

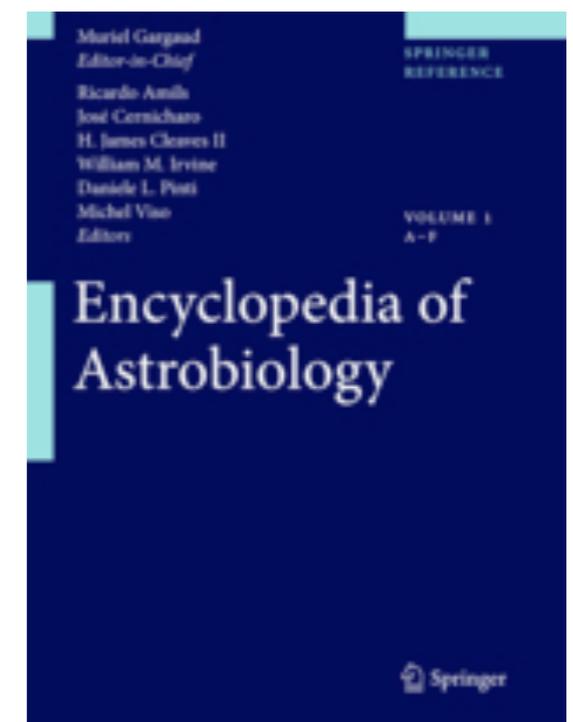
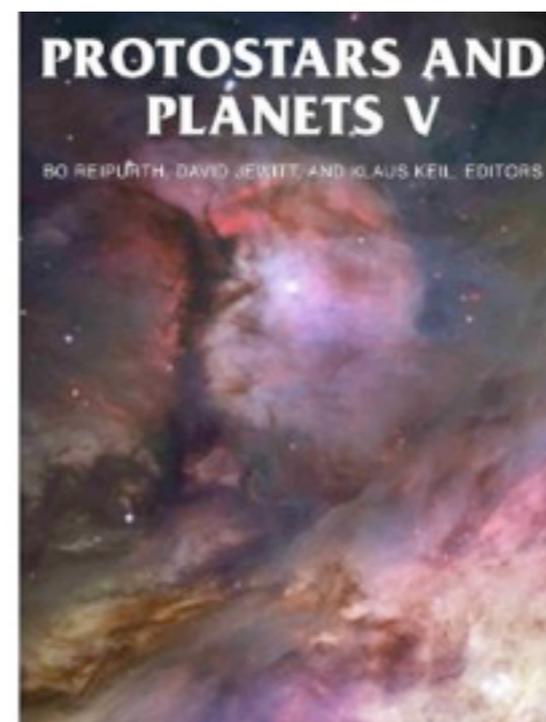
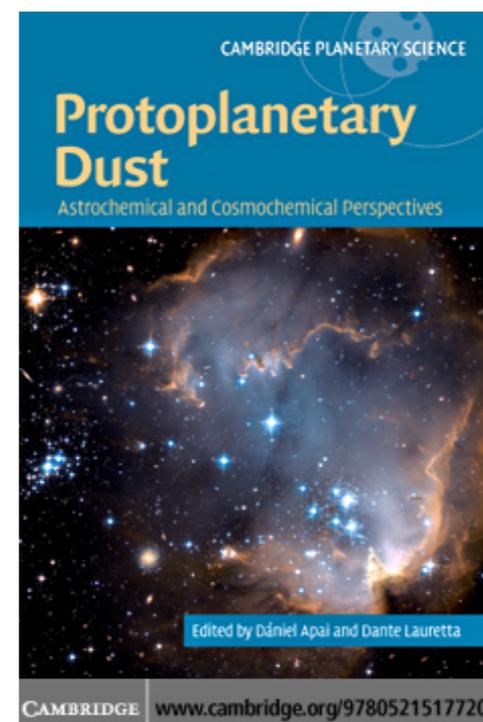
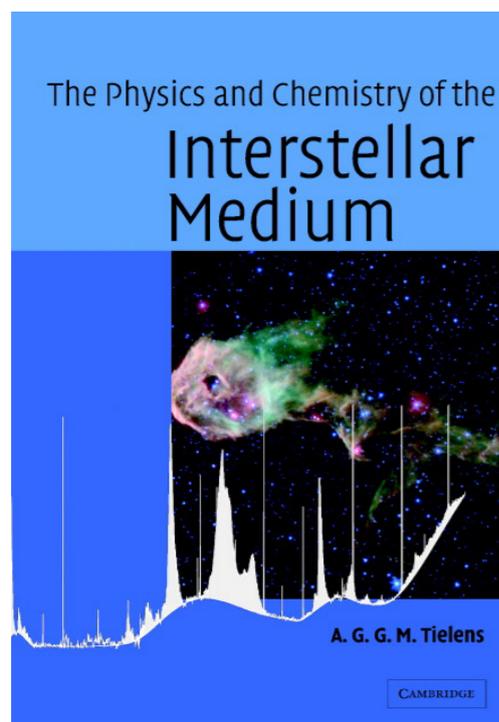
Gas in protoplanetary disks

Dmitry Semenov
Max Planck Institute for Astronomy
Heidelberg, Germany



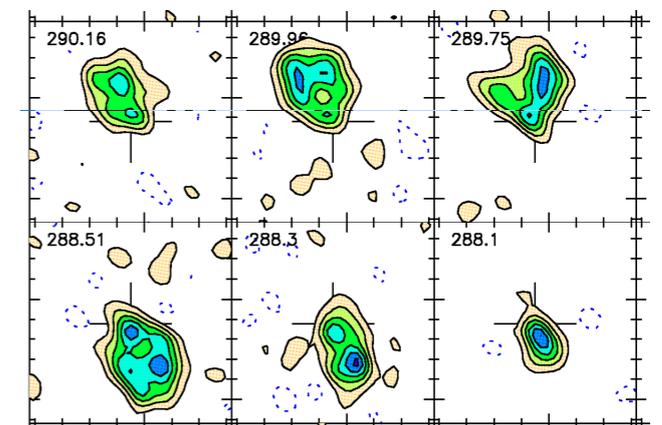
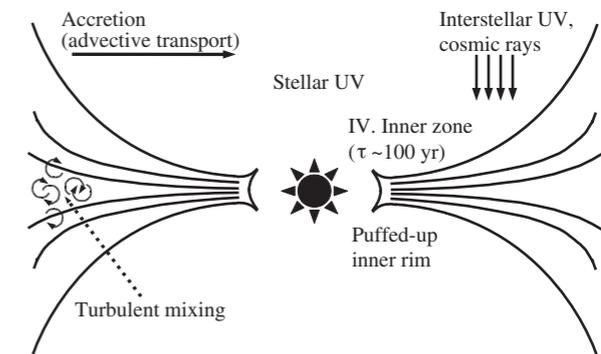
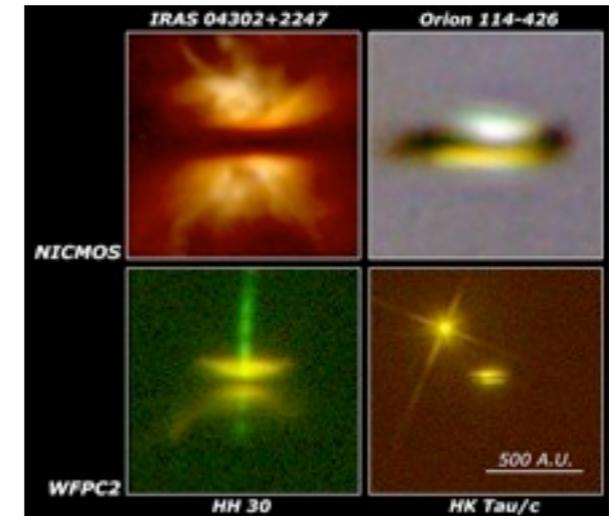
Suggested literature

- 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: $\sim 10^6$ (~ 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

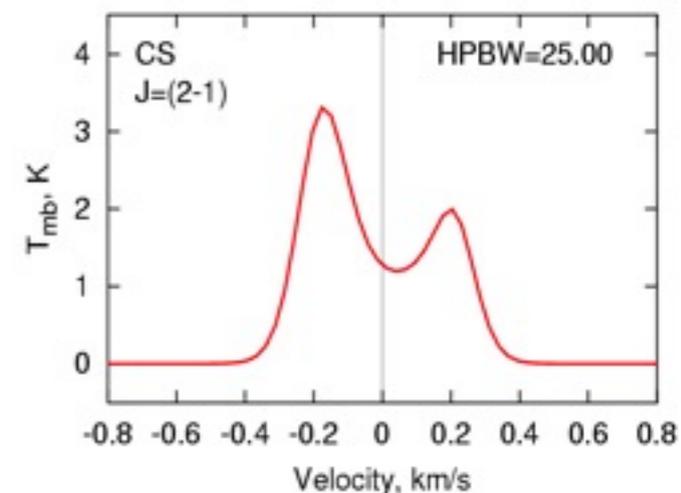
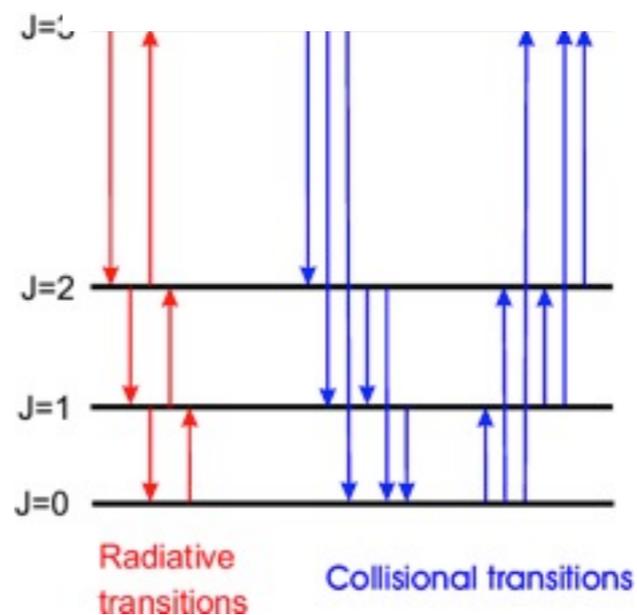
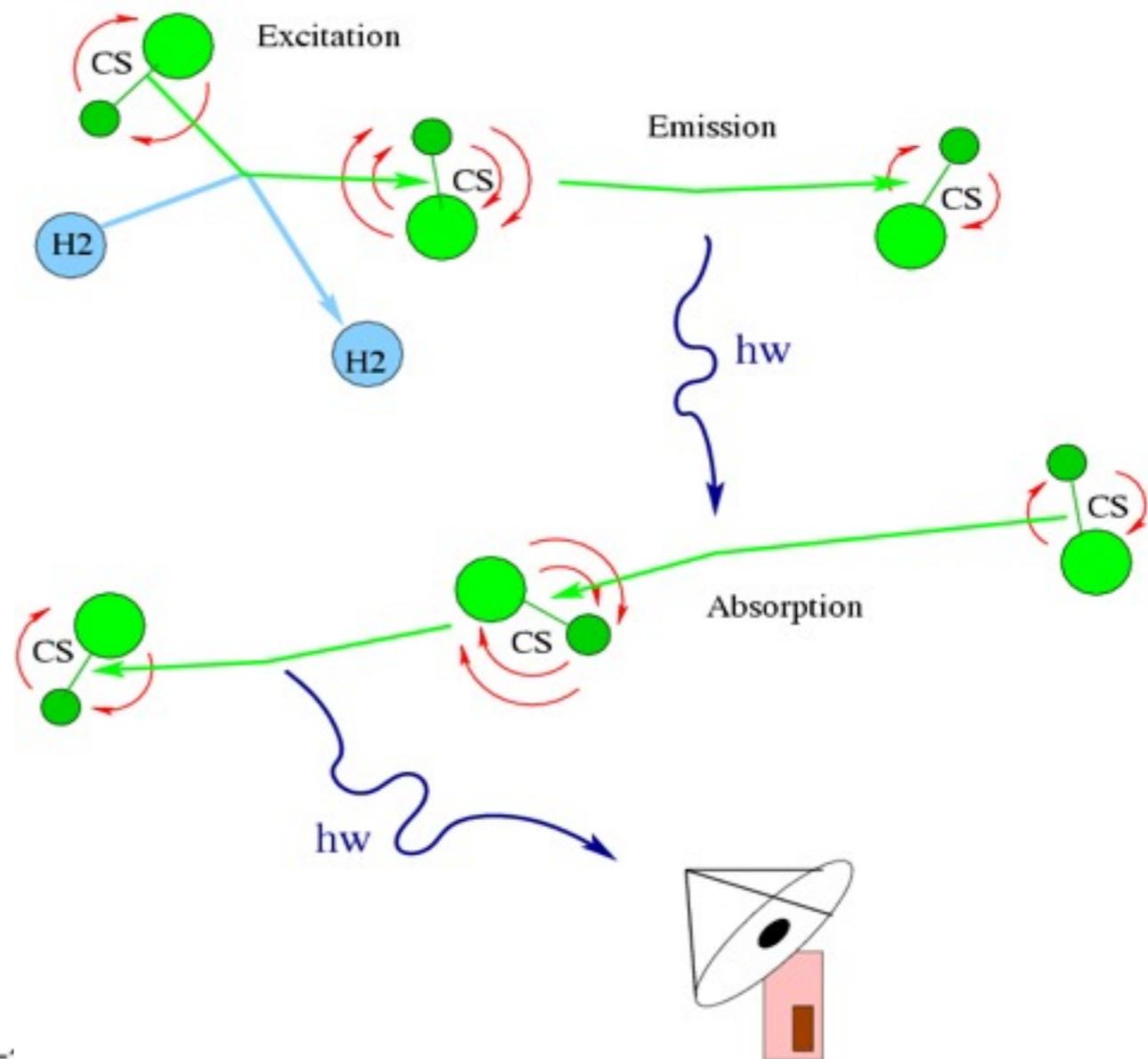


- Plateau de Bure interferometer, Submillimeter Array, Very Large Array, CARMA, ATCA
- IRAM 30-m, Apex 12-m, Effelsberg 100-m, Aresibo 100-m, JCMT 15m, Nobeyama 45-m

I. Basics of line excitation and line analysis

Analysis of emission line data

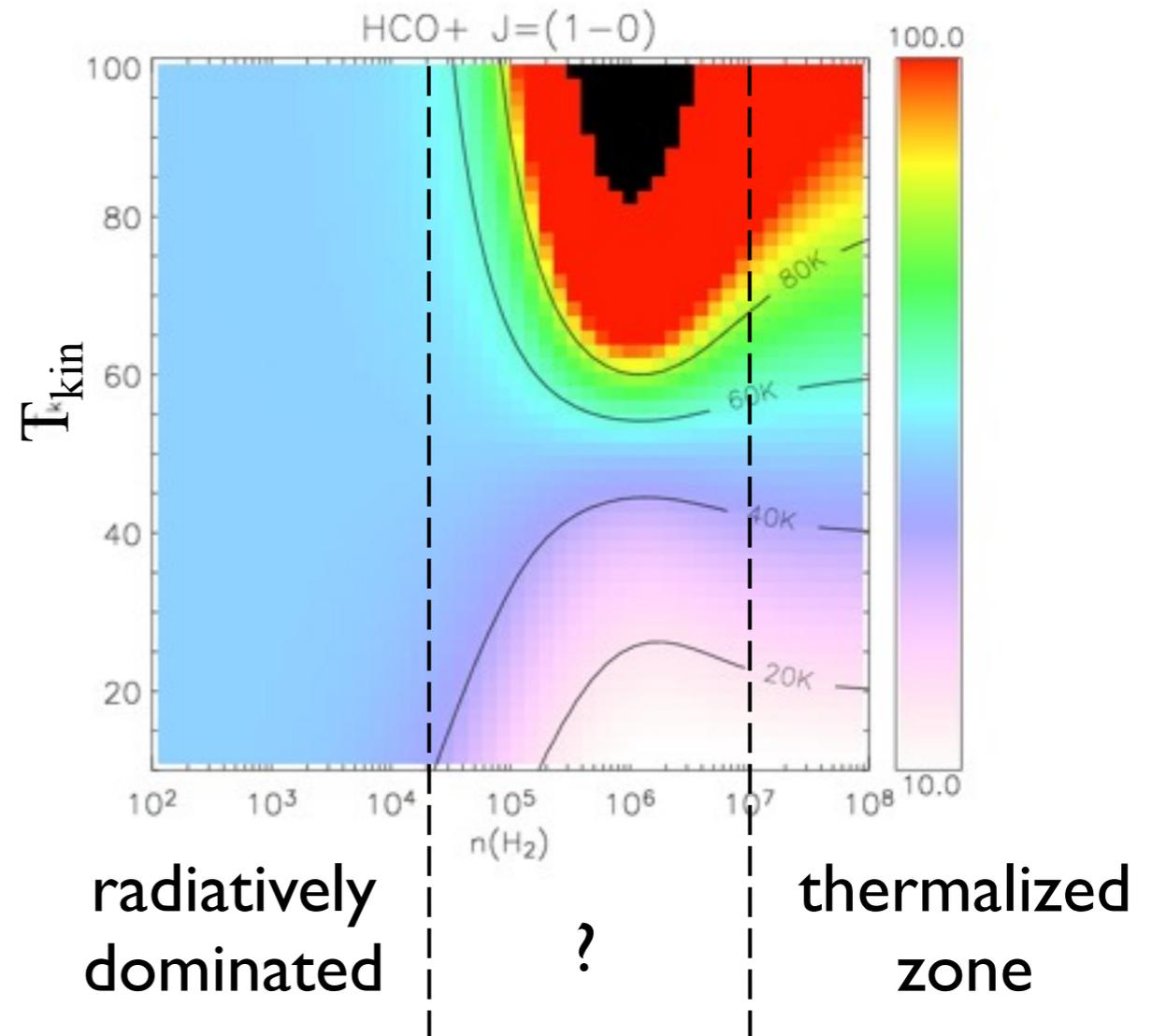
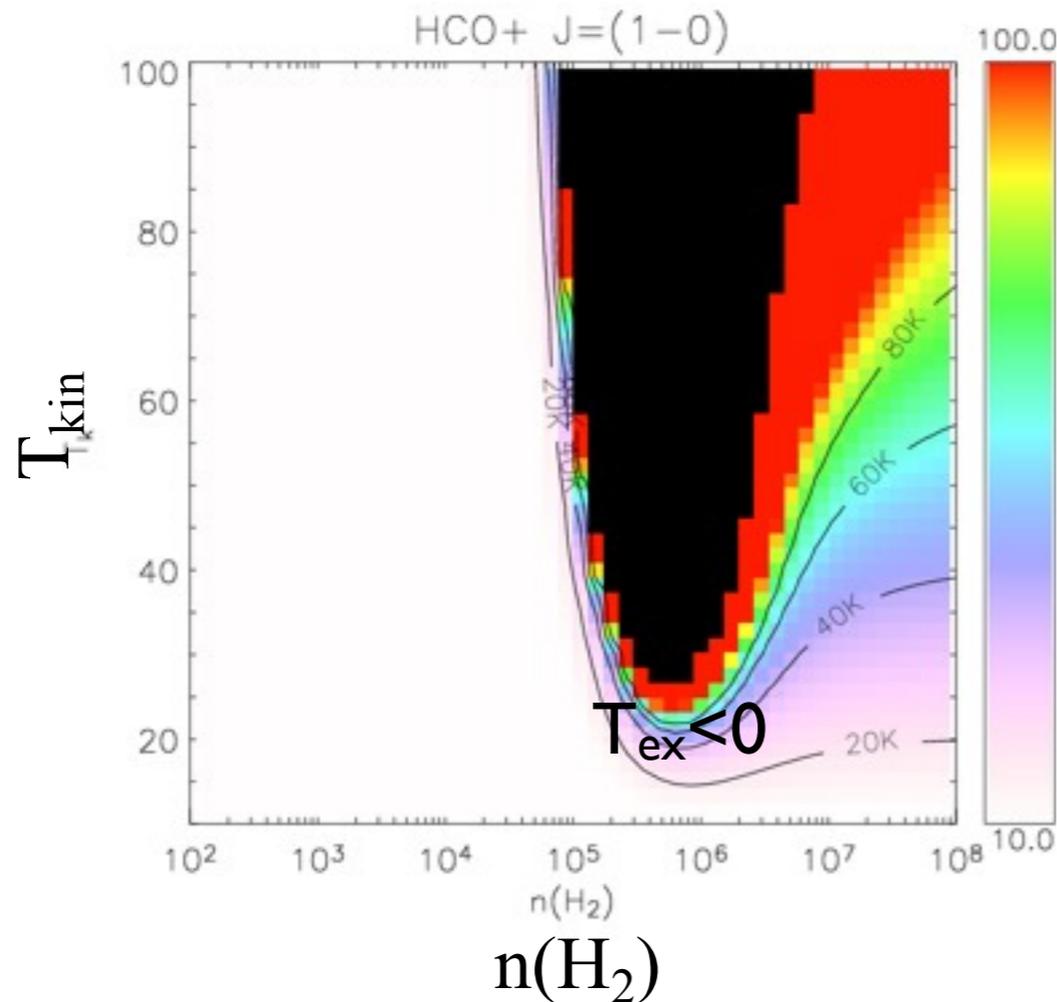
- n, T + chemistry + excitation + kinematics + radiative transfer: line
- Excitation: radiation & collisions
- Excitation & RT: non-local problem
- 6D: 3D n, T + 1D v + 2D sky plane
- Incomplete coverage of (u, v) plane
- Optically thick lines: Intensity $\sim T_{\text{exc}}$ (^{12}CO , H_2O)
- Optically thin lines: Intensity $\sim \tau^* T_{\text{exc}}$



Excitation temperatures: HCO⁺(1-0)

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

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



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

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

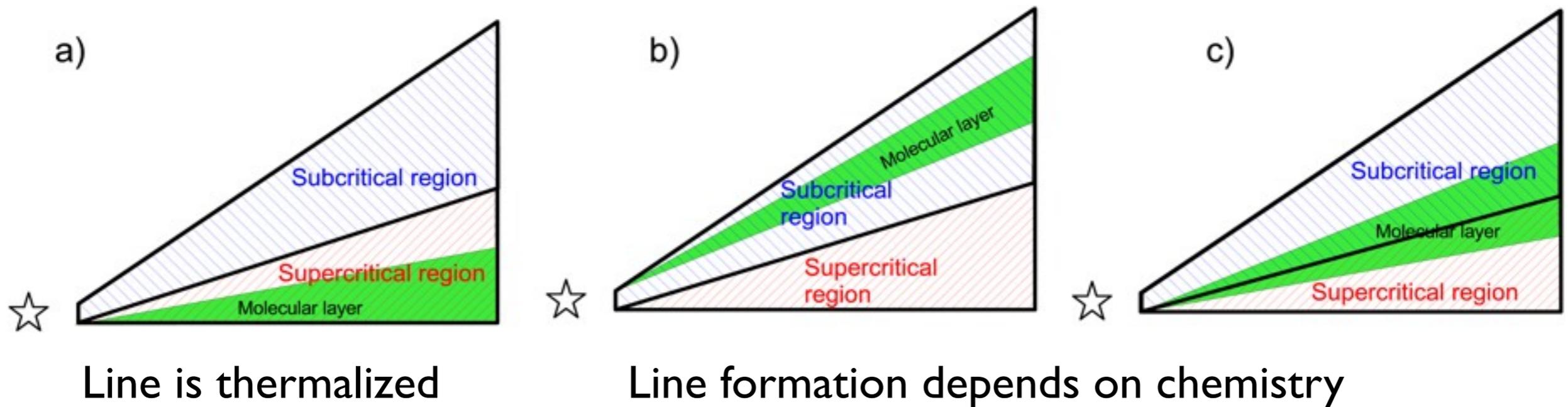
Non-LTE

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

LTE

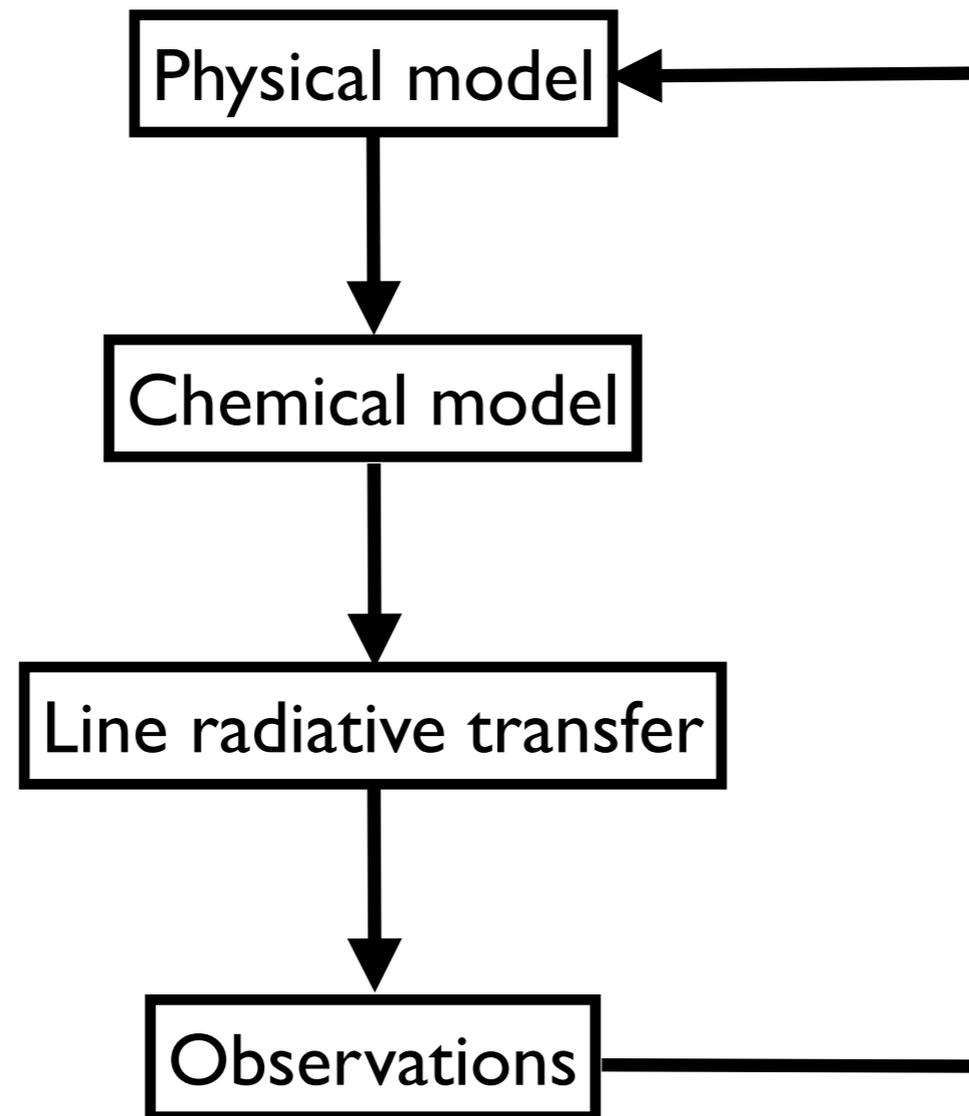
Excitation conditions in PPDs

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

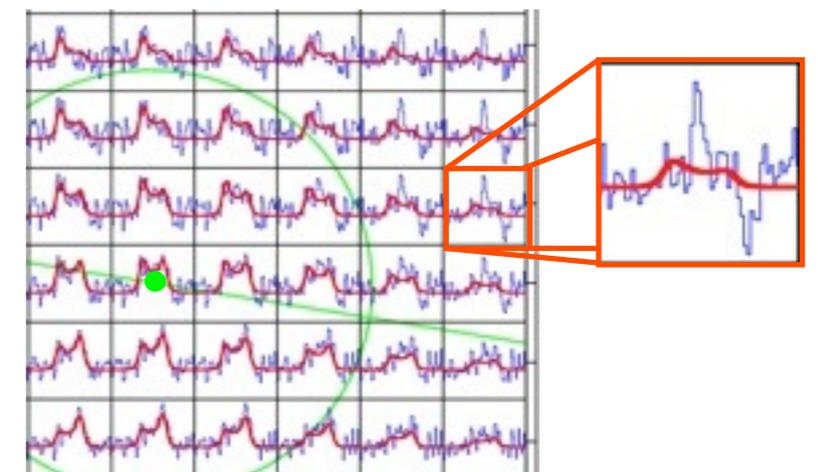
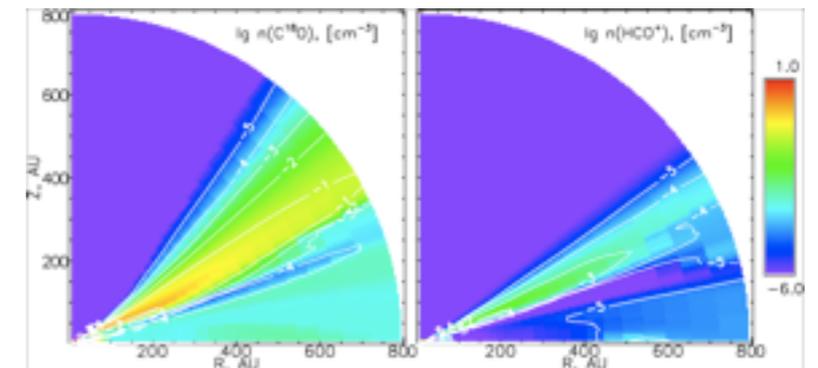
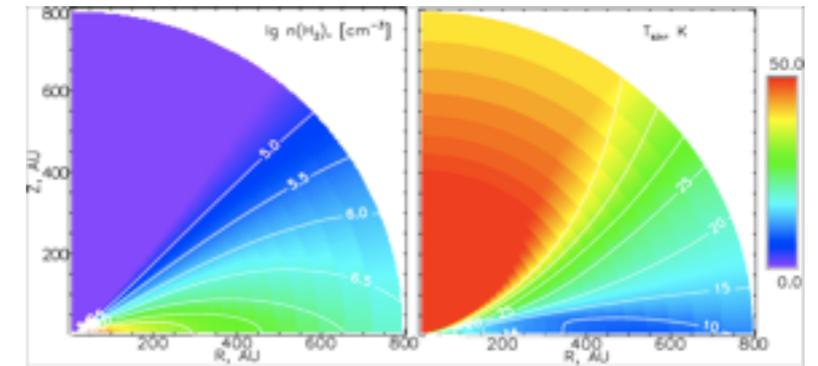


- Molecules in disks populate dense regions: $n_{\text{H}} > 10^5 - 10^6 \text{ cm}^{-3}$
- Thermalized: low-lying transitions of observed molecules
- Asymmetric molecules have perplex level structure: H_2O
- High-lying transitions: LTE or non-LTE?

Analysis of emission line data



Iterative fitting



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

http://www.astrochymist.org/astrochymist_mole.html

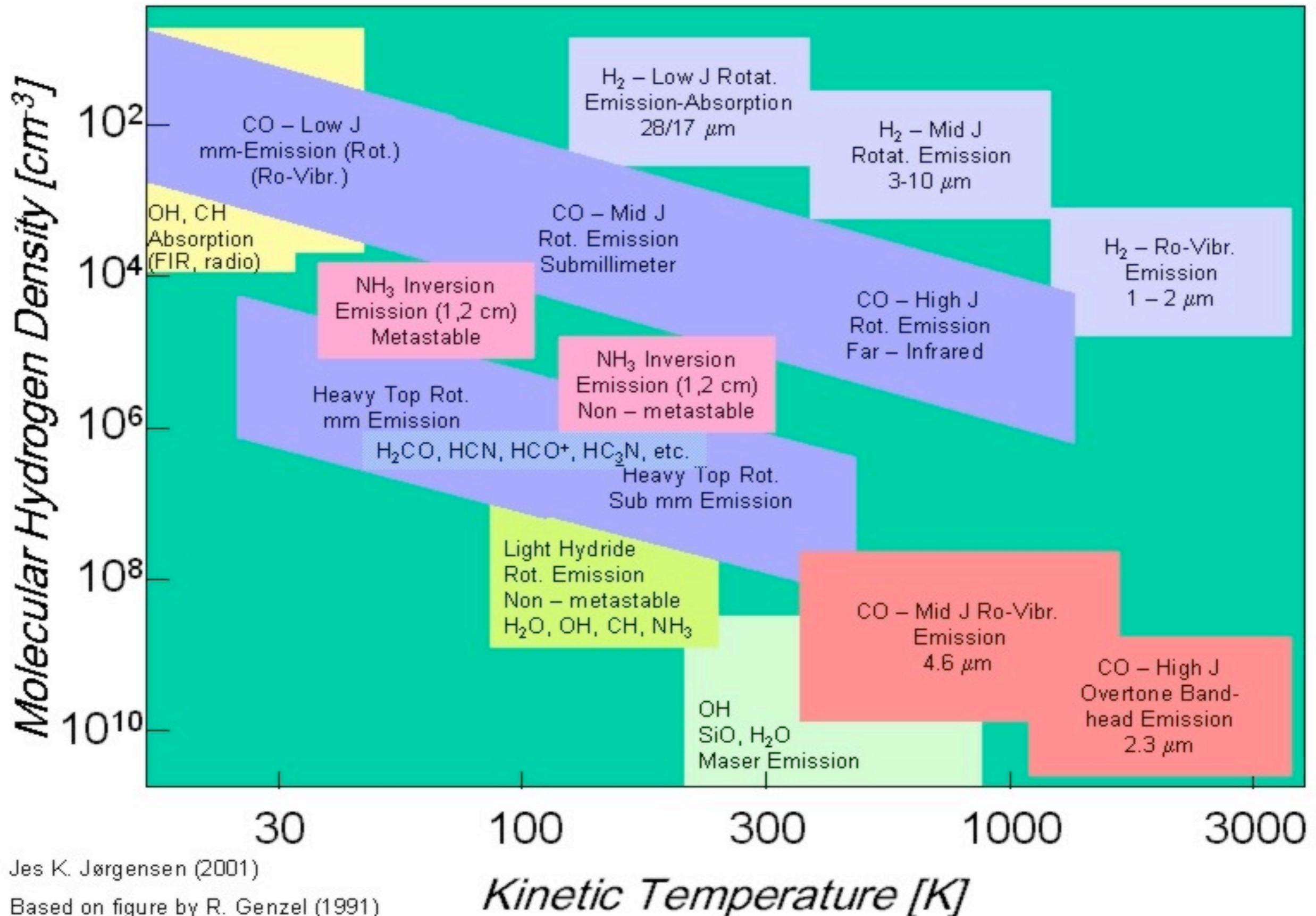
<http://www.astro.uni-koeln.de/cdms/molecules>

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⁺, DCO⁺, CN, HCN, DCN, HNC, N₂H⁺,

H₂CO, CS, HDO, C₂H₂, CO₂, OH, H₂O, Ne, Fe, Si, H₂

Molecules as probes of T and n_H



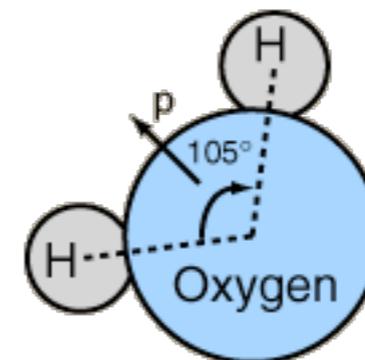
Jes K. Jørgensen (2001)

Based on figure by R. Genzel (1991)

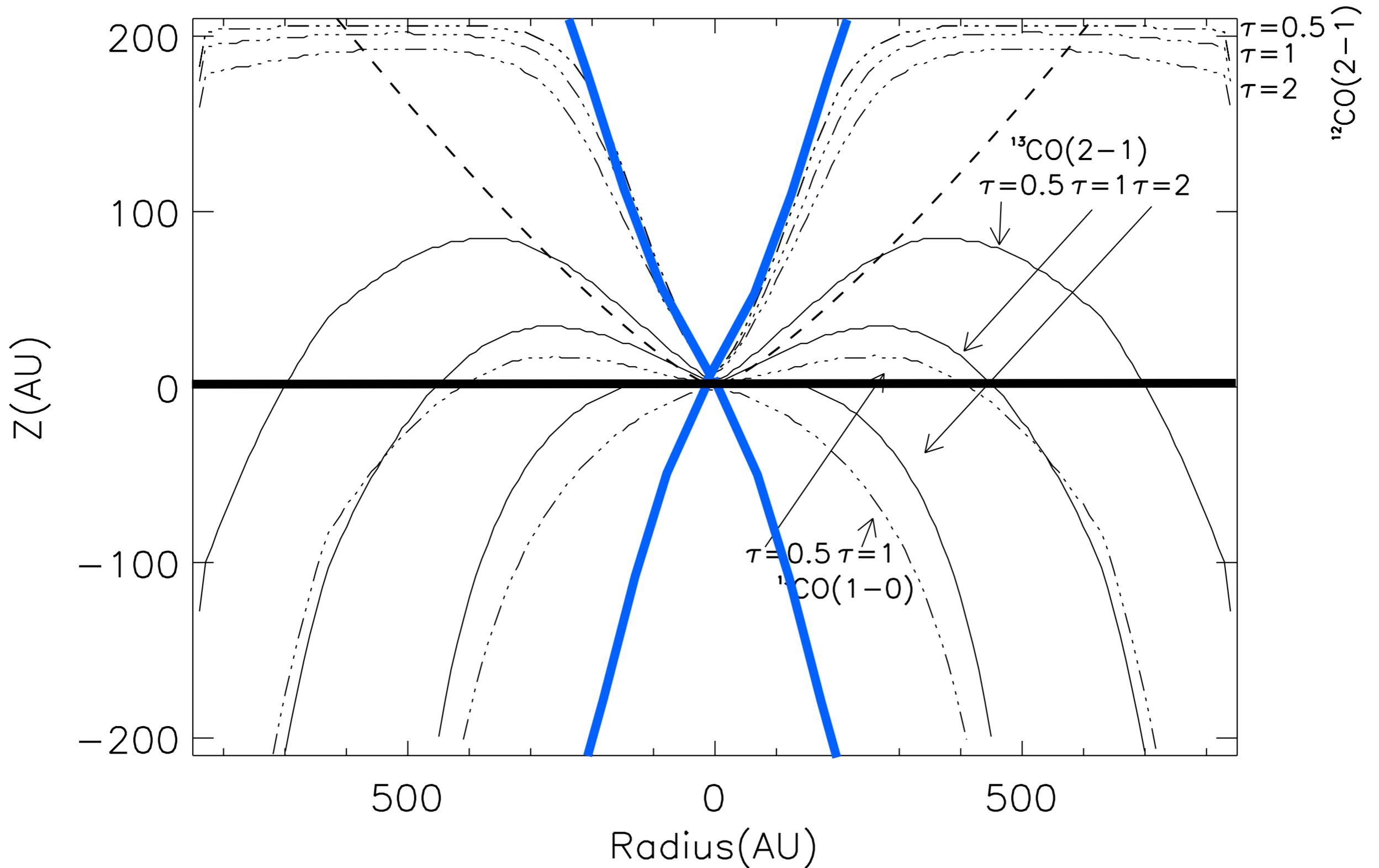
Other molecular tracers

Tracer	Quantity
^{12}CO , ^{13}CO	Temperature
H_2	—
NH_3	—
CS , H_2CO	Density
CCH , HCN , CN	Photochemistry
HCO^+	Ionization
N_2H^+ , H_2D^+	—
C^+	—
Metal ions	—
Complex organics	Surface processes
DCO^+ , DCN , H_2D^+	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

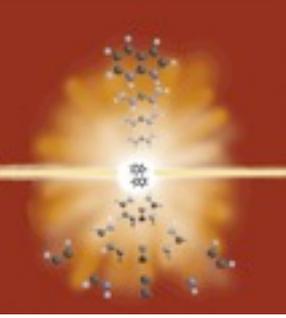


CO isotopologues in disks: $T_{\text{kin}}(z)$





Reactions in disks



Radiative association:



Surface reactions:



Neutral-neutral:



Ion-molecule:



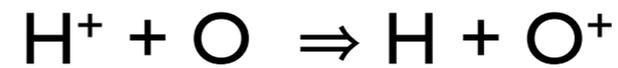
Ionization:



Photodissociation:



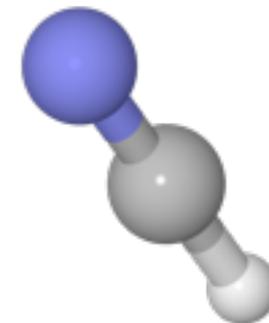
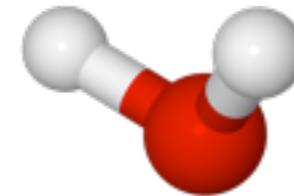
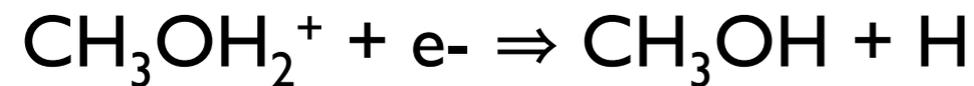
Charge exchange:



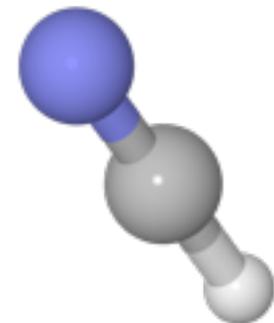
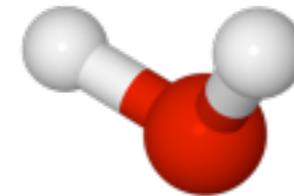
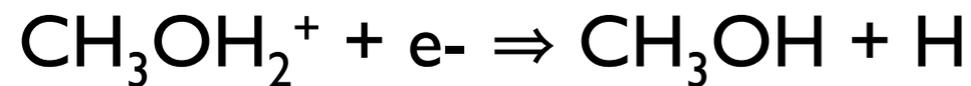
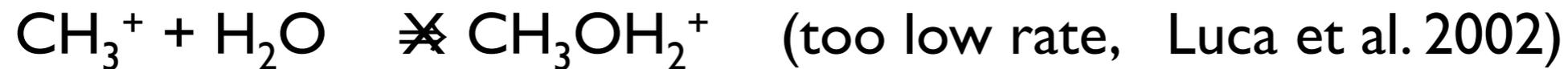
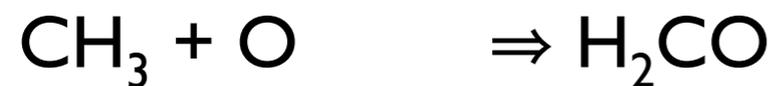
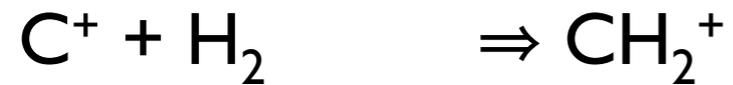
Dissociative recombination: $\text{H}_3\text{O}^+ + e^- \Rightarrow \text{H}_2\text{O} + \text{H}$

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

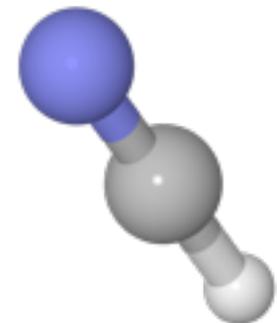
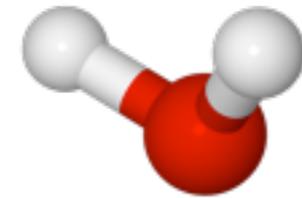
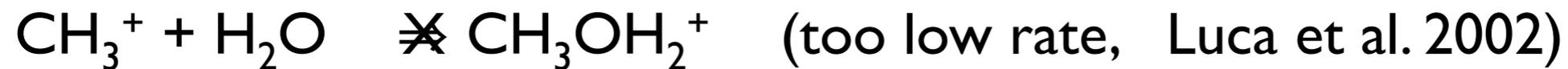
Gas-phase formation of complex molecules



Gas-phase formation of complex molecules



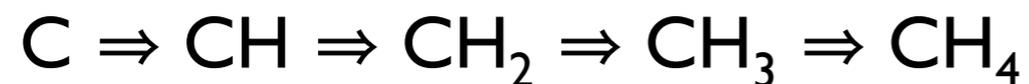
Gas-phase formation of complex molecules



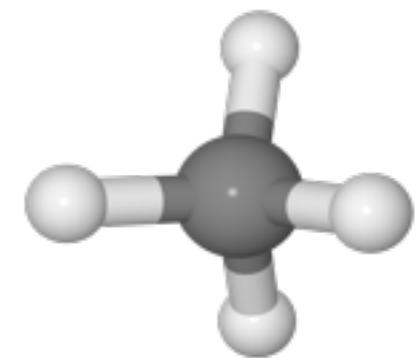
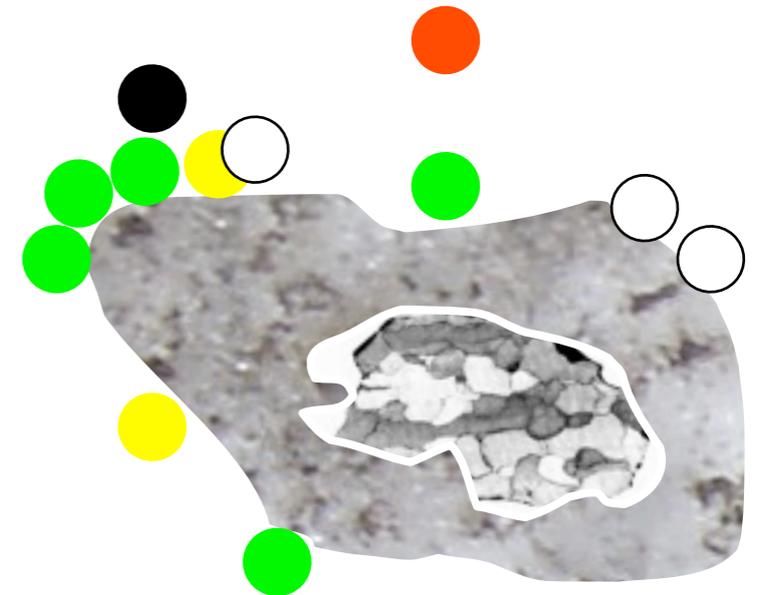
Surface formation of complex molecules

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

Surface chemistry:



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

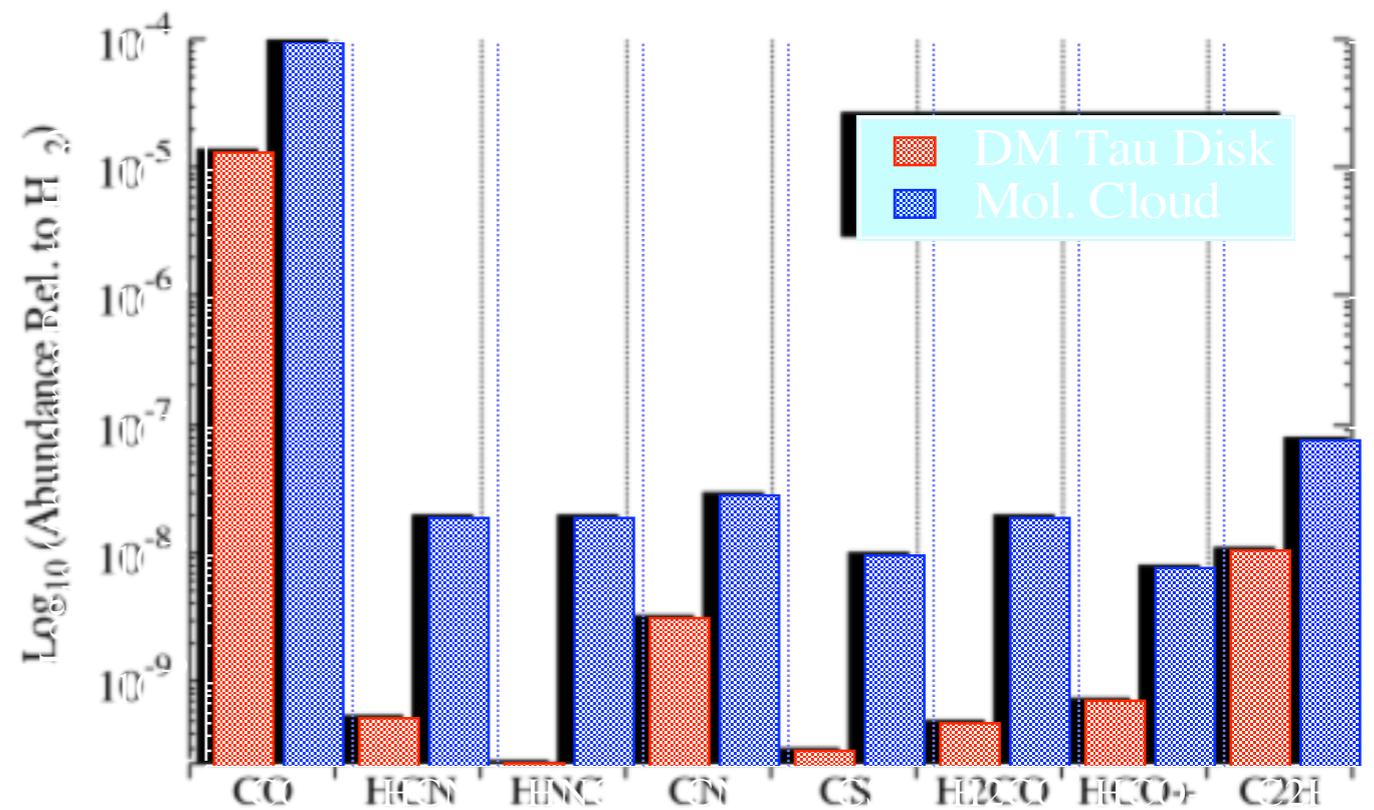


III. Observations of molecules in PPDs

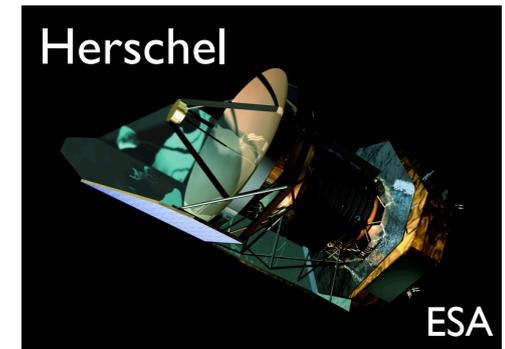
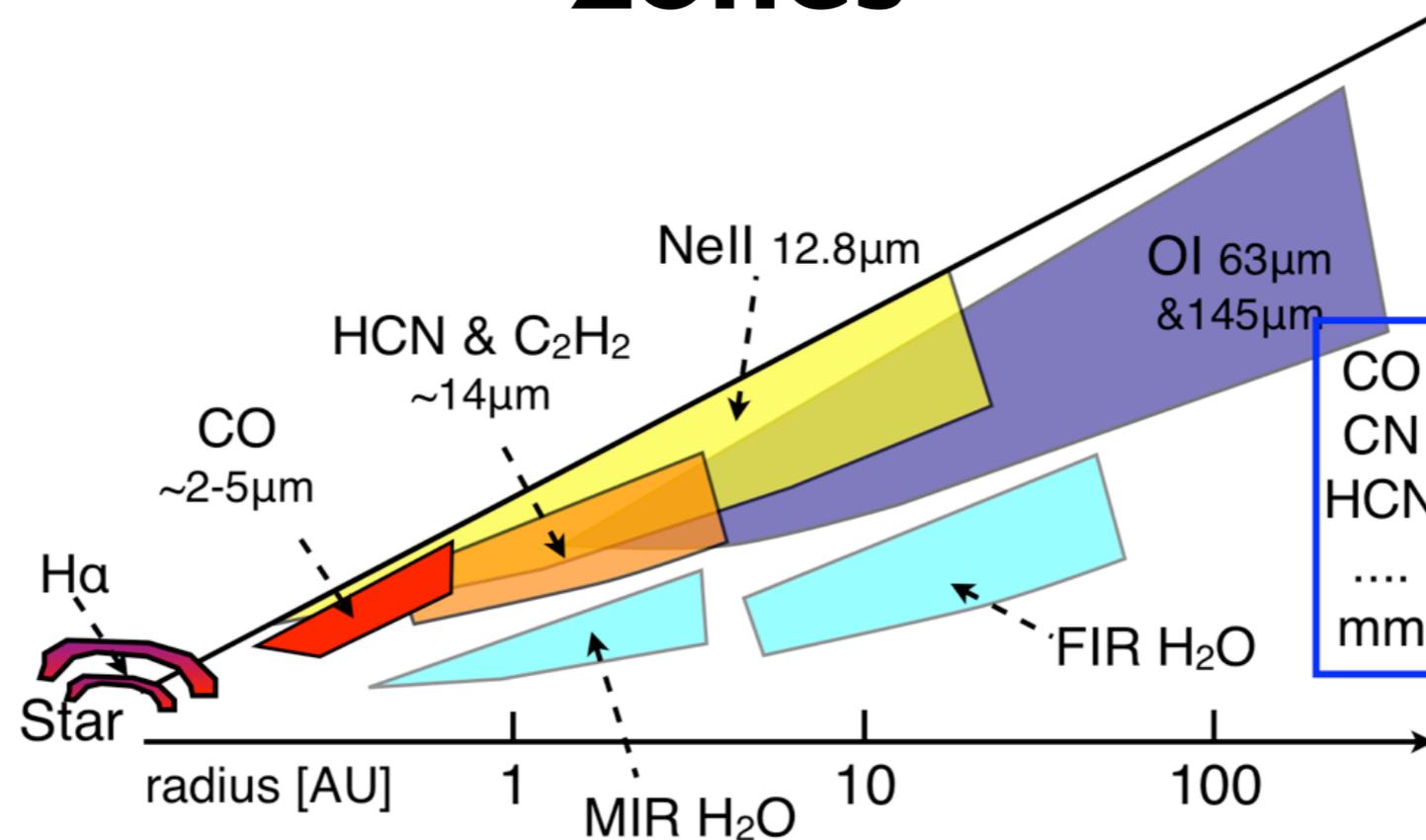
- IR (space) spectroscopy:
 - inner regions: <20 AU
 - rotational/vibrational lines
 - absorption/emission
 - Boltzmann diagrams, LTE, T_{kin}
- (Sub-)millimeter observations:
 - outer regions: >50–100 AU
 - rotational/vibrational lines
 - emission lines
 - antennas: no spatial information, surveys
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

Observational findings: outer disks

- Gas: depletion of molecules
- Ices: H_2O , NH_3 , CH_4 , H_2CO , CH_3OH
- Vertical gradients of T
- Photo-dominated chemistry
- Cold CO, CCH, HCN
- "Dry" interiors: where is water?
- Keplerian rotation
- Non-thermal line broadening

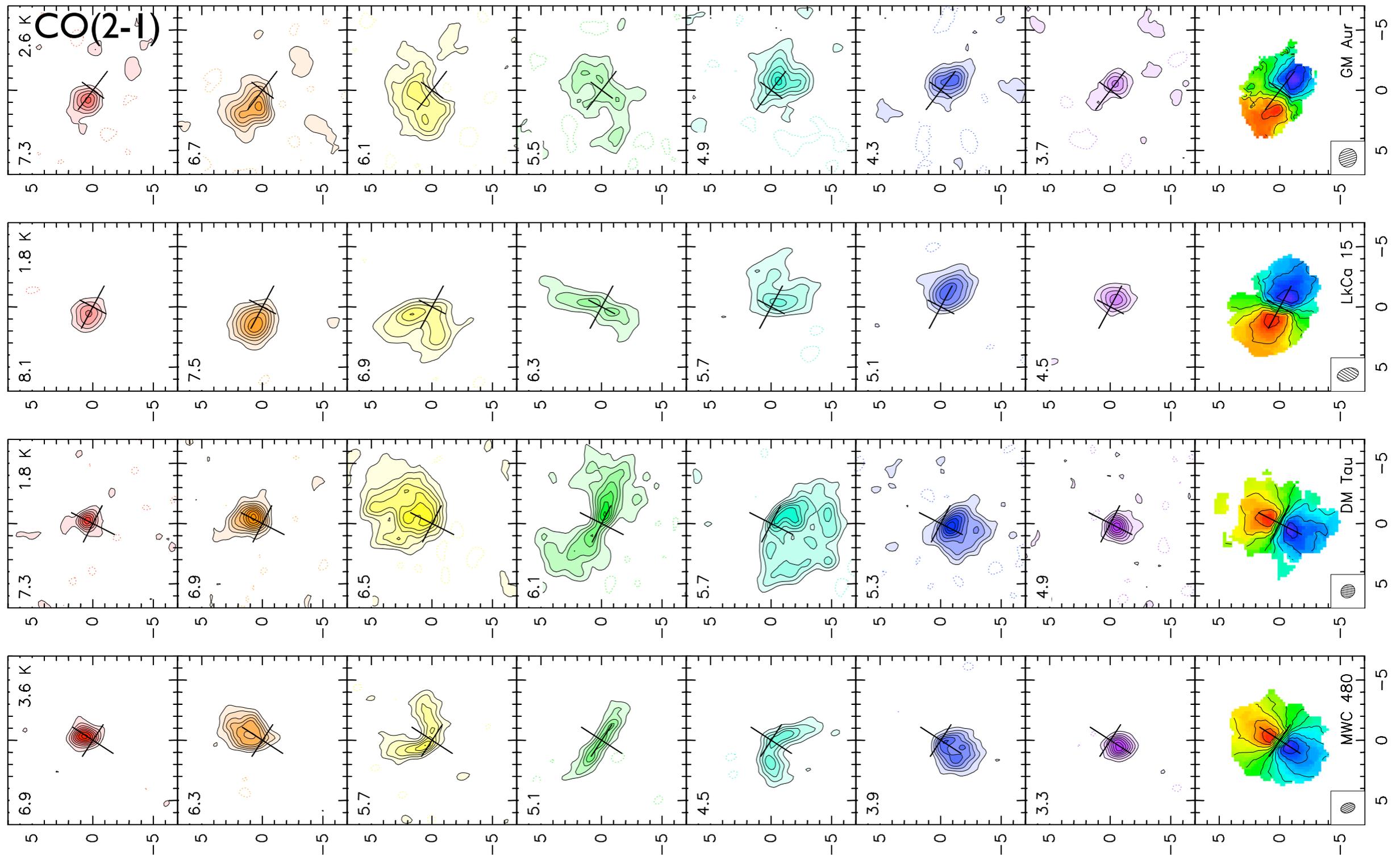


IR revolution: molecules in planet-forming zones



- Nell, Fell, OI, H₂, OH, H₂O, CO₂, HCN and C₂H₂
- Warm gas: $T \gtrsim 100 - 5000 \text{ K}$
- No depletion
- Non-Keplerian profiles: disk wind?
- Herbig Ae disks appears to be deficient in H₂O and organics

Kinematics: weighting stars



- M_* from high SNR measurements of Ω_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

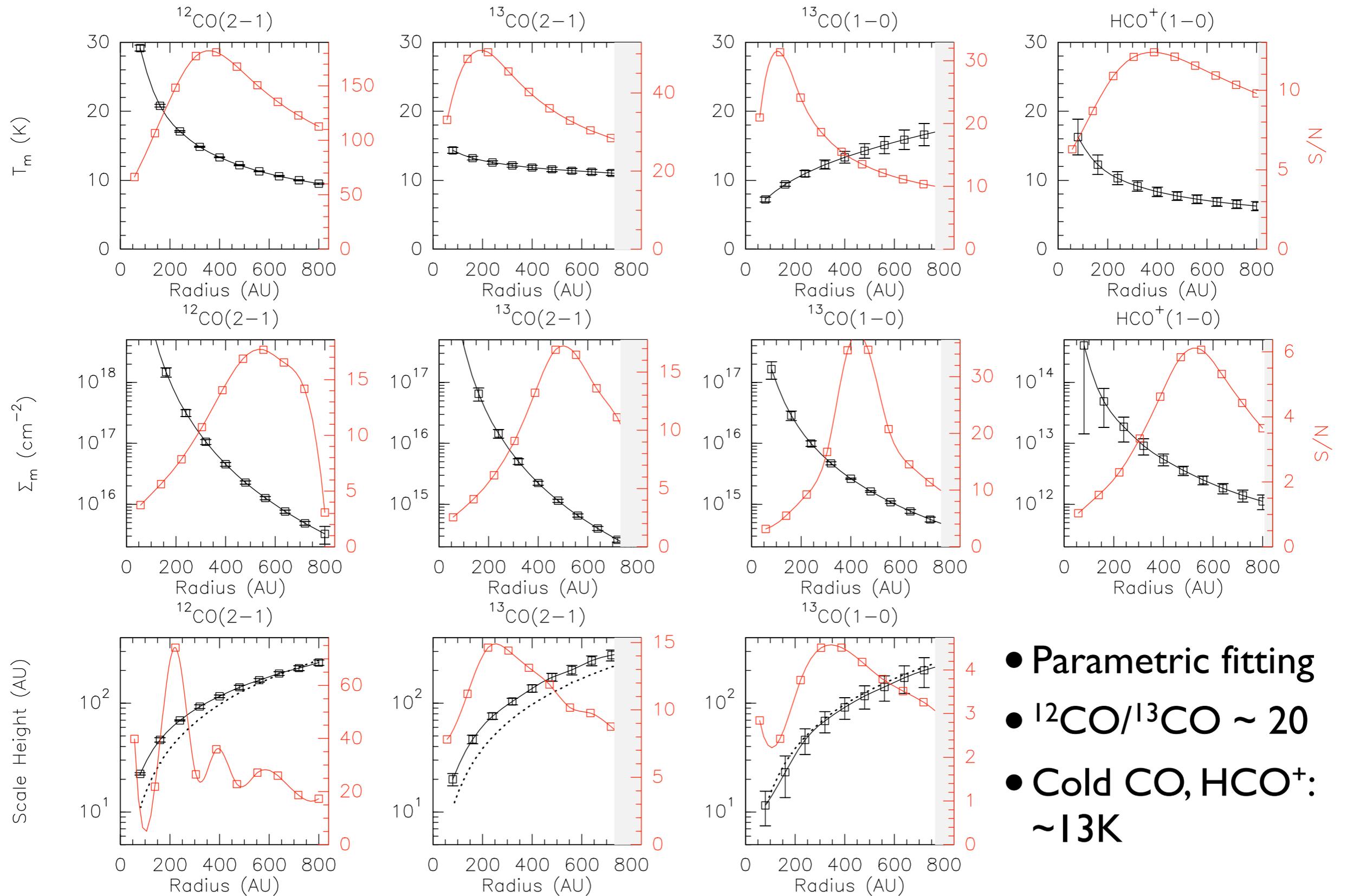


- Limited sample: large, face-on disks (~6)
- Lines are weak: ~0.3–3K (0.1–1Jy)
- 1 line: ~1–10 hours



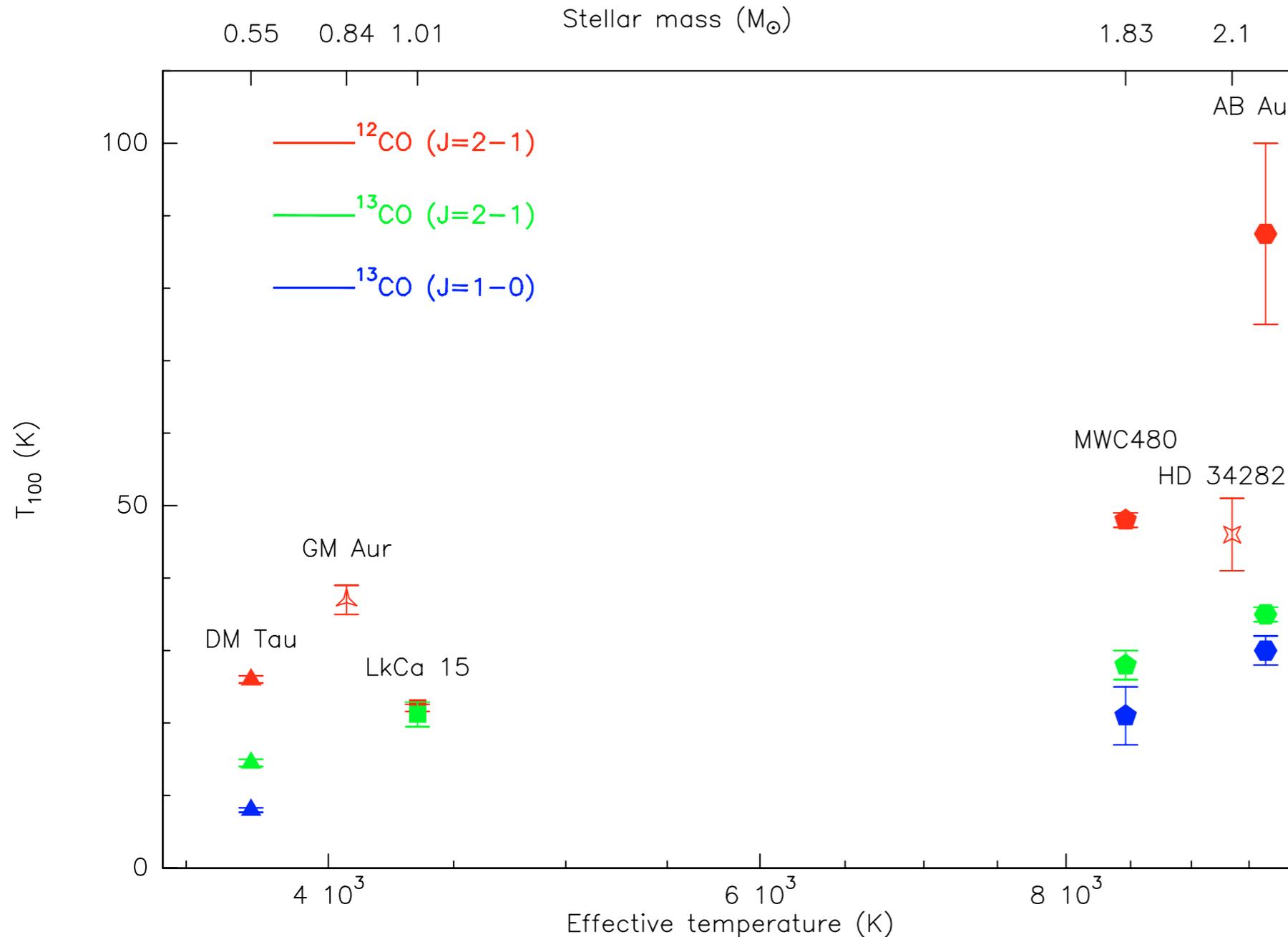
- Herbig Ae: CO, HCO⁺, CN, HCN
- T Tau: CO, HCO⁺, HCN, N₂H⁺, CCH, CS, H₂CO, DCO⁺, DCN

Resolved surface density & T: DM Tau



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

Temperature in T Tau and Herbig Ae disks



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

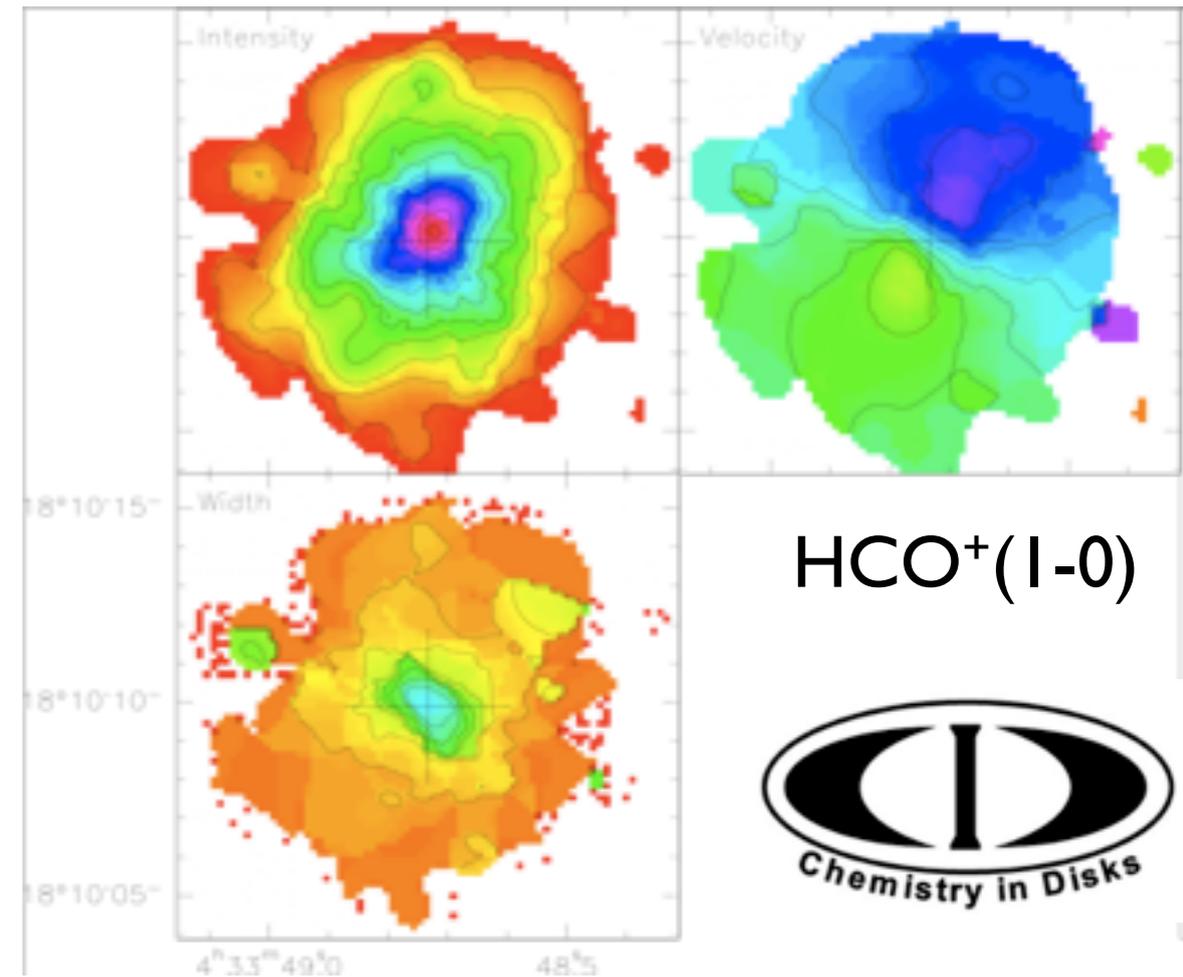
- "Cool" T Tauri disks:
 $T_{\text{kin}} \sim 10\text{--}30\text{K}$

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

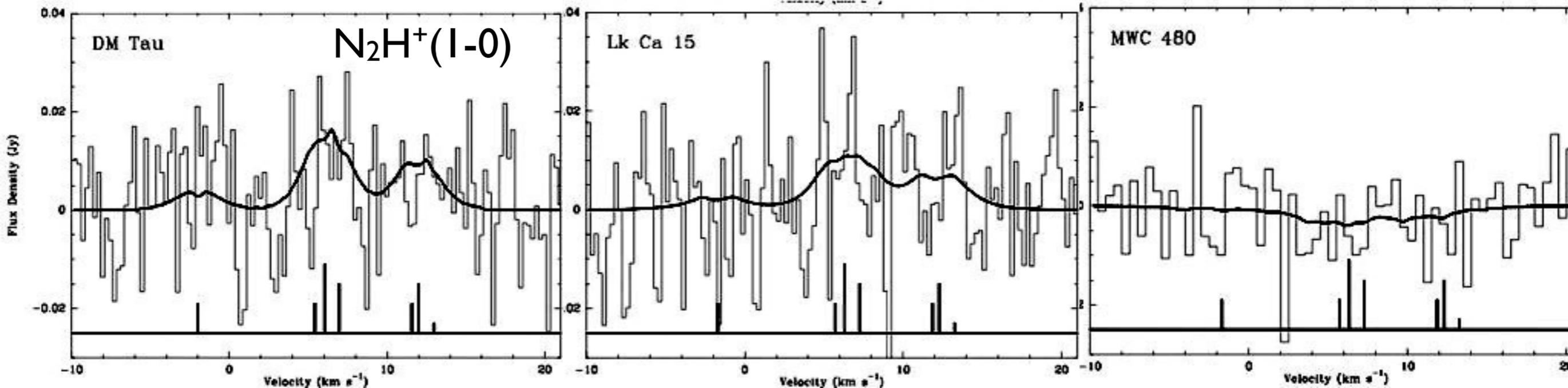
- Are transitional disks peculiar?

Ionization: HCO^+ and N_2H^+

- LkCa 15 (K5), DM Tau (M1) and MWC480 (A4)
- $J=1-0, 2-1$
- Two 5σ detections: N_2H^+ in LkCa 15 & DM Tau
- Upper limit: MWC480



Dutrey et al. (2007)



Ionization: HCO^+ and N_2H^+

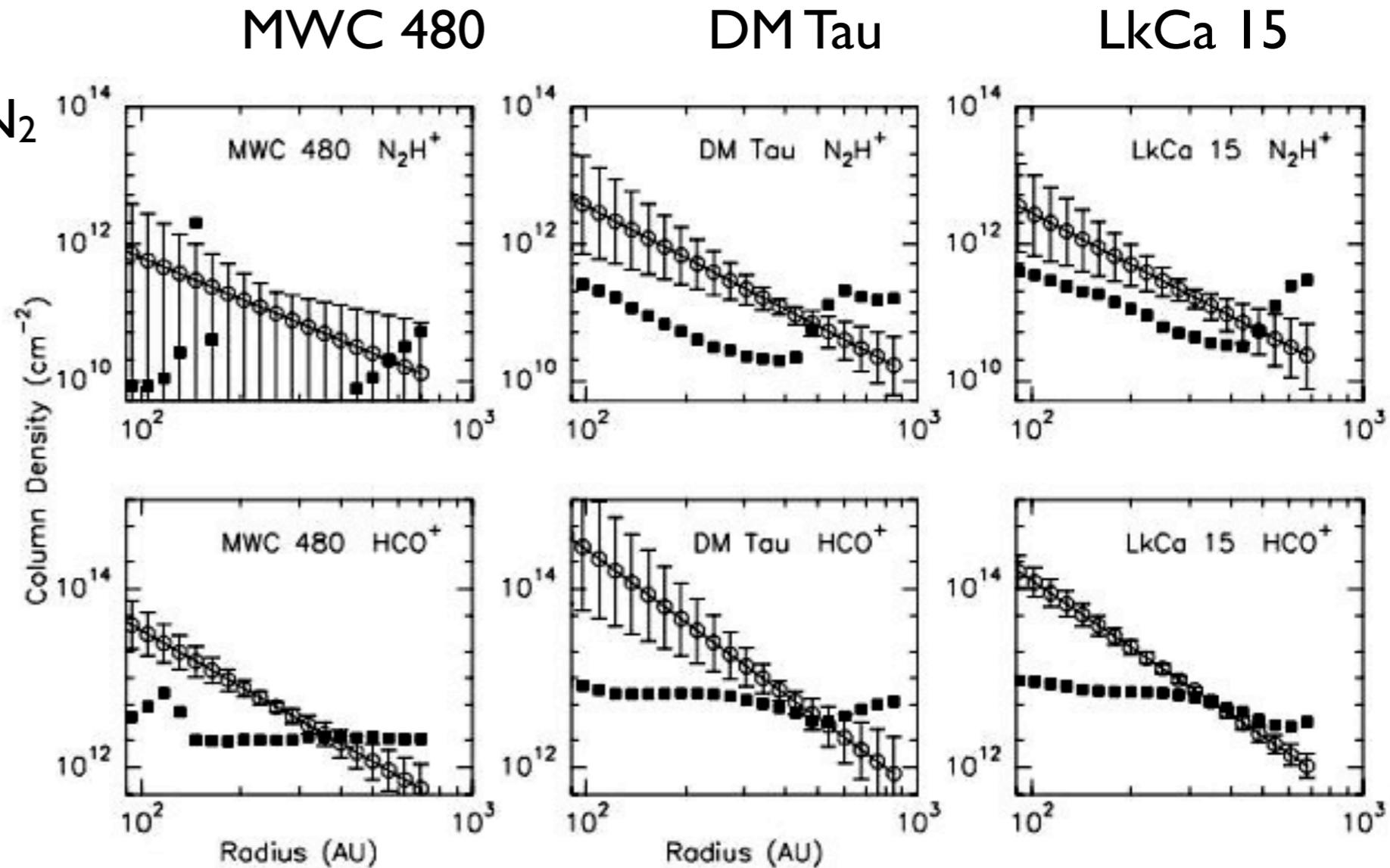
- HCO^+ is dominant ion:
 $\text{N}_2\text{H}^+ + \text{CO} \Rightarrow \text{HCO}^+ + \text{N}_2$

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

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

- Radial profiles are poorly reproduced

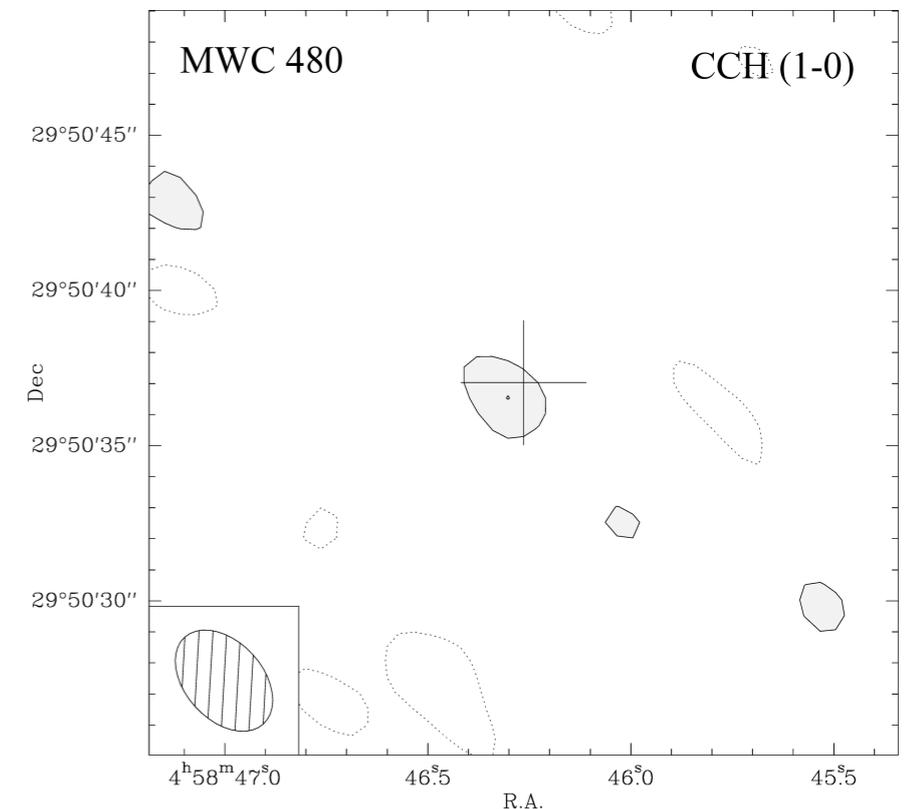
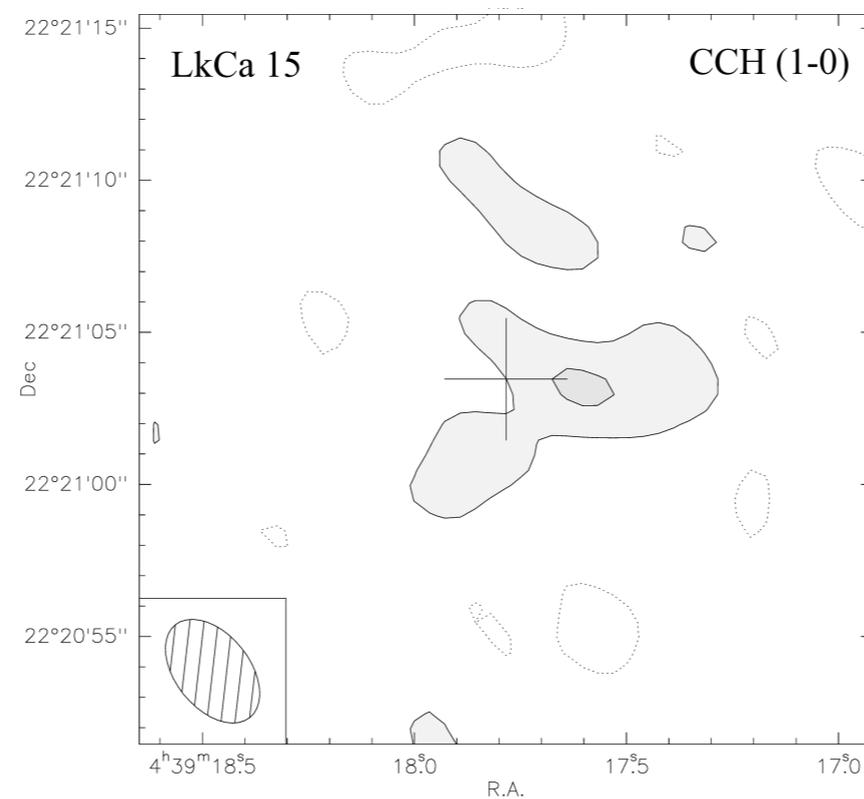
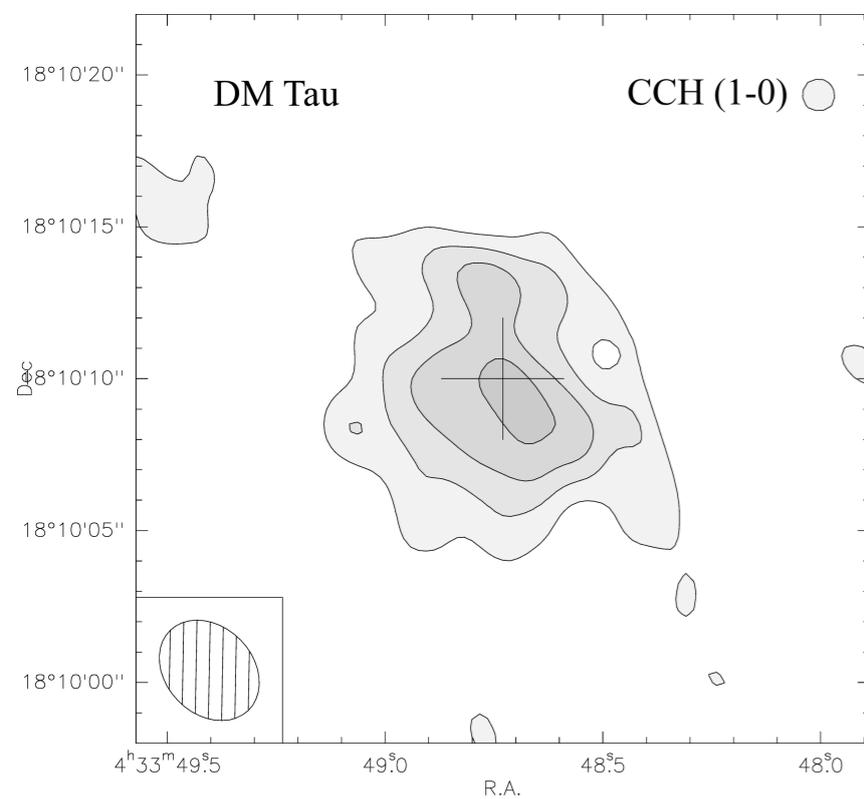
- Absolute values are in qualitative agreement



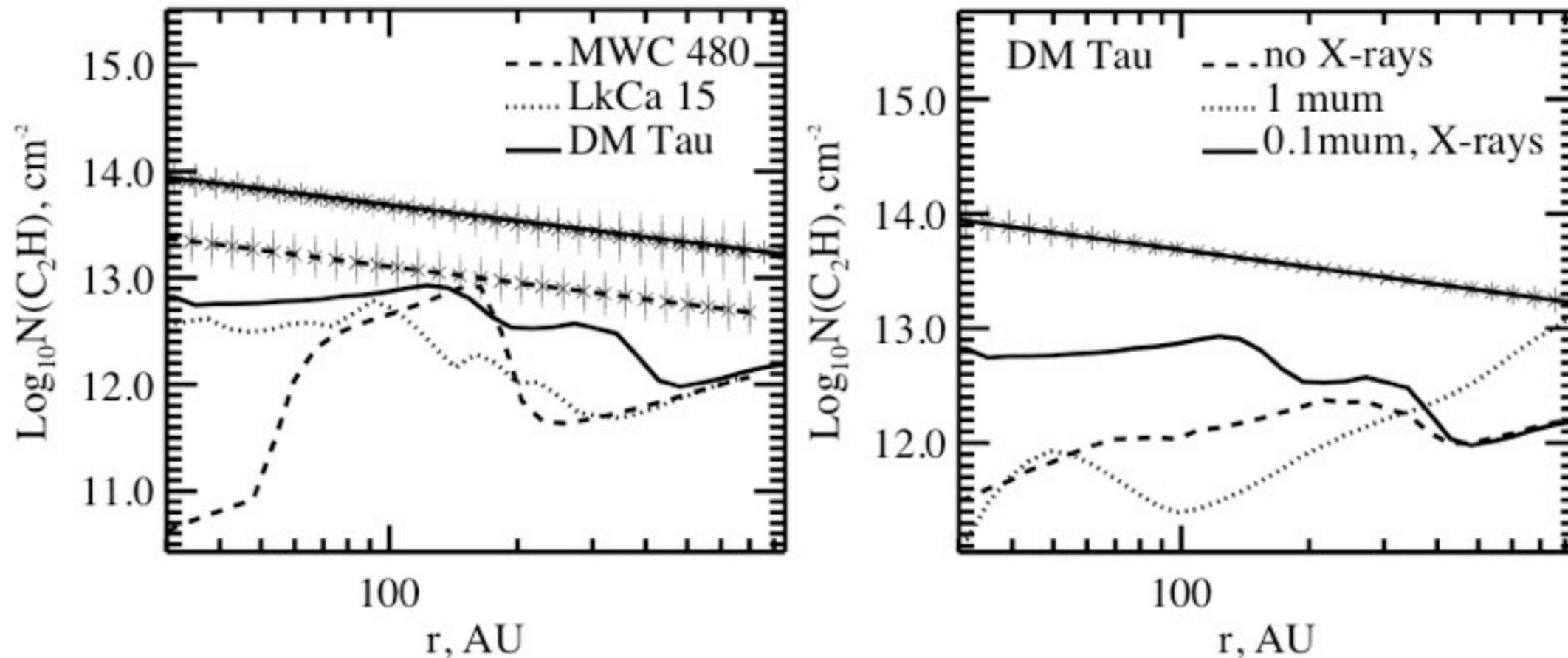
X-ray-driven chemistry in disks



- 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



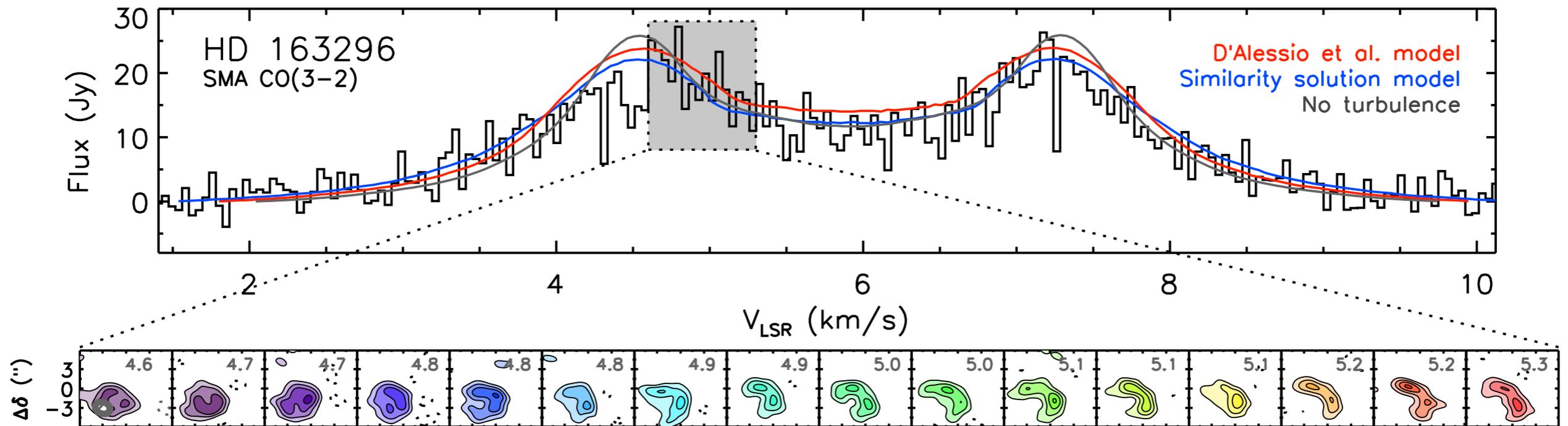
- T_{exc} : ~ 6 K
- Large-scale mixing or sub-thermal excitation?
- Less CCH in MWC 480
- Strong photodissociation by the Herbig Ae star?
- Low L_X in MWC 480: less efficient ion-molecule chemistry?

Chemistry in T Tau and Herbig Ae disks

Molecule	χ^2 -minimization method			Chemical model		DM Tau
	N [cm ⁻²]	1 σ error	N/N(¹³ CO) ^(1*)	N [cm ⁻²]	N/N(¹³ CO) ^(2*)	N/N(¹³ CO) ^(1*)
H ₂	6 10 ²²	1 10 ²²	1.5 10 ⁶	5 10 ²²	1.3 10 ⁶	1 10 ⁷
¹³ CO ^(*3)	4 10 ¹⁶	5 10 ¹⁵	1	4 10 ¹⁶	1	1
HCO ⁺	6 10 ¹²	3 10 ¹¹	1.5 10 ⁻⁴	1.5 10 ¹³	4 10 ⁻⁴	2 10 ⁻³
HCN	5 10 ¹¹	3 10 ¹¹	1.3 10 ⁻⁵	4 10 ¹¹	10 ⁻⁵	7 10 ⁻⁴
CS	3 10 ¹²	3 10 ¹²	< 8 10 ⁻⁵	2 10 ¹¹	5 10 ⁻⁶	3 10 ⁻⁴
C ₂ H	2 10 ¹³	2 10 ¹³	< 5 10 ⁻⁴	10 ¹⁰	2.5 10 ⁻⁷	10 ⁻³
CH ₃ OH	0	7 10 ¹⁵	< 2 10 ⁻¹	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_X: less efficient ion-molecule chemistry
- CO + He⁺ ⇒ C⁺ + O + He⁺

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

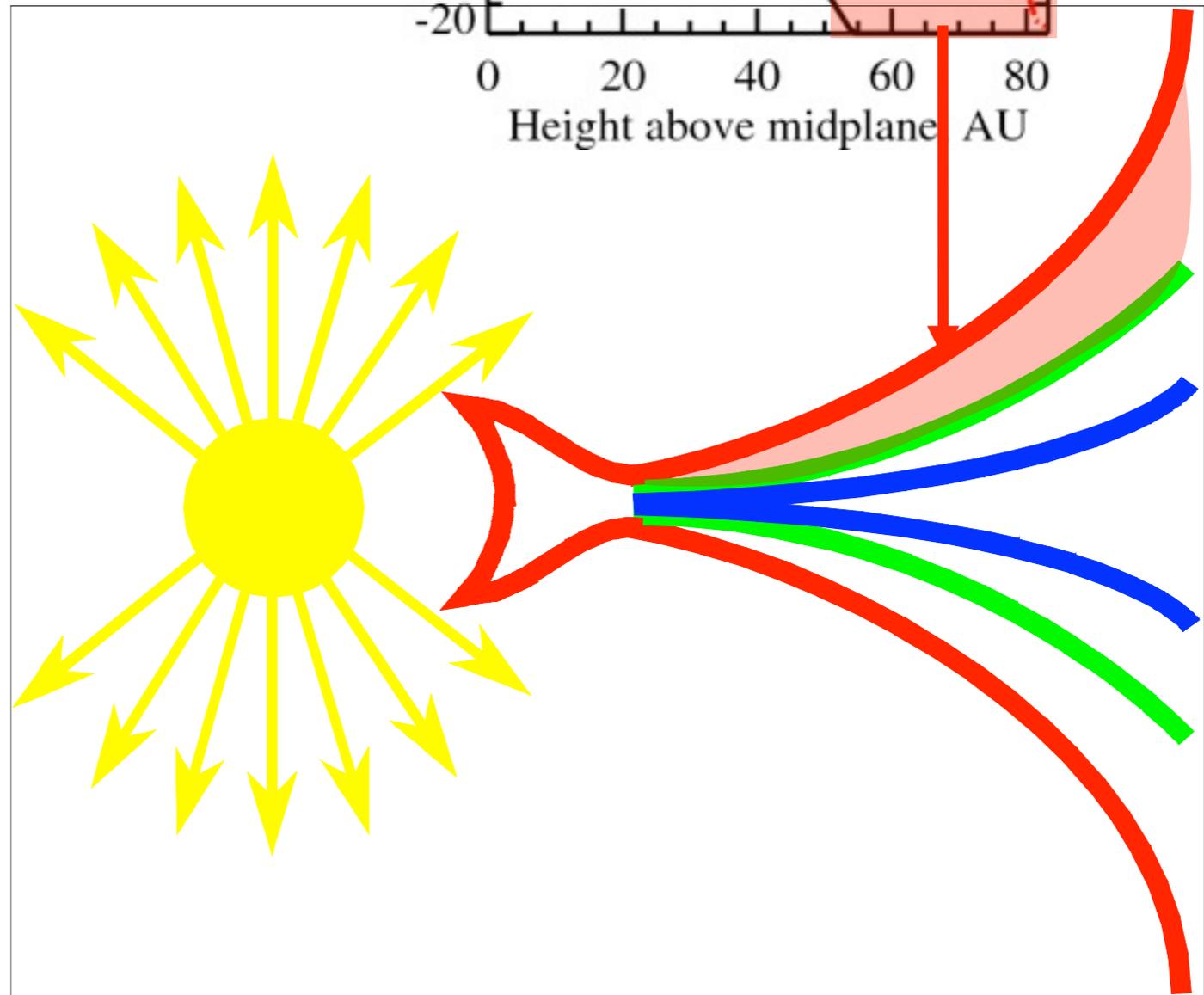
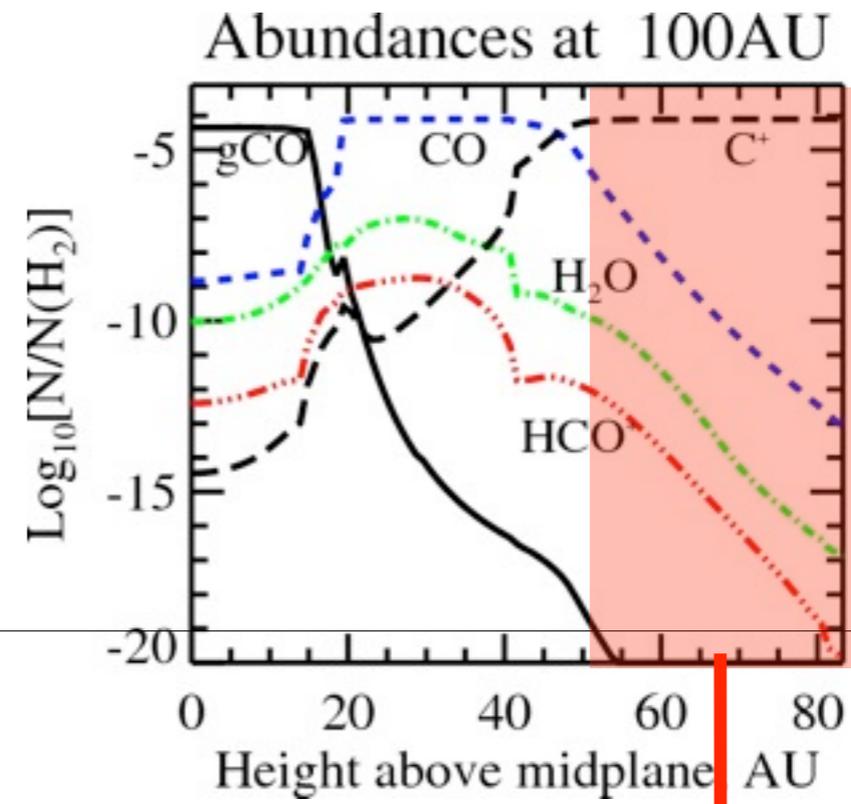
III. Observations of molecules in PPDs: Summary

- 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

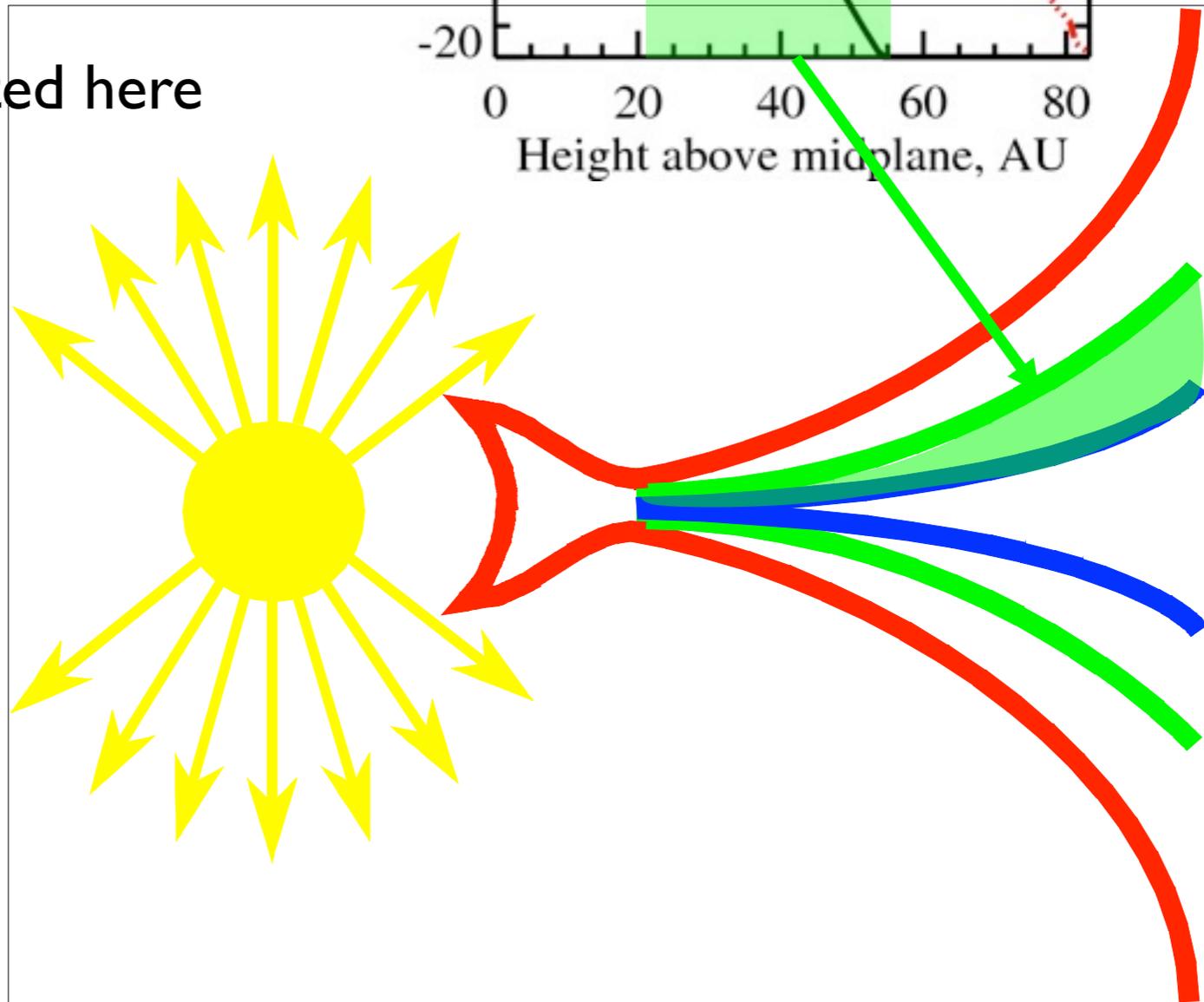
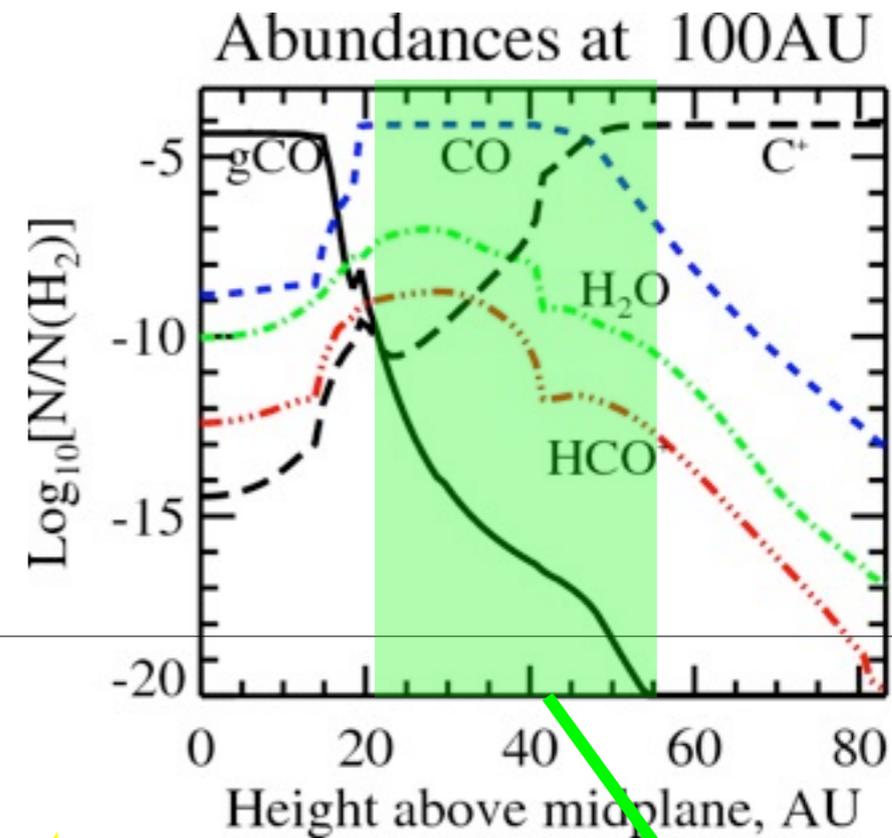
Zone of ions and radicals (atmosphere)

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



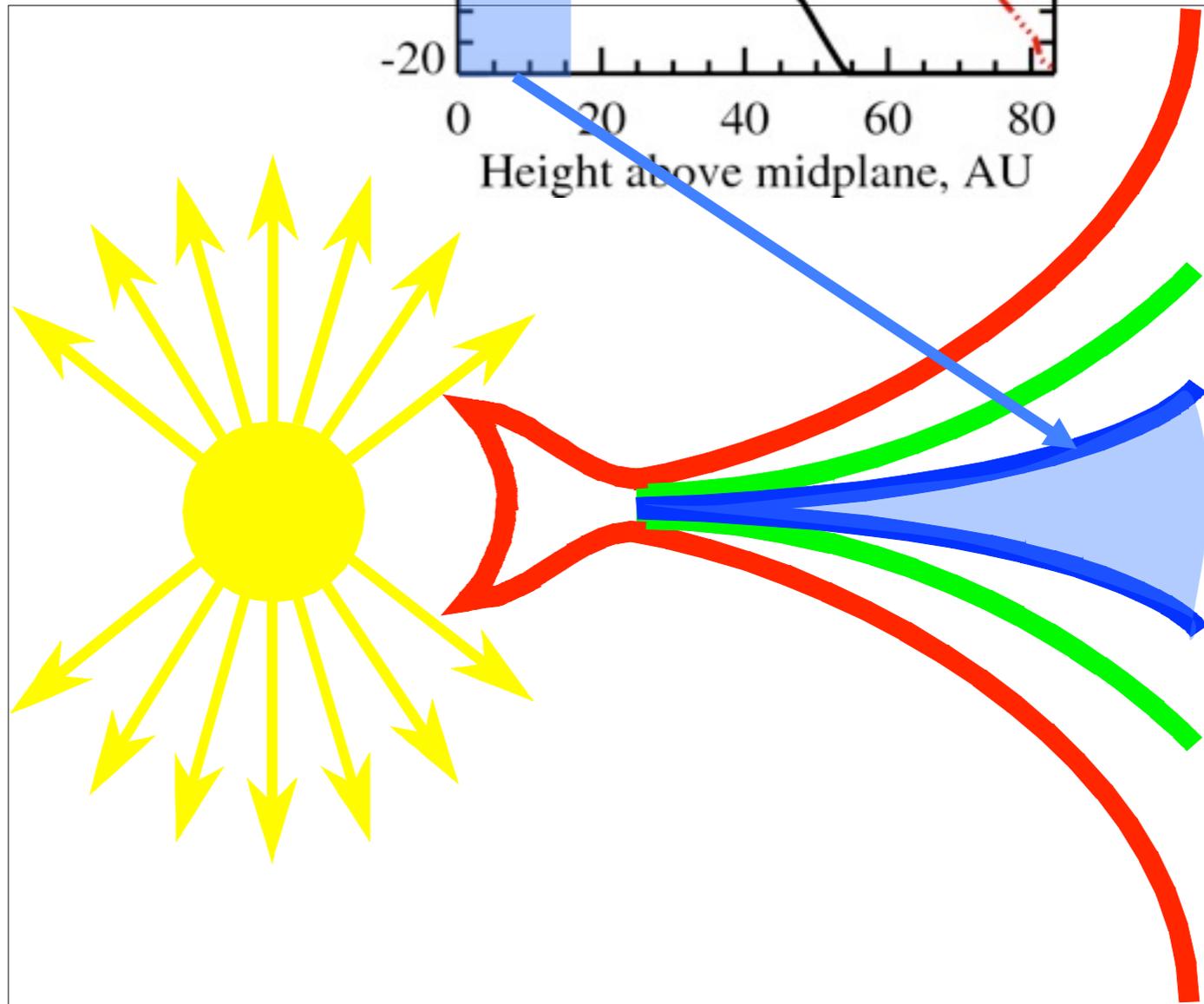
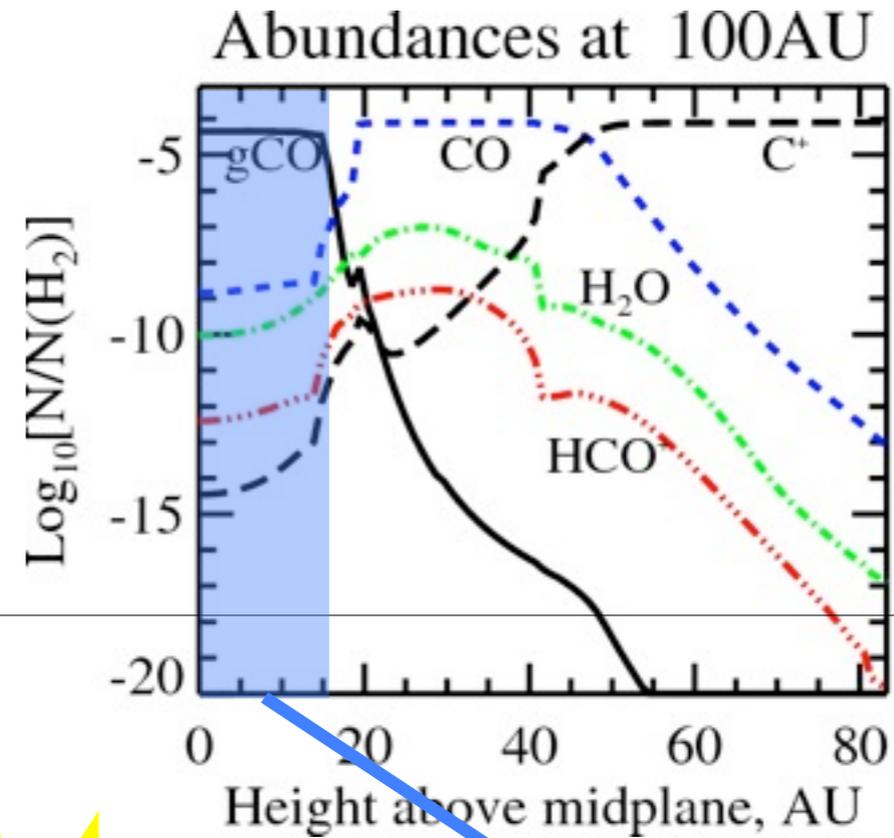
Zone of molecules (intermediate layer)

- 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



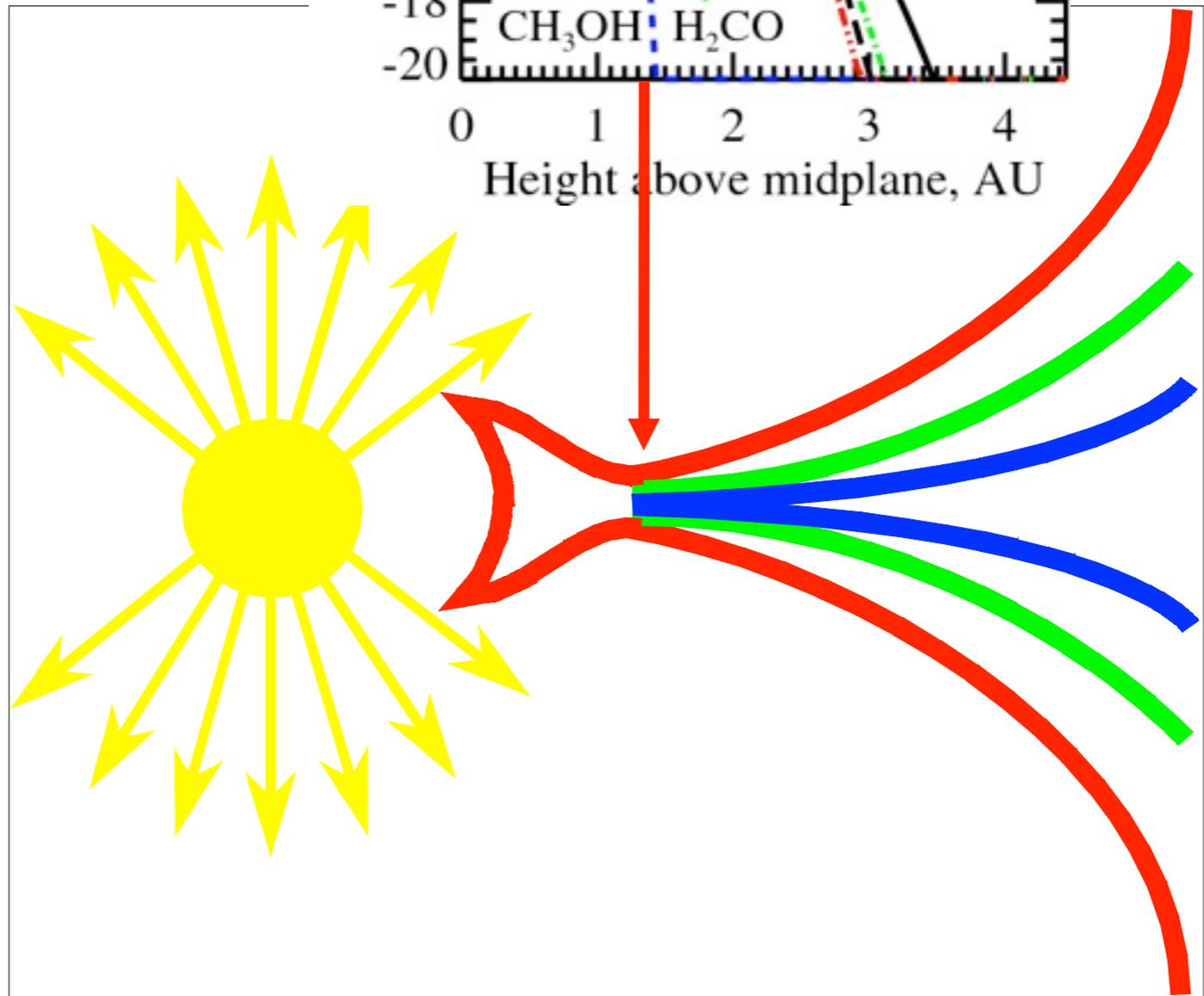
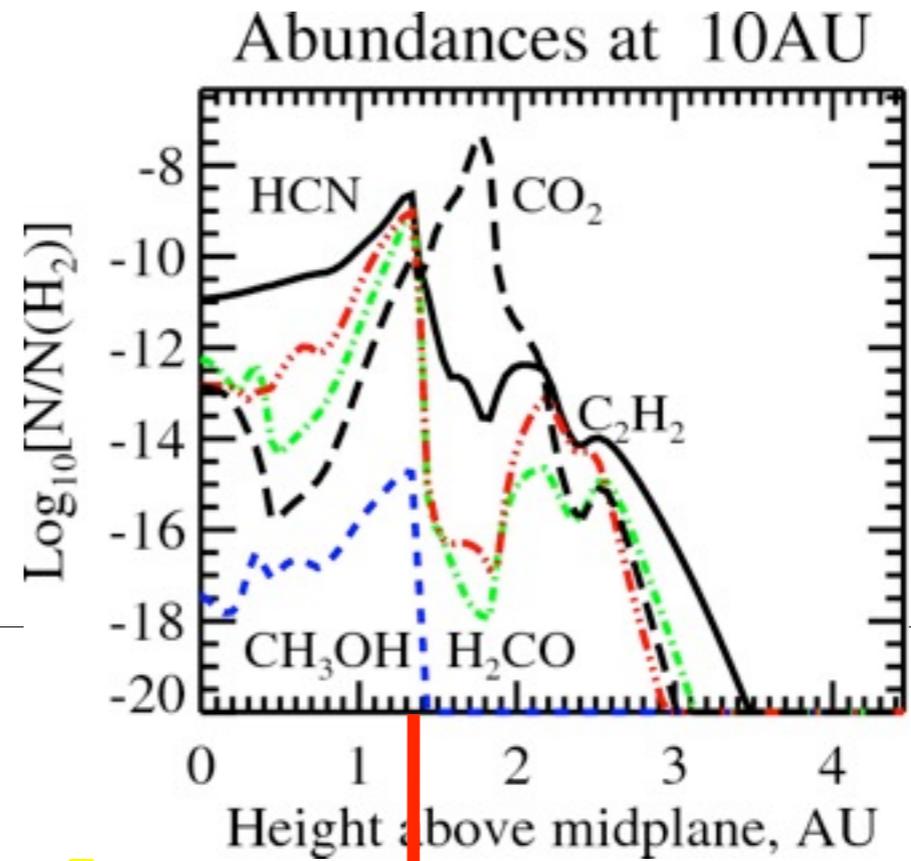
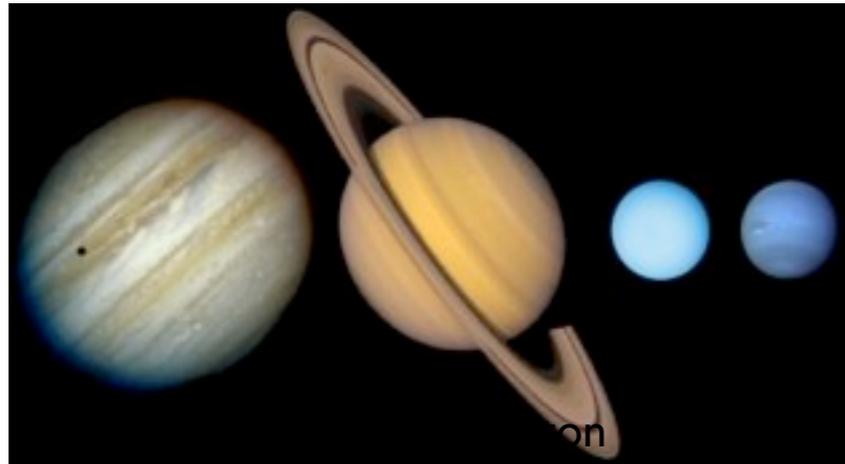
Zone of ices (midplane)

- 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

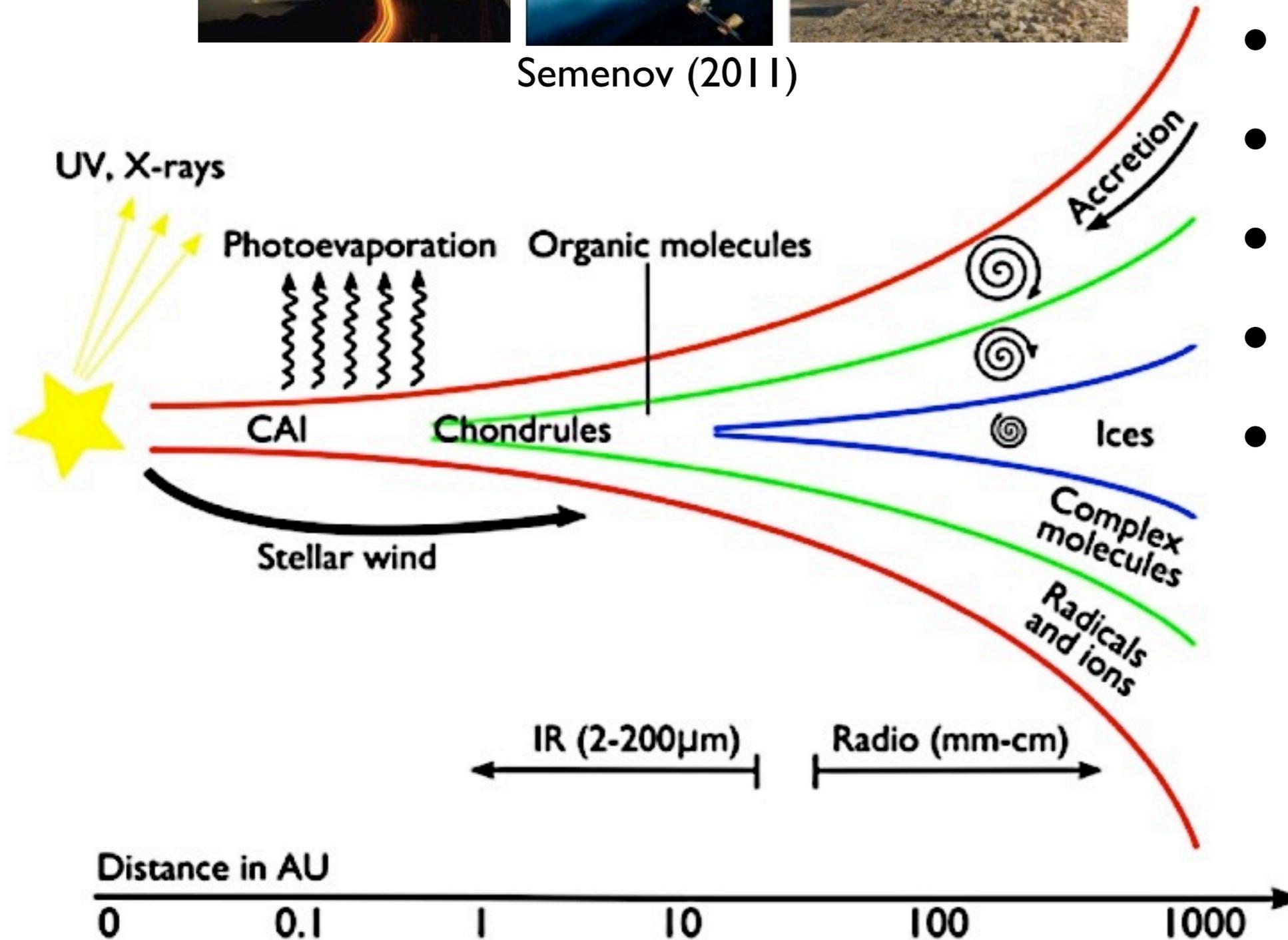


A scheme of disk structure



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

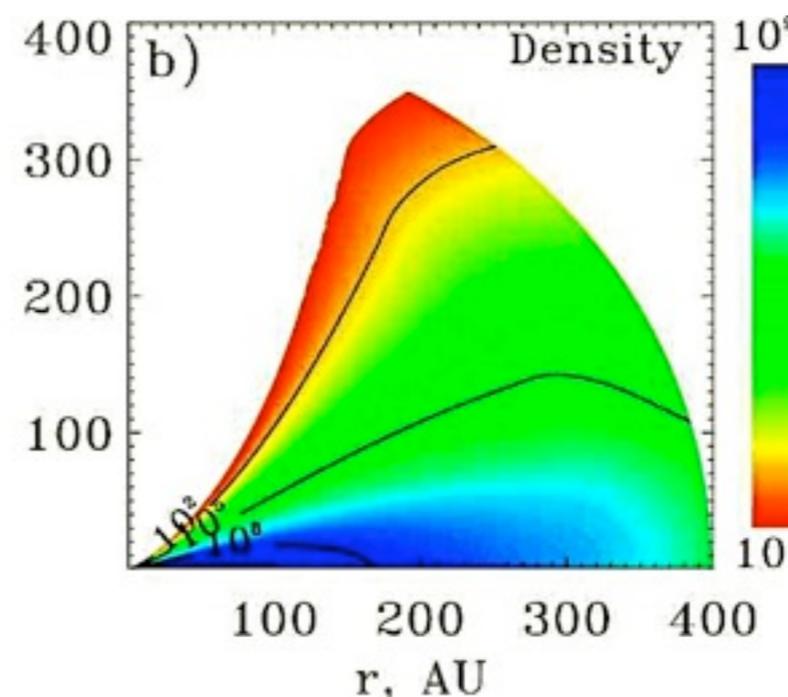
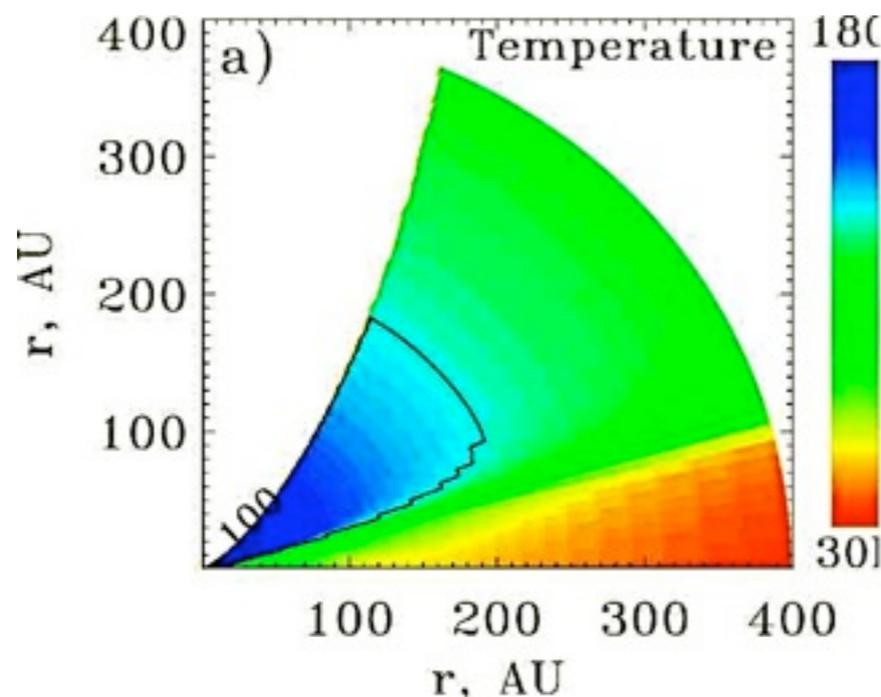
V. Modeling disk chemistry

Chemical kinetics equations

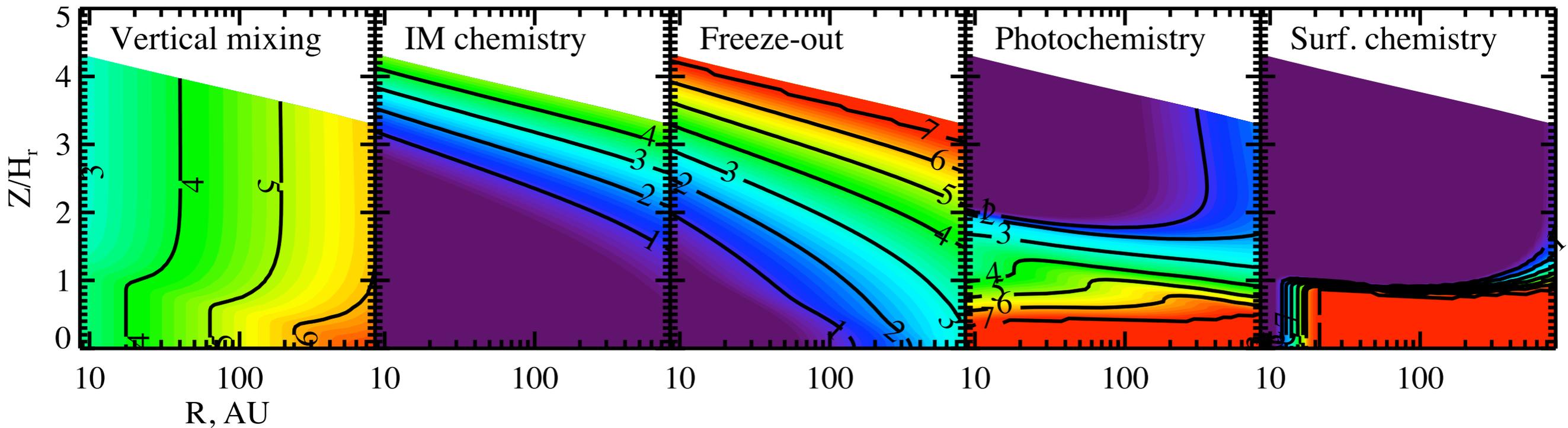
$$\frac{\partial n_i}{\partial t} = \sum_{j,k \neq i} k_{jk} n_j n_k - n_i \sum_l k_{li} n_l + \nabla D n_H \nabla n_i / n_H - \nabla U n_i$$

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

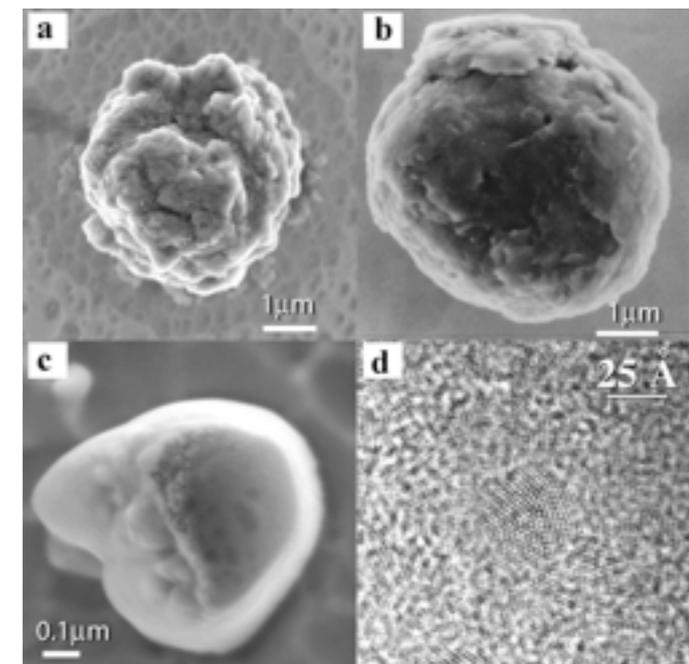
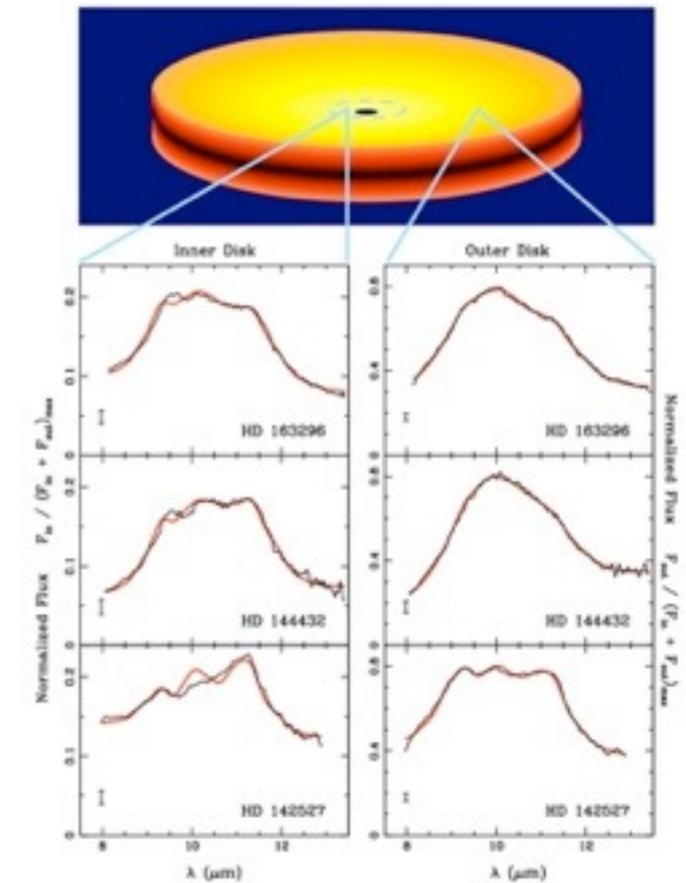


Characteristic Timescales: Outer Disk (250 AU)

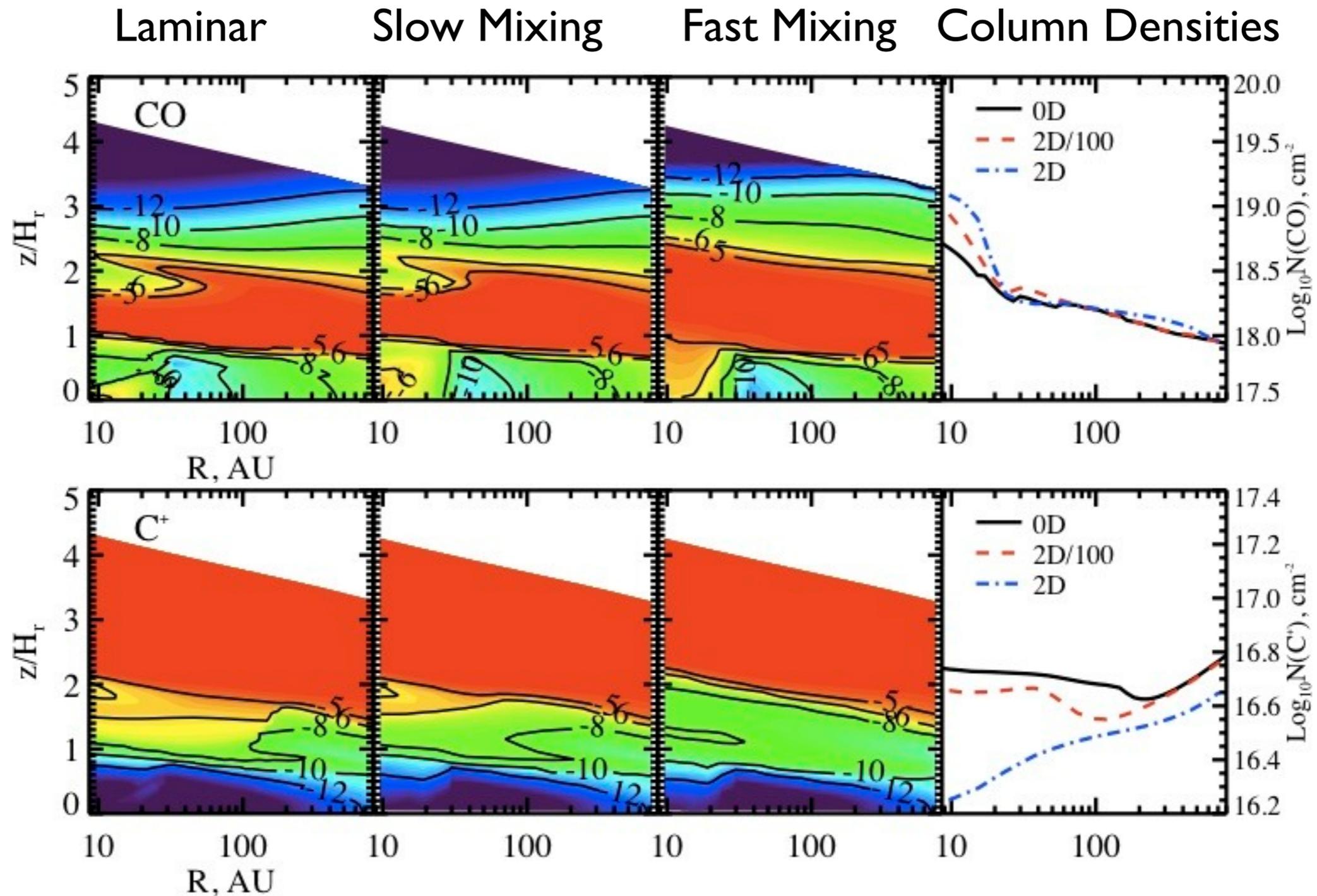
Processes	Midplane [yr]	Warm layer* [yr]	Atmosphere* [yr]
Mixing	1.0 (6)	2.5 (5)	1.4 (5)
Gas-phase	2.0 (-2)	1.8 (-1)	2.9 (0)
UV	>1.0 (7)	1.2 (6)	3.1 (1)
Accretion	2.7 (1)	1.8 (2)	2.3 (3)
Desorption	1.0 (6)	4.3 (0)	<1.0 (-7)
Surface*	>1.0 (7)	>1.0 (7)	1.4 (5)

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

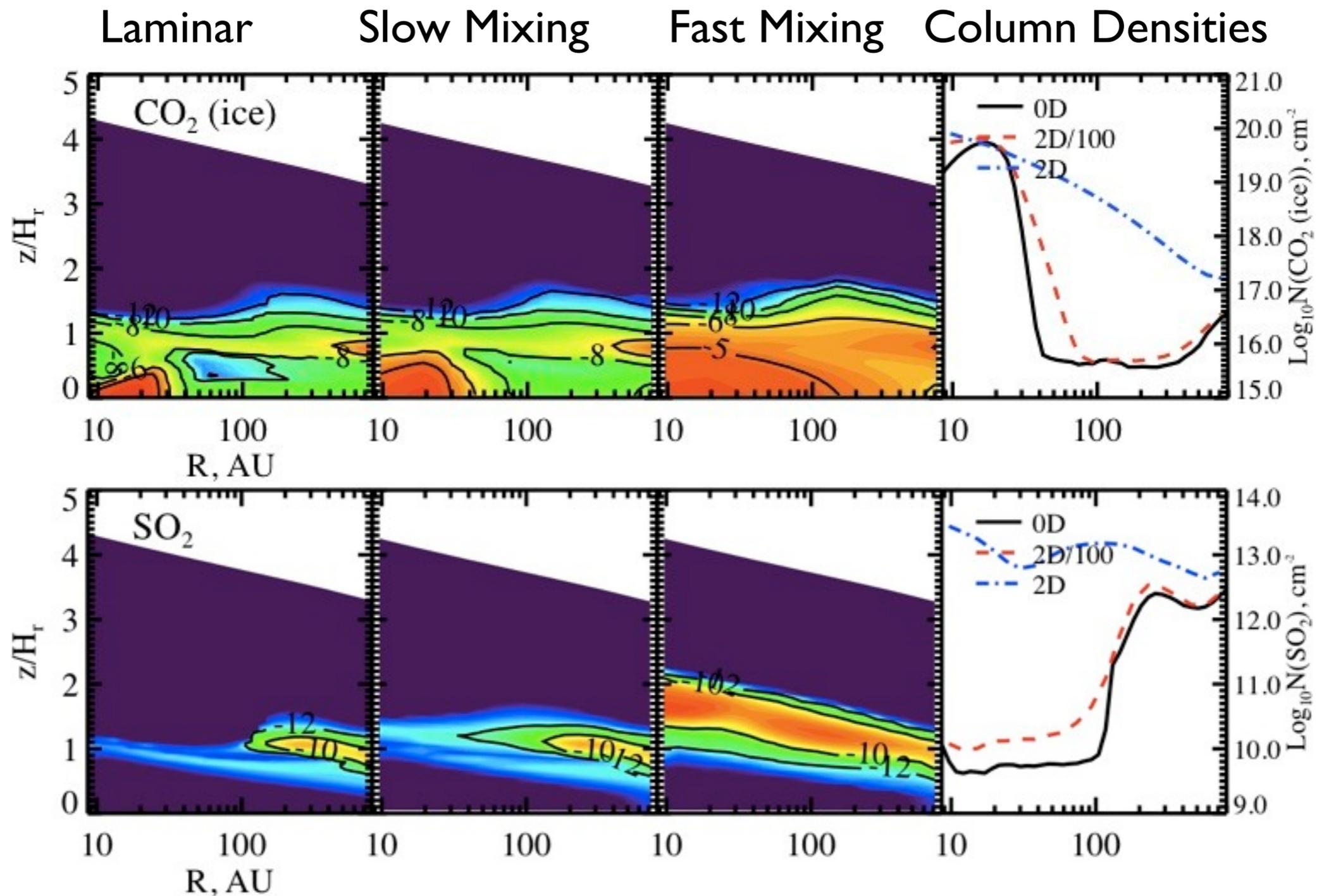


Turbulence: Steadfast species



- Fast gas-phase formation and destruction
- t : Gas-phase chemistry < Dynamics
- Example: CO, OH, H₂O ice, CCH, C⁺, CN, HCN

Turbulence: Sensitive species



- Slow surface formation & desorption
- τ : Surface chemistry $>$ Dynamics
- Hydrocarbons (C_2H_2), organics (HCOOH), SO , SO_2 , C_2S , C_3S

VI. The Brave New World: ALMA

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

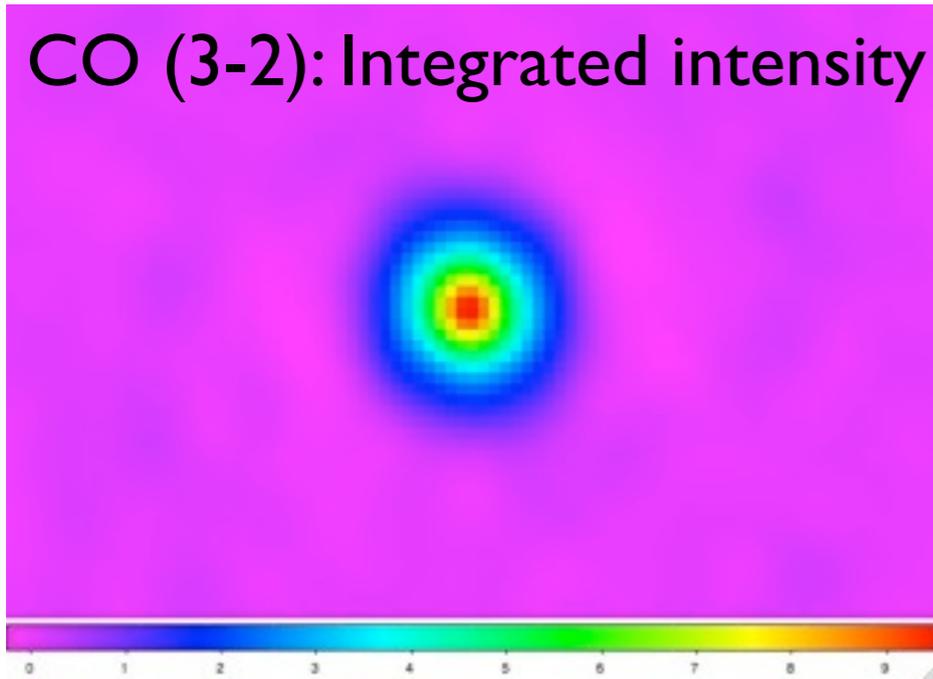


ALMA imaging of gas in PPDs:

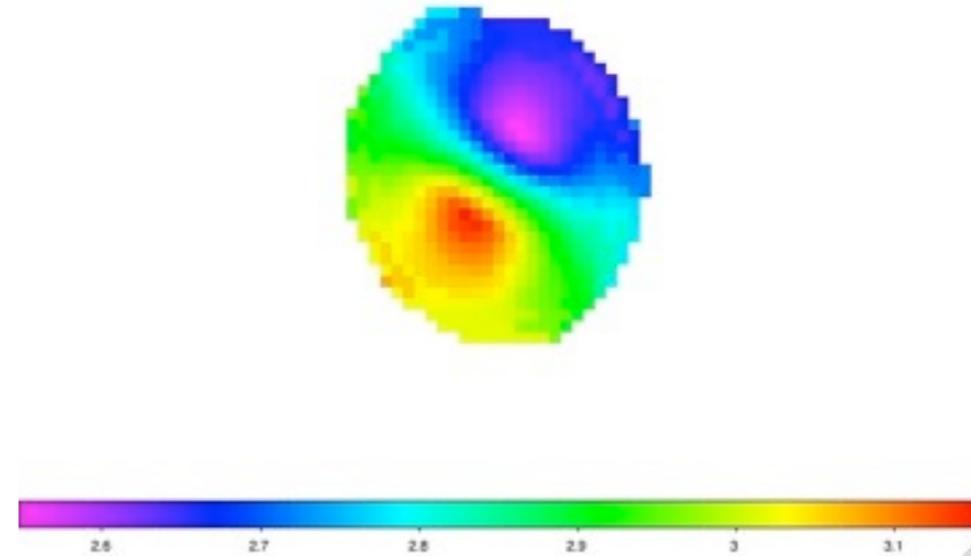
- "Hot core/corinos"-like complex molecules: $>\text{CH}_3\text{OH}$, C_nH_m
- Molecules with S, P, Si, Cl, ...
- Anions: C_8H^-
- Isotopologues: ^{15}N , ^{34}S , $^{17,18}\text{O}$, D, ^{13}C
- Ionization structure
- Planet-forming inner regions
- Molecular layers
- Large- and small-scale dynamics
- Large surveys
- Unknown unknowns!

ALMA is working: TW Hya

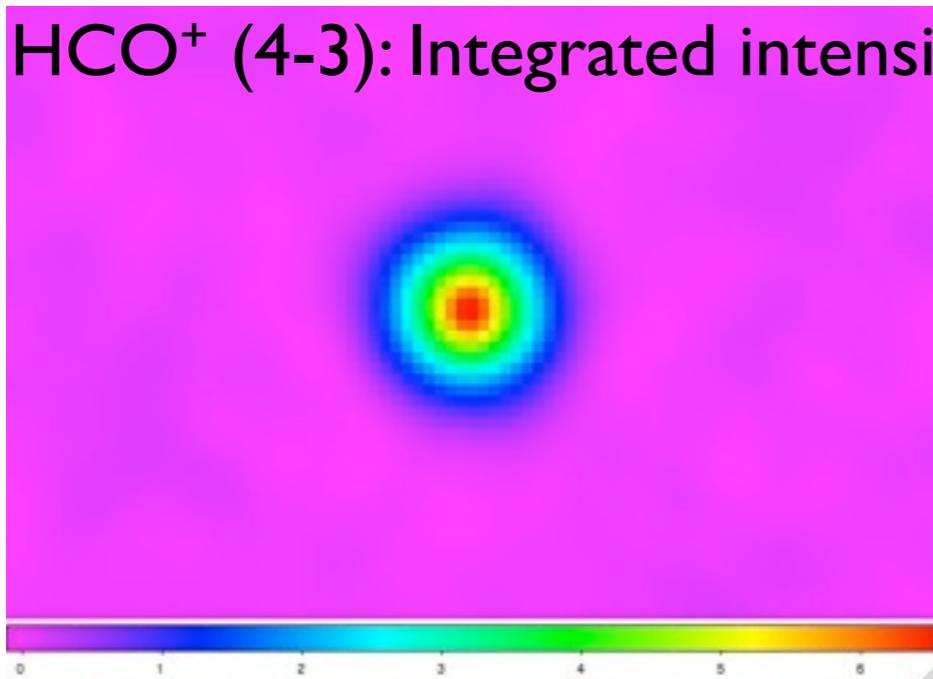
CO (3-2): Integrated intensity



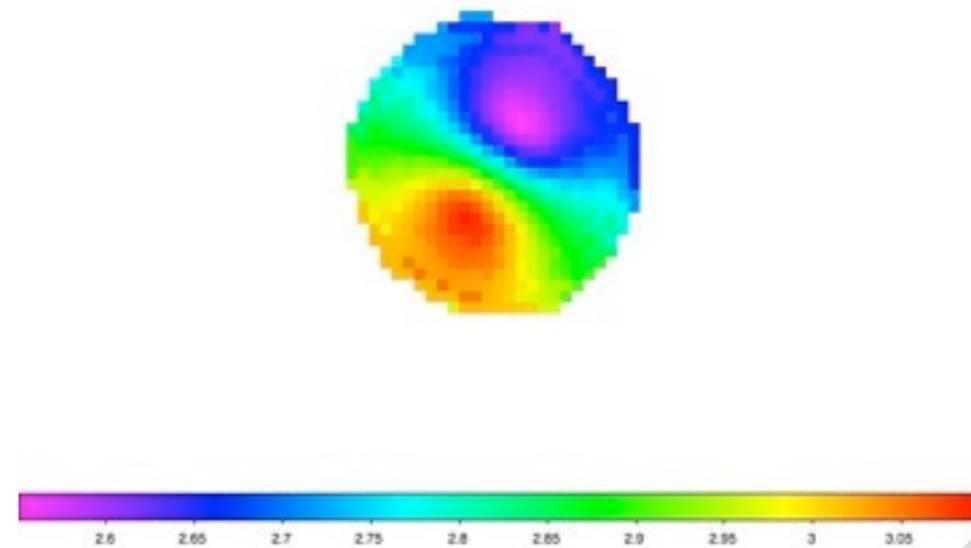
CO (3-2): Rotation



HCO⁺ (4-3): Integrated intensity



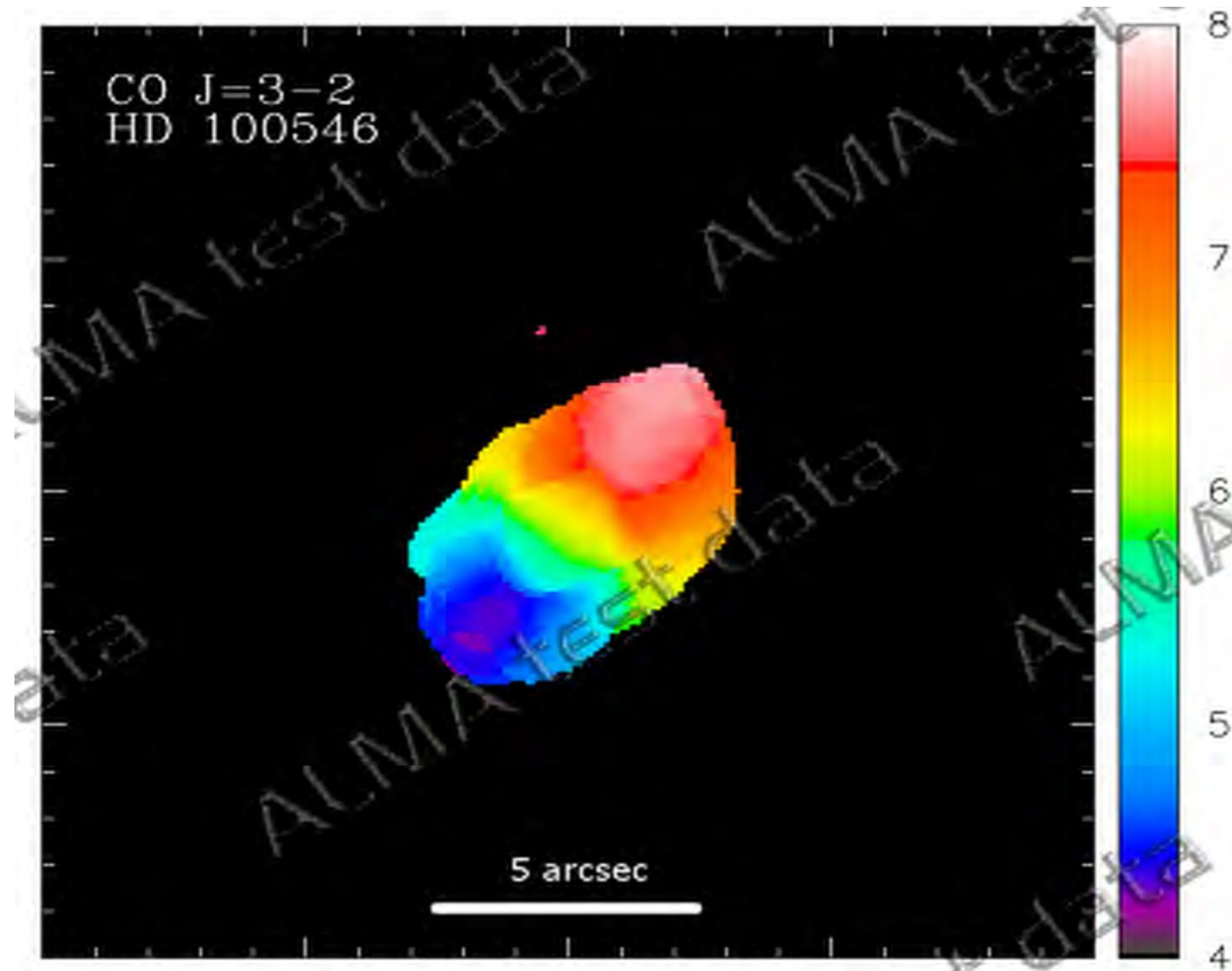
HCO⁺ (4-3): Rotation



Science Verification observations of TW Hya at 345 GHz

ALMA is working: HD 100546

CO (3-2): Rotation

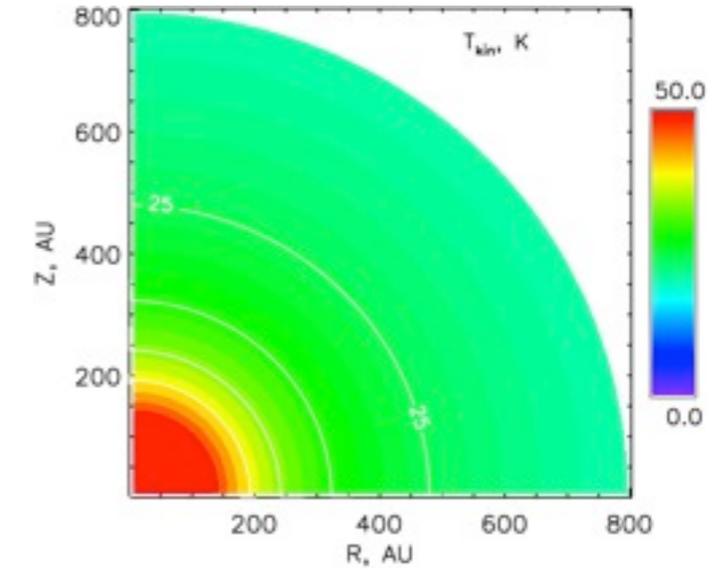
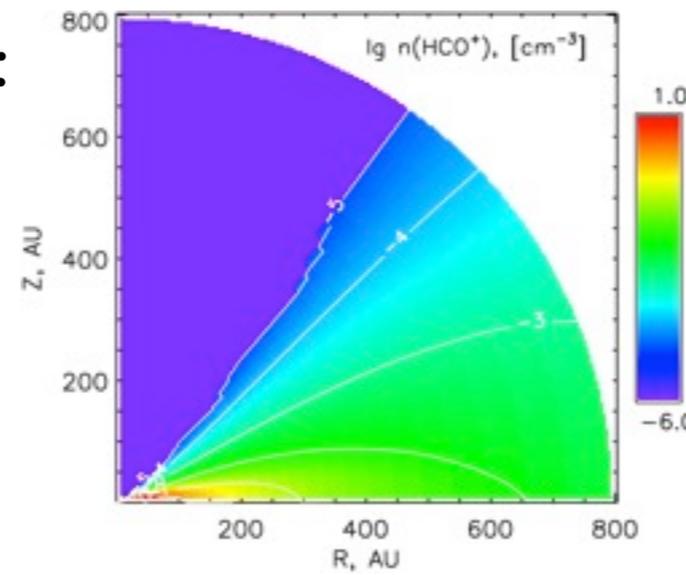


ALMA commissioning

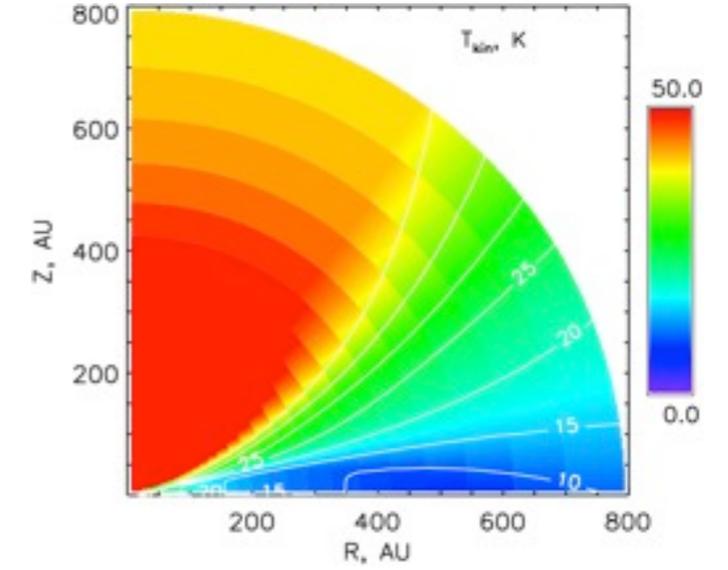
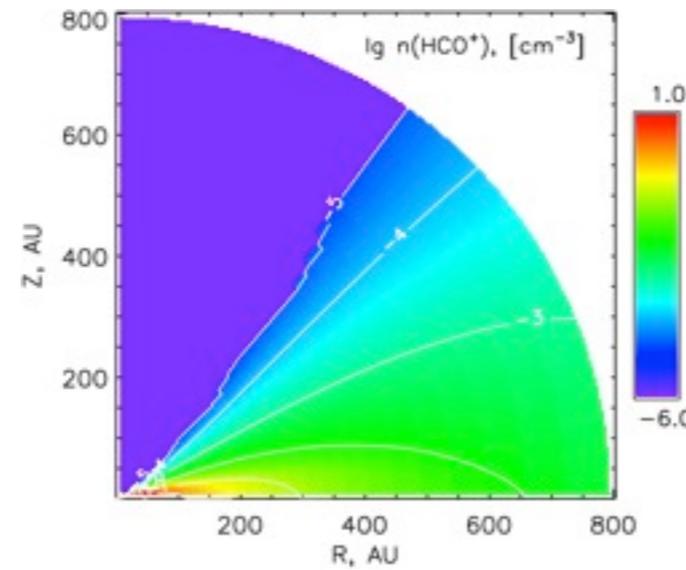
Disk models for ALMA: HCO⁺ (4-3)

2D Monte-Carlo LRT calculations:

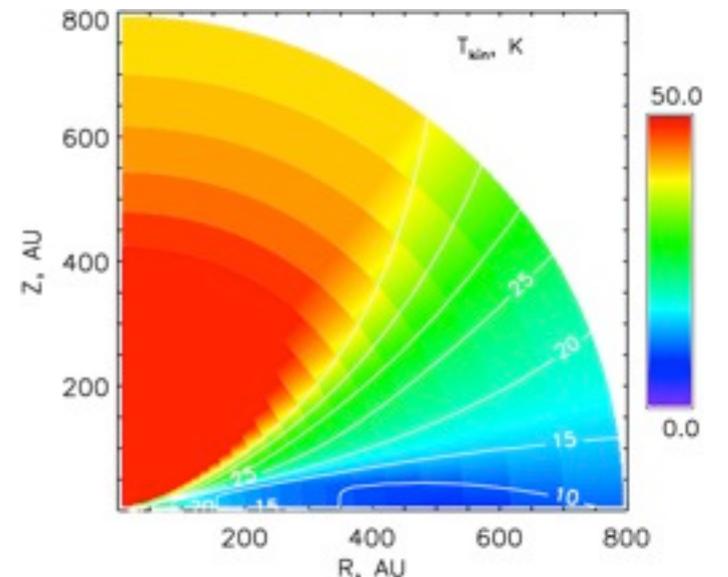
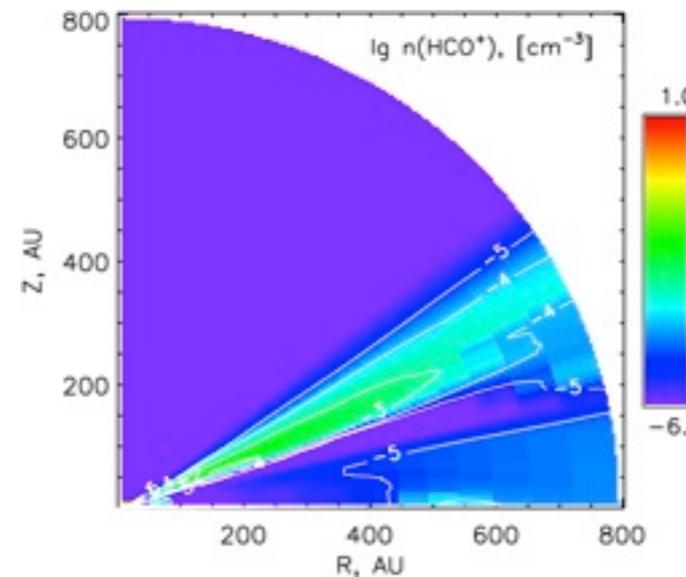
Uniform abundances,
radial T-gradient



Uniform abundances,
2D T-gradient



Chemical abundances,
2D T-gradient

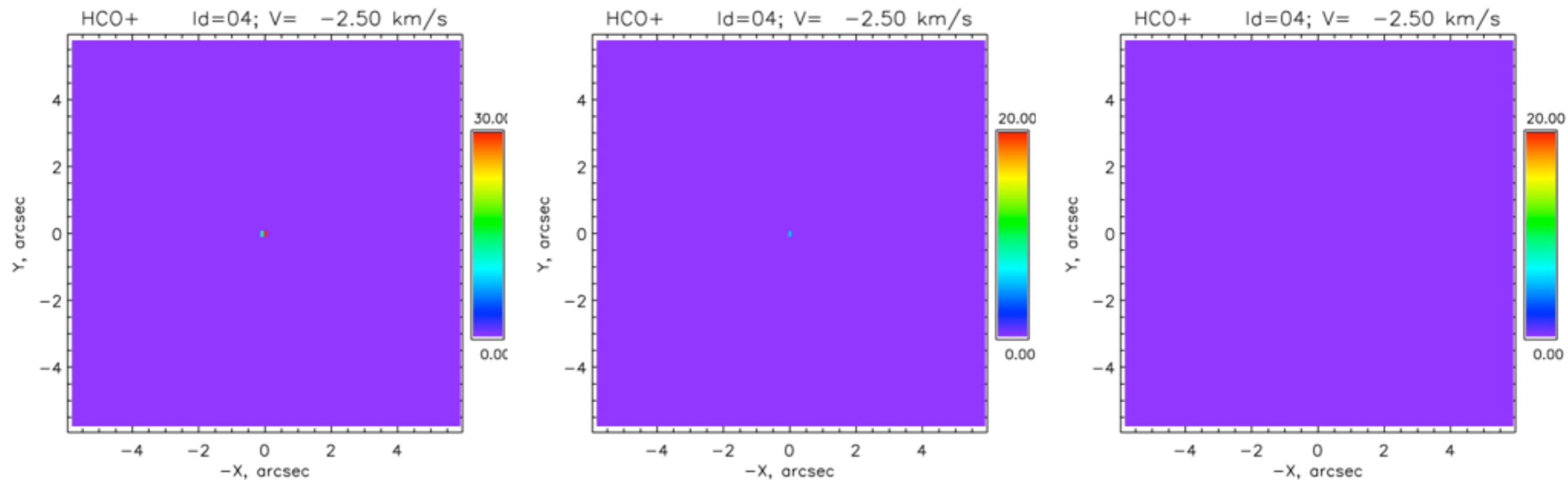


Channel maps of HCO⁺ (4-3)@ 20°

“UNIFORM”

“THERMAL”

“CHEMICAL”



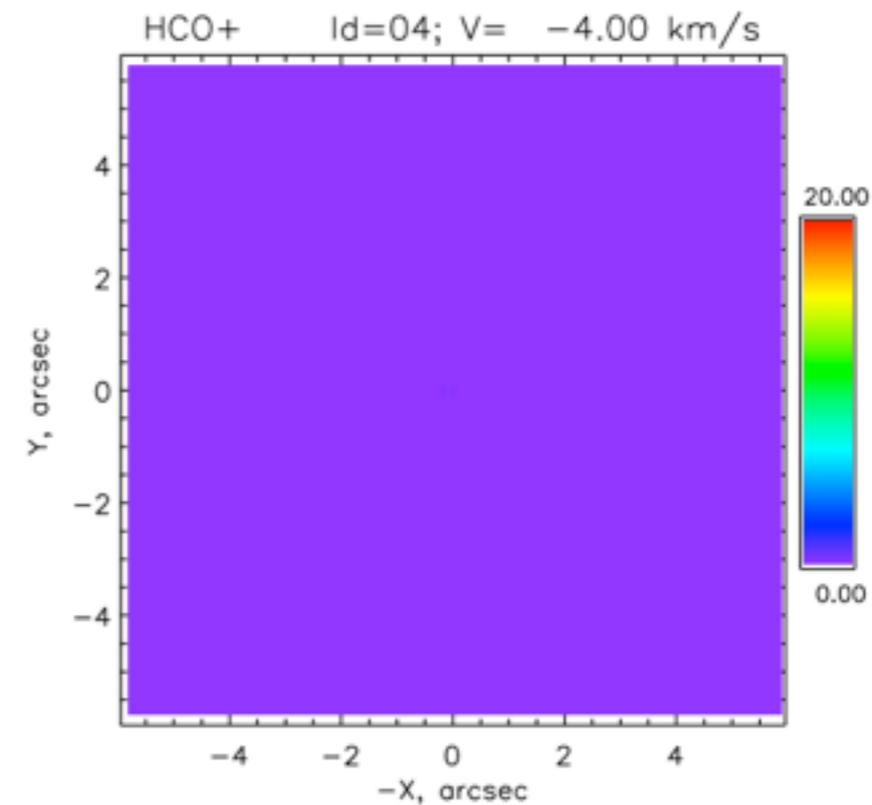
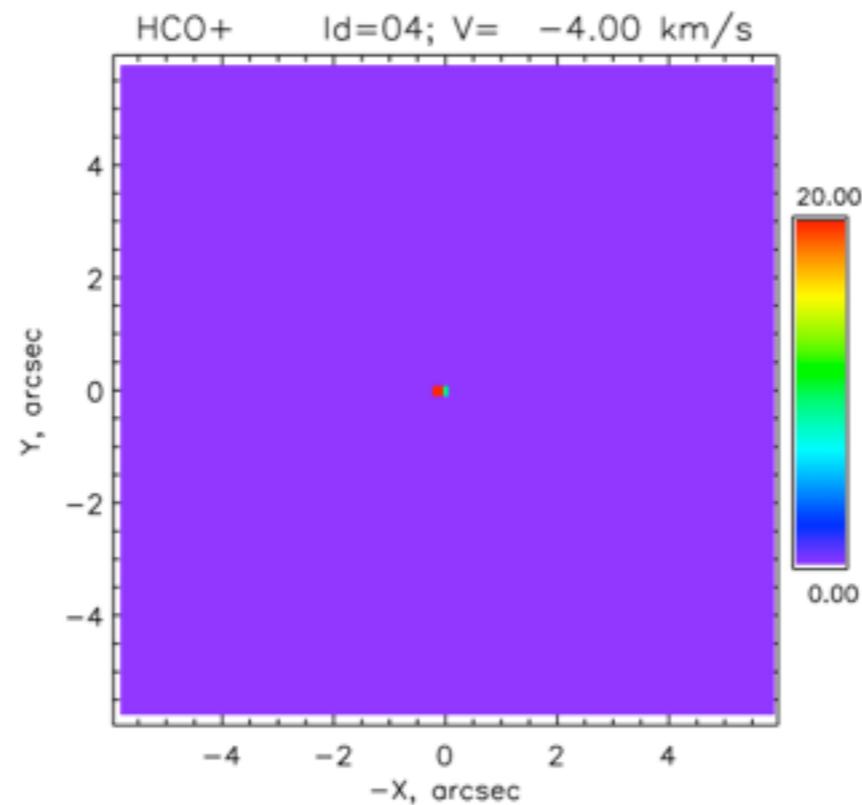
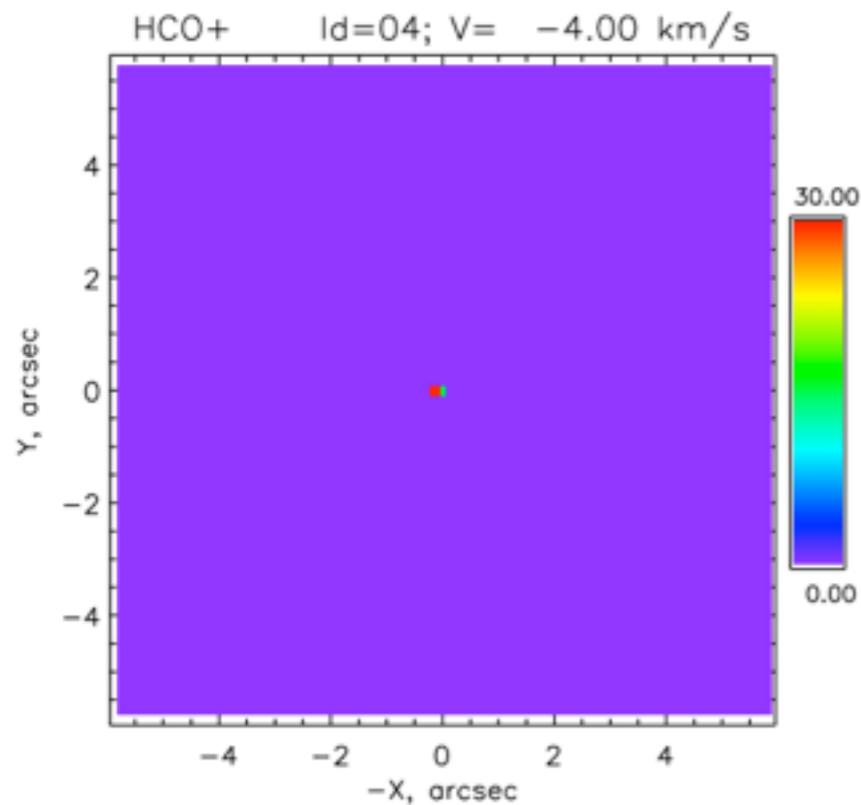
Face-on disks: no big difference

Channel maps of HCO⁺ (4-3)@ 60°

“UNIFORM”

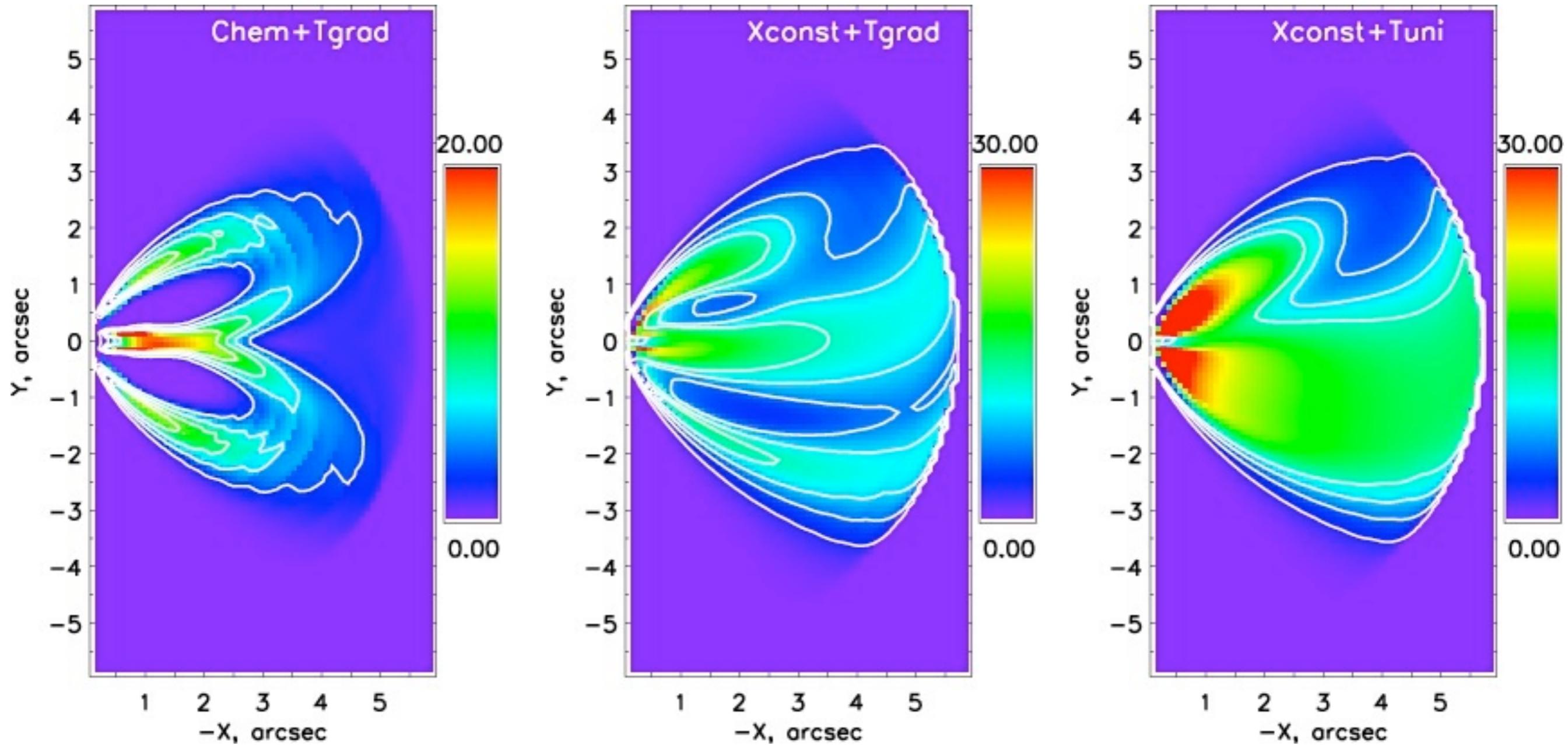
“THERMAL”

“CHEMICAL”



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

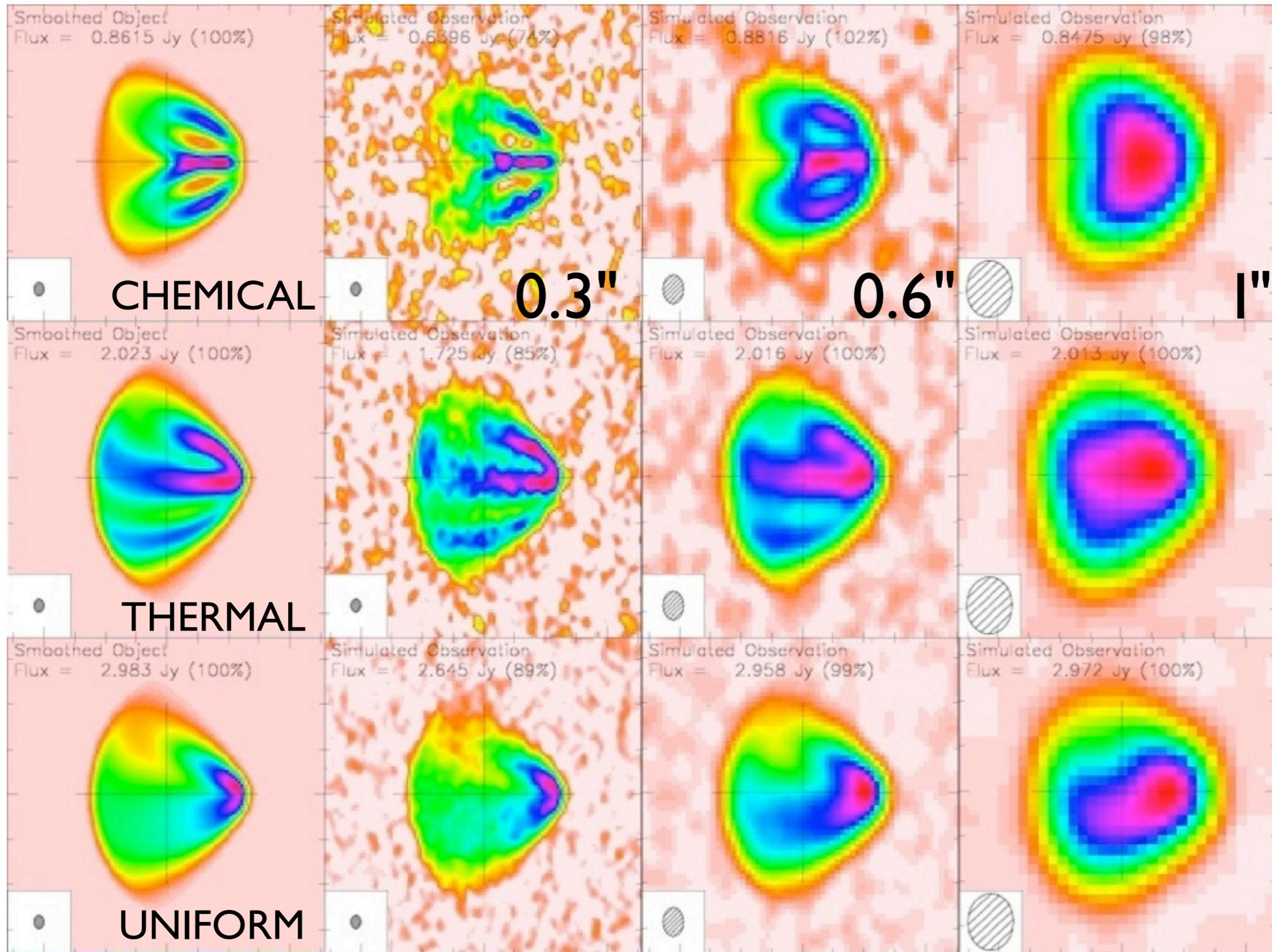
Chemical vs. Temperature Gradients: 0.68 km/s channel of HCO+ (4-3)@ 60°



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 ⁺ (1–0)	89	30	Zoom-c (4 hr) ^a
C ¹⁸ O(2–1)	220	75	Zoom-d (1 hr)	Zoom-c (<0.5 hr)	Zoom-c (4 hr)	Zoom-c (10 hr)
¹³ CO(2–1)	220	75	Zoom-d (<0.5 hr)	Zoom-d (<0.5 hr)	Zoom-c (2 hr)	Zoom-c (3.5 hr) ^a
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 ⁺ (4–3)	357	120	Zoom-d (<0.5 hr)	Zoom-e (<0.5 hr)	Zoom-c (2 hr)	Zoom-c (3 hr)
HCO ⁺ (7–6)	624	210	Zoom-e (<0.5 hr)	Zoom-e (1.5 hr)	Zoom-c (12 hr)	Zoom-d (>12 hr)
¹³ 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