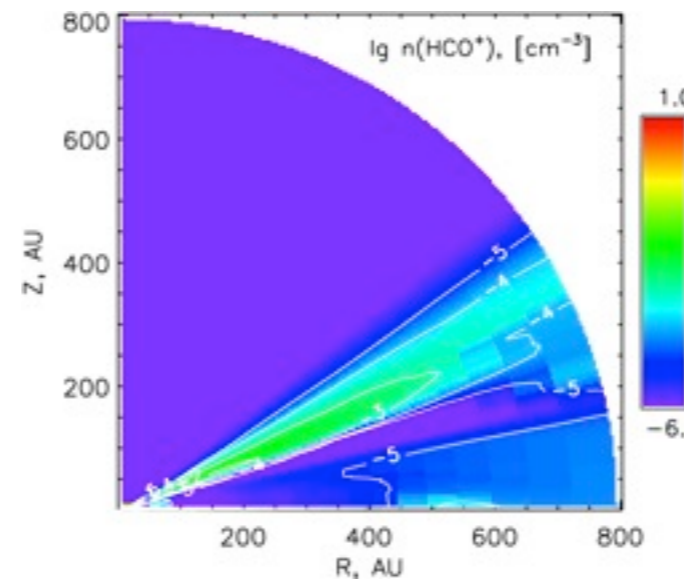
Uniform abundances,  
radial T-gradient



Uniform abundances,  
2D T-gradient



Chemical abundances,  
2D T-gradient

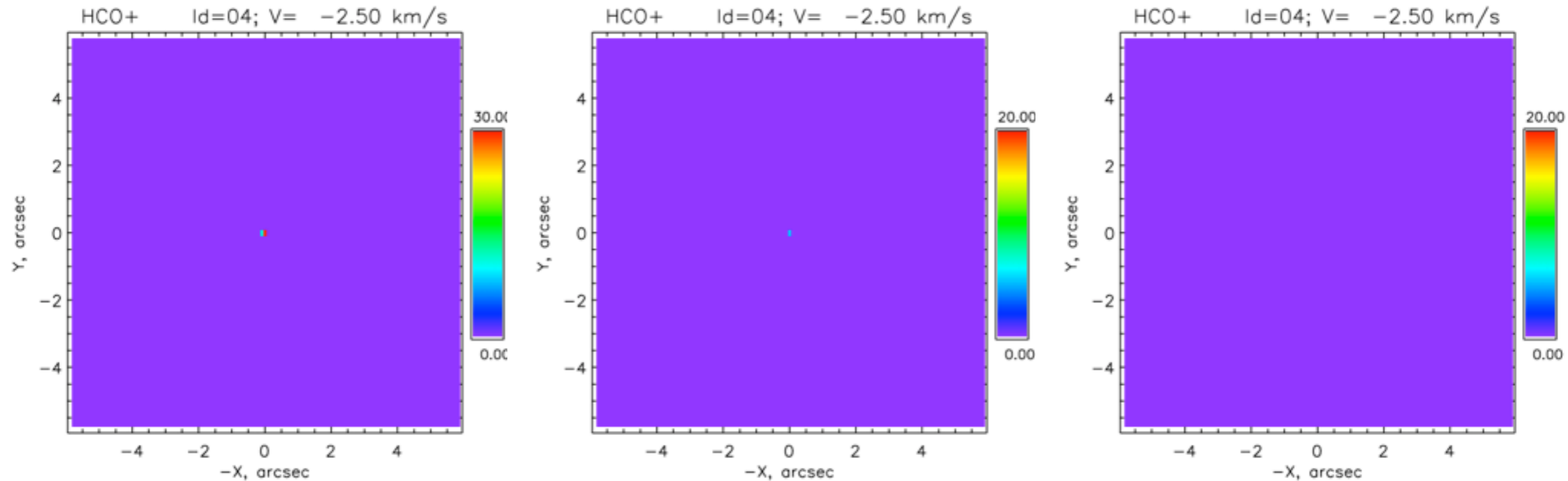


# Channel maps of HCO<sup>+</sup> (4-3)@ 20°

“UNIFORM”

“THERMAL”

“CHEMICAL”



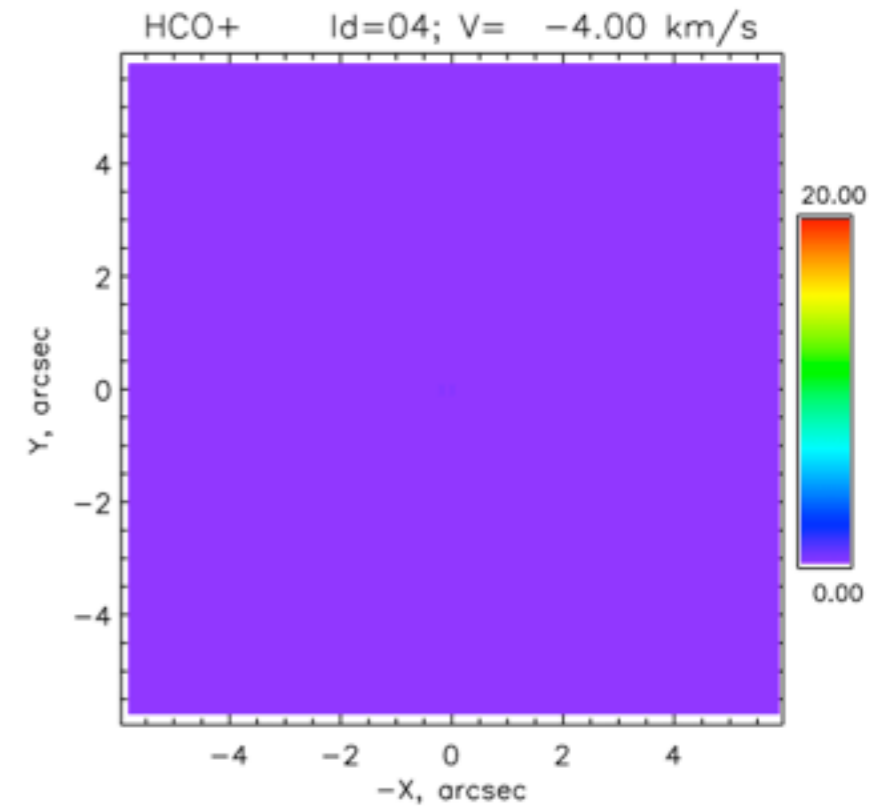
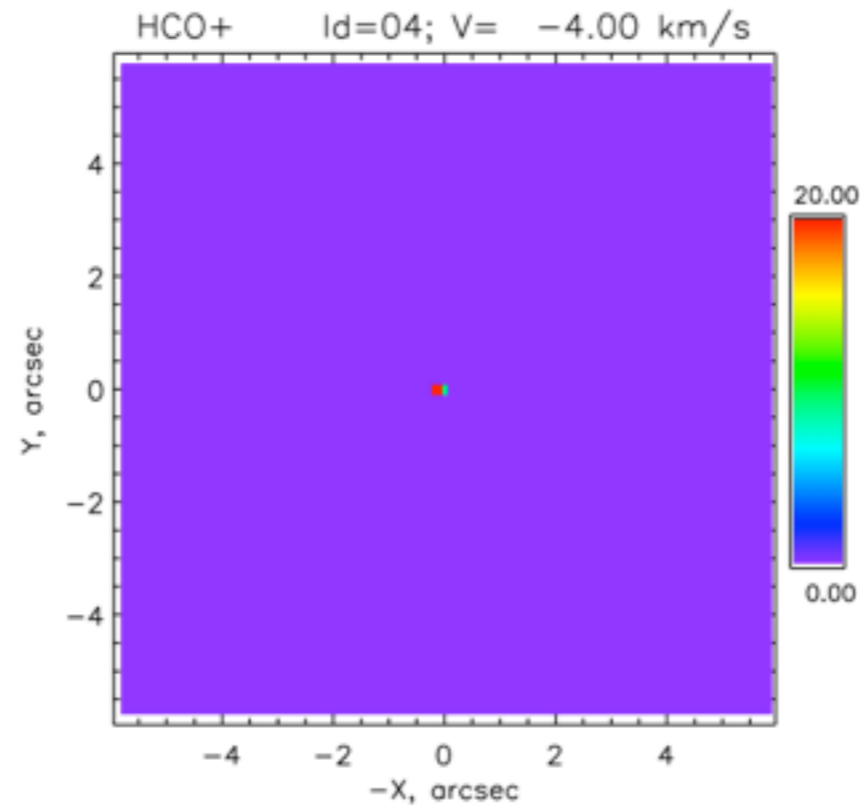
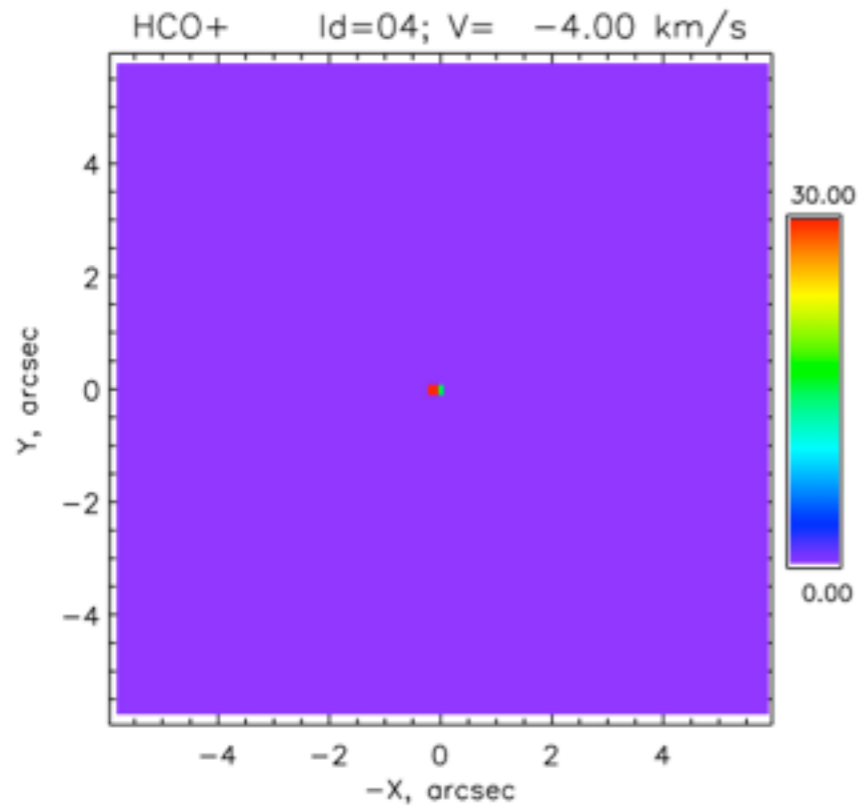
Face-on disks: no big difference

# Channel maps of HCO<sup>+</sup> (4-3)@ 60°

“UNIFORM”

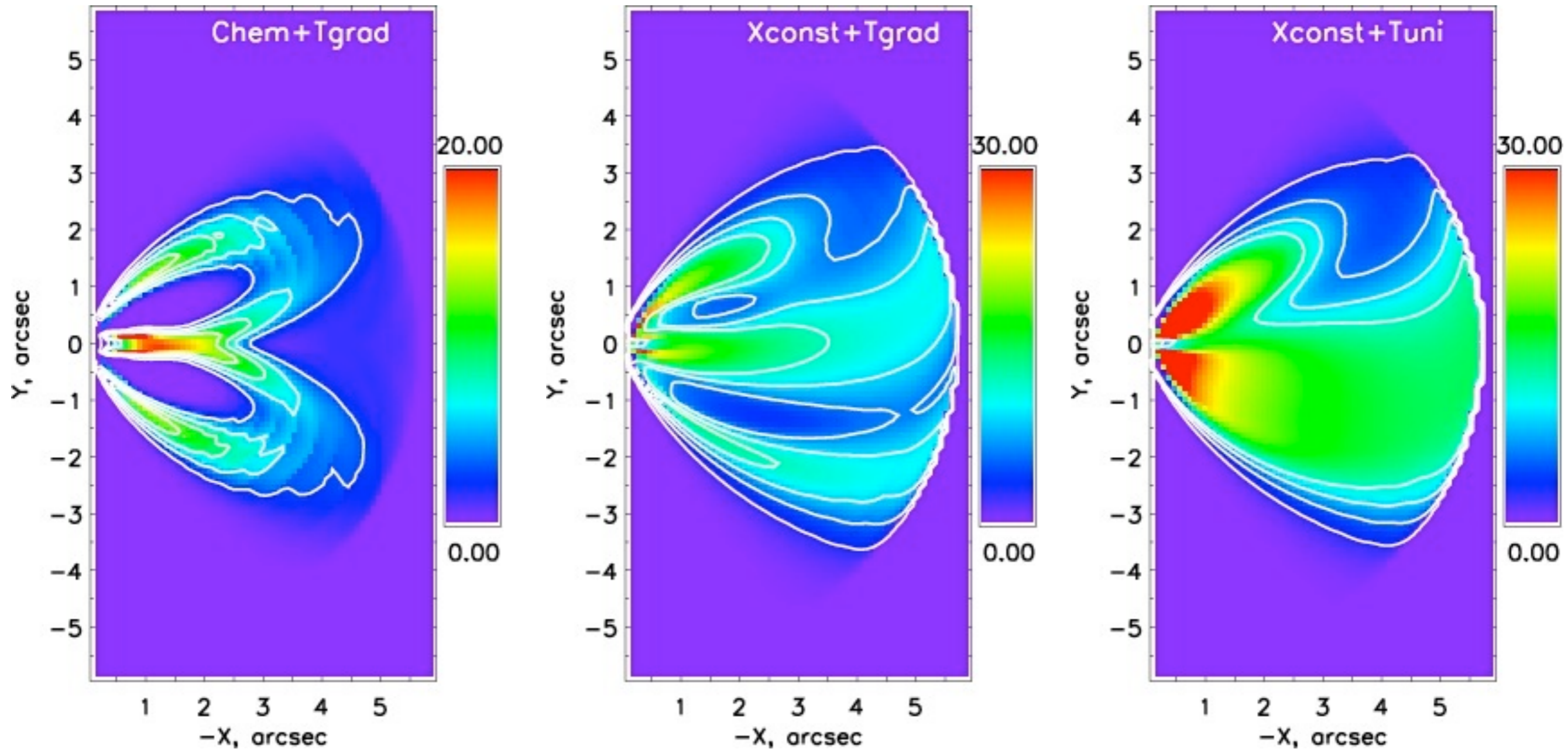
“THERMAL”

“CHEMICAL”



Edge-on disks: molecular layers & T-gradients become visible

# Chemical vs. Temperature Gradients: 0.68 km/s channel of HCO+ (4-3)@ 60°

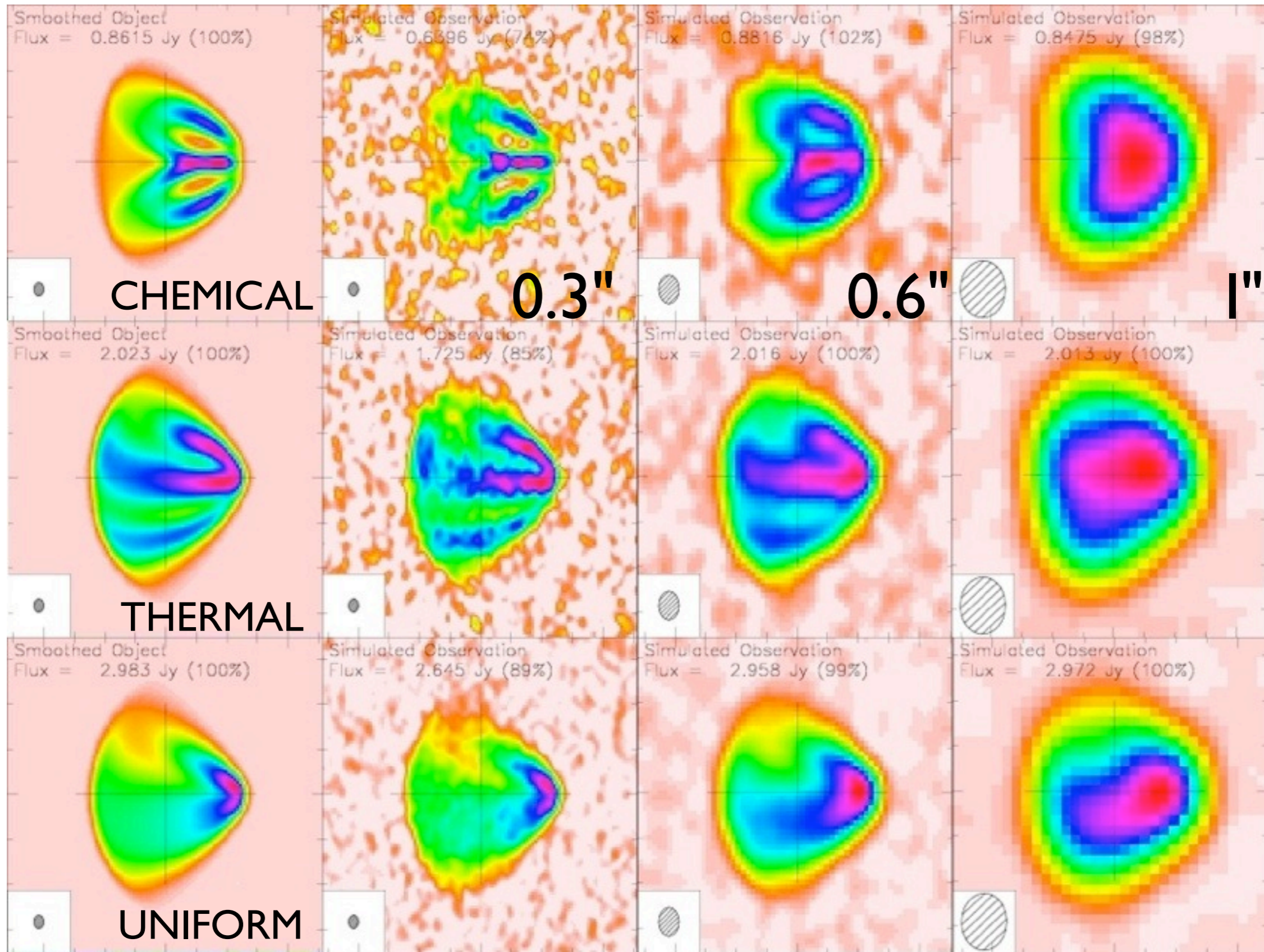




# ALMA simulations

Ideal image

Reconstructed images



# ALMA simulations (other transitions, disk sizes, and inclinations)

SPECIES	FREQUENCY (GHz)	BANDWIDTH (kHz)	$R_{\text{disk}} = 800 \text{ AU}$		$R_{\text{disk}} = 250 \text{ AU}$	
			$i = 20^\circ$	$i = 60^\circ$	$i = 20^\circ$	$i = 60^\circ$
			HCO <sup>+</sup> (1–0) .....	89	30	Zoom-c (4 hr) <sup>a</sup>
C <sup>18</sup> O(2–1) .....	220	75	Zoom-d (1 hr)	Zoom-c (<0.5 hr)	Zoom-c (4 hr)	Zoom-c (10 hr)
<sup>13</sup> CO(2–1) .....	220	75	Zoom-d (<0.5 hr)	Zoom-d (<0.5 hr)	Zoom-c (2 hr)	Zoom-c (3.5 hr) <sup>a</sup>
CS(5–4) .....	245	80	Zoom-e (3 hr)	Zoom-d (12 hr)	Zoom-b (>12 hr)	Zoom-b (>12 hr)
HCN(3–2) .....	266	90	Zoom-e (<0.5 hr)	Zoom-d (1 hr)	Zoom-c (4 hr)	Zoom-b (>12 hr)
HCO <sup>+</sup> (4–3) .....	357	120	Zoom-d (<0.5 hr)	Zoom-e (<0.5 hr)	Zoom-c (2 hr)	Zoom-c (3 hr)
HCO <sup>+</sup> (7–6) .....	624	210	Zoom-e (<0.5 hr)	Zoom-e (1.5 hr)	Zoom-c (12 hr)	Zoom-d (>12 hr)
<sup>13</sup> CO(6–5) .....	661	220	Zoom-e (<0.5 hr)	Zoom-e (1 hr)	Zoom-d (1 hr)	Zoom-c (6 hr)

Thermal gradients and chemical stratification in disks will become observable