Chemistry as a Tool to Study Protoplanetary Disks: A Modeler's View

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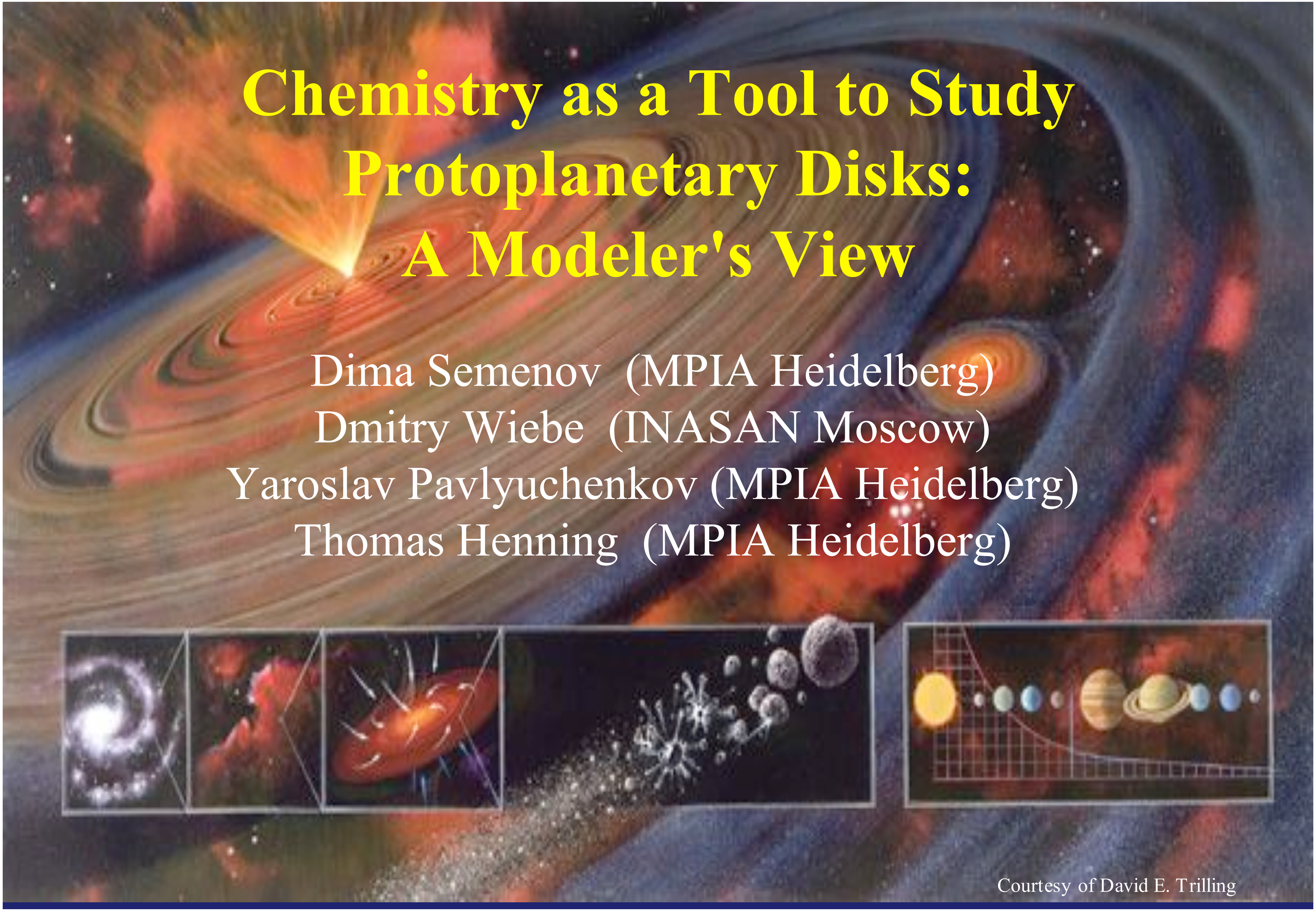


Courtesy of David E. Trilling

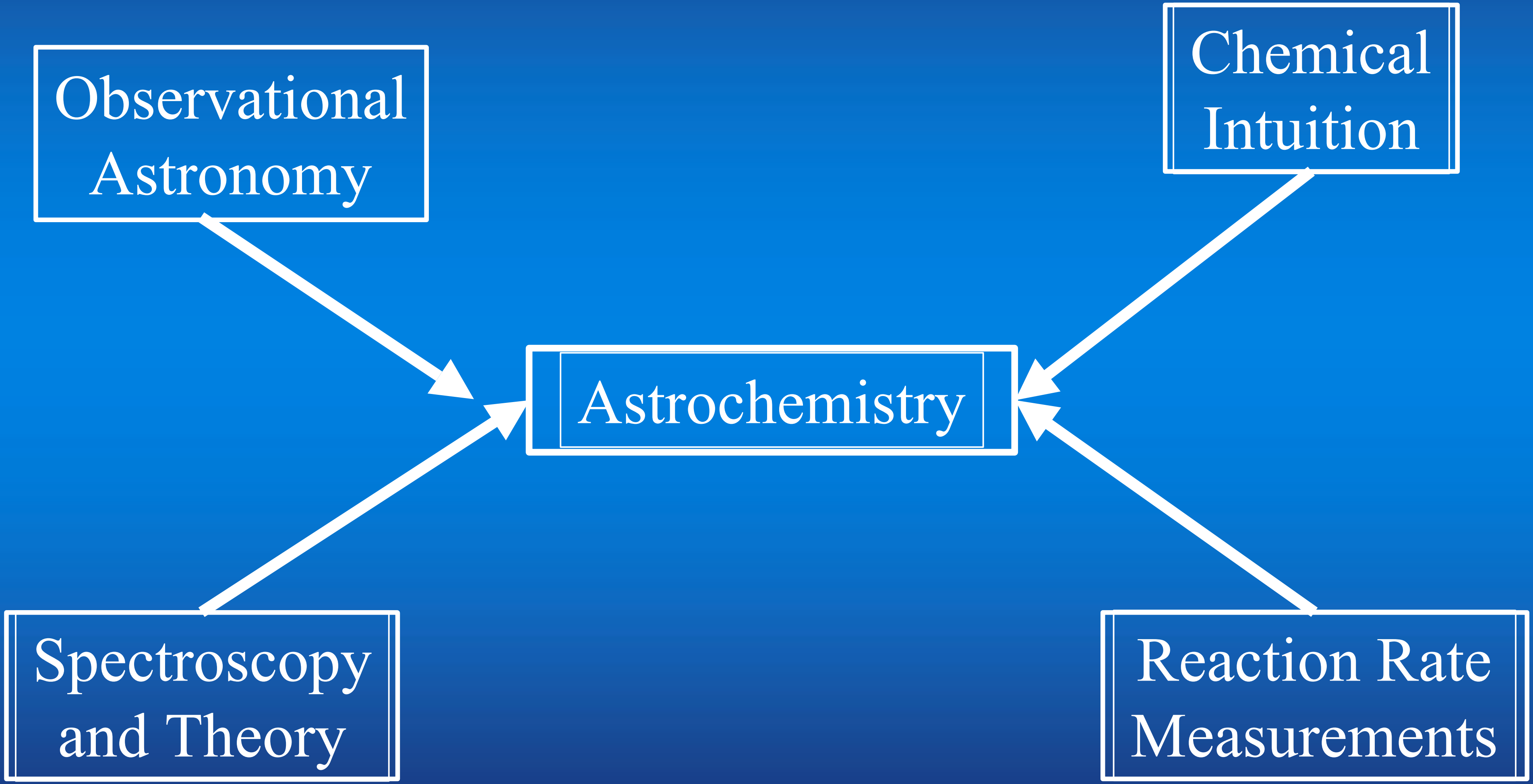
Outline

"All science is either physics or stamp collecting."

Ernest Rutherford (1871-1937)

- Basics of cosmochemistry
- Motivation to study disks
- Ionization state in disks
- Importance of disk dynamics for chemistry
- Disk and envelope around AB Aur
- Conclusions

A Difficult Topic For Discussion



Observational Astronomy

Chemical Intuition

Astrochemistry

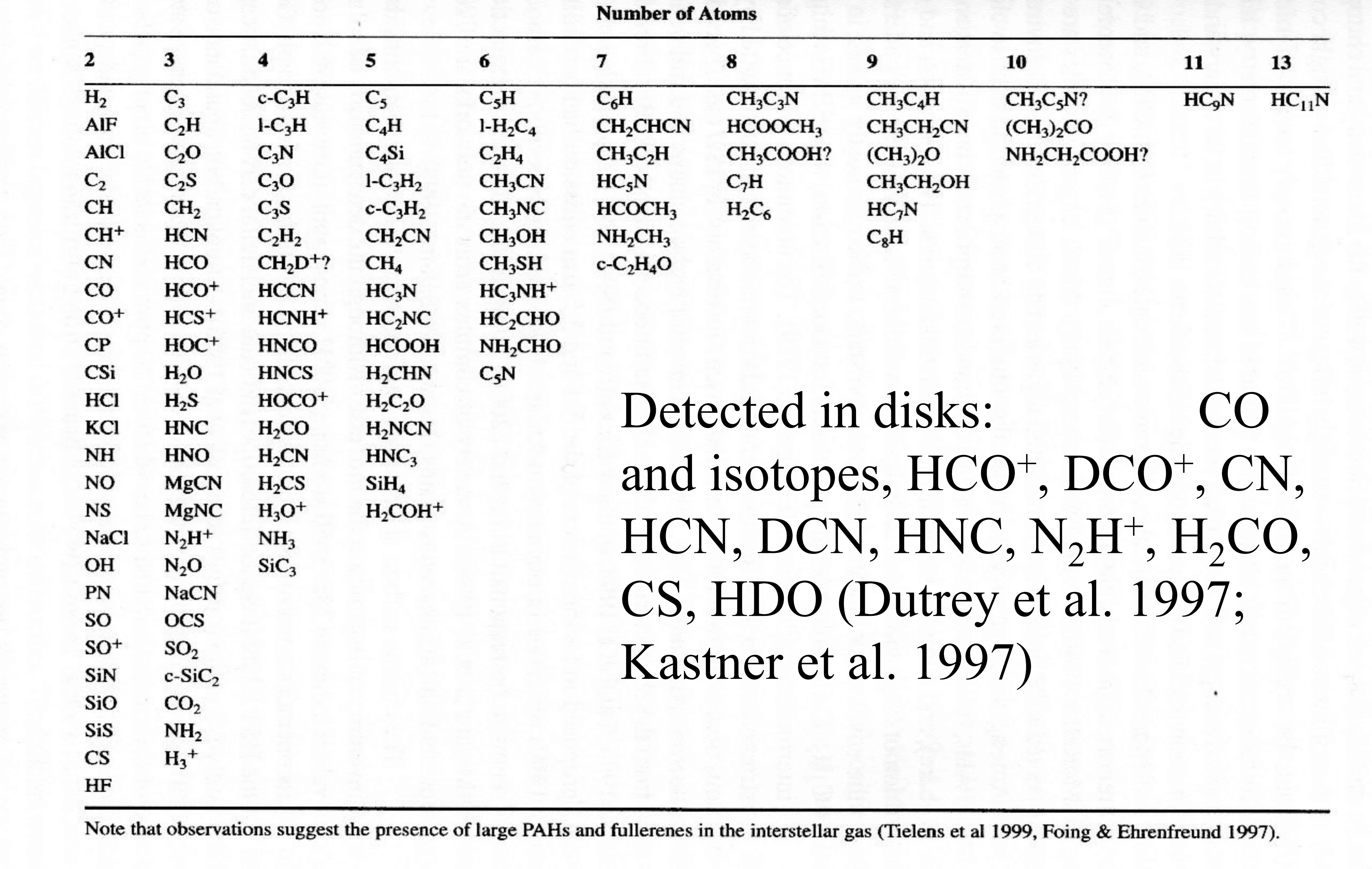
Spectroscopy and Theory

Reaction Rate Measurements

Brief History of Atoms and Molecules

- 460 BC: concept of “atom” (Democritus)
- 1800’s: experimental proof (J. Dalton)
- 1870’s: periodic table (D. Mendeleev)
- First IS atoms are claimed in 1921
- First IS molecules: CH, CN, CH^+ (1937-41)
- First theory by Bates and Spitzer (1951)
- First IS molecule in radio: OH (1963)
- 1963-72: NH_3, H_2O, H_2, H_2CO, HCO^+, etc.

Detected Interstellar Species



Number of Atoms										
2	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**13**
H_2	C_3	c-C_3H	C_5	C_5H	C_6H	CH_3C_3N	CH_3C_4H	CH_3C_5N?	HC_9N	$HC_{11}N$
AlF	C_2H	l-C_3H	C_4H	l-H_2C_4	CH_2CHCN	$HCOOCH_3$	CH_3CH_2CN	$(CH_3)_2CO$		
AlCl	C_2O	C_3N	C_4Si	C_2H_4	CH_3C_2H	CH_3COOH?	$(CH_3)_2O$	NH_2CH_2COOH?		
C_2	C_2S	C_3O	l-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2OH			
CH	CH_2	C_3S	c-C_3H_2	CH_3NC	$HCOCH_3$	H_2C_6	HC_7N			
CH^+	HCN	C_2H_2	CH_2CN	CH_3OH	NH_2CH_3		C_8H			
CN	HCO	CH_2D^+?	CH_4	CH_3SH	c-C_2H_4O					
CO	HCO^+	HCCN	HC_3N	HC_3NH^+						
CO^+	HCS^+	$HCNH^+$	HC_2NC	HC_2CHO						
CP	HOC^+	HNCO	HCOOH	NH_2CHO						
CSi	H_2O	HNCS	H_2CHN	C_5N						
HCl	H_2S	$HOCO^+$	H_2C_2O							
KCl	HNC	H_2CO	H_2NCN							
NH	HNO	H_2CN	HNC_3							
NO	MgCN	H_2CS	SiH_4							
NS	MgNC	H_3O^+	H_2COH^+							
NaCl	N_2H^+	NH_3								
OH	N_2O	SiC_3								
PN	NaCN									
SO	OCS									
SO^+	SO_2									
SiN	c-SiC_2									
SiO	CO_2									
SiS	NH_2									
CS	H_3^+									
HF										

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

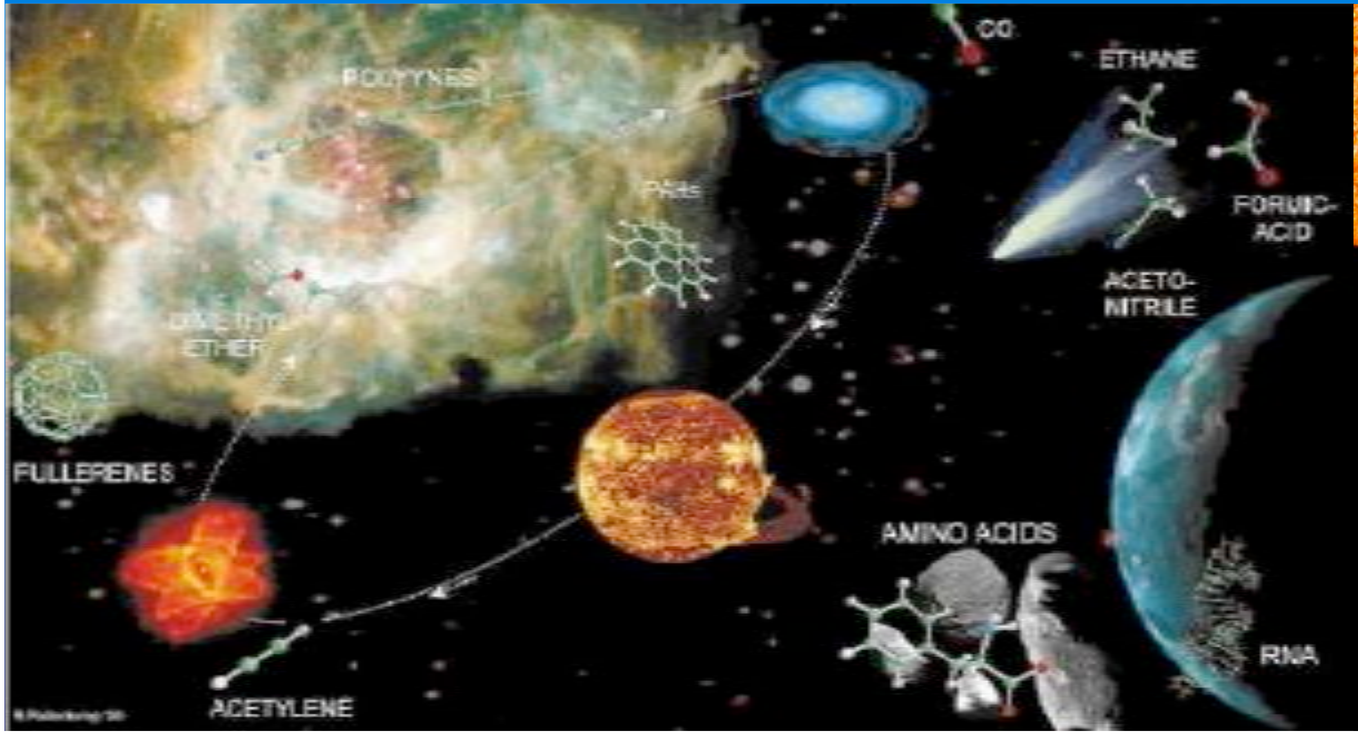
Detected in disks: CO and isotopes, HCO^+, DCO^+, CN, HCN, DCN, HNC, N_2H^+, H_2CO, CS, HDO (Dutrey et al. 1997; Kastner et al. 1997)

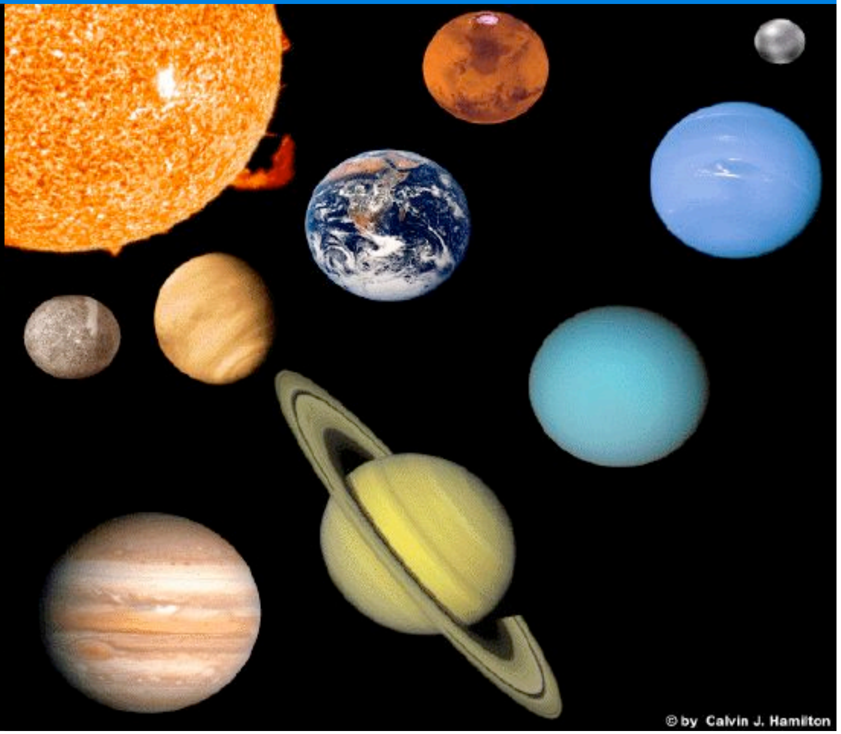
The Astronomer's Periodic Table

Courtesy of Ben McCall and Steve Charnley

Role of Molecules

- Probes of physical conditions of the source
- Cooling of gas
- Detailed information about the source (cosmic rays, elemental abundances, dust properties, ionization/magnetic fields, etc.)

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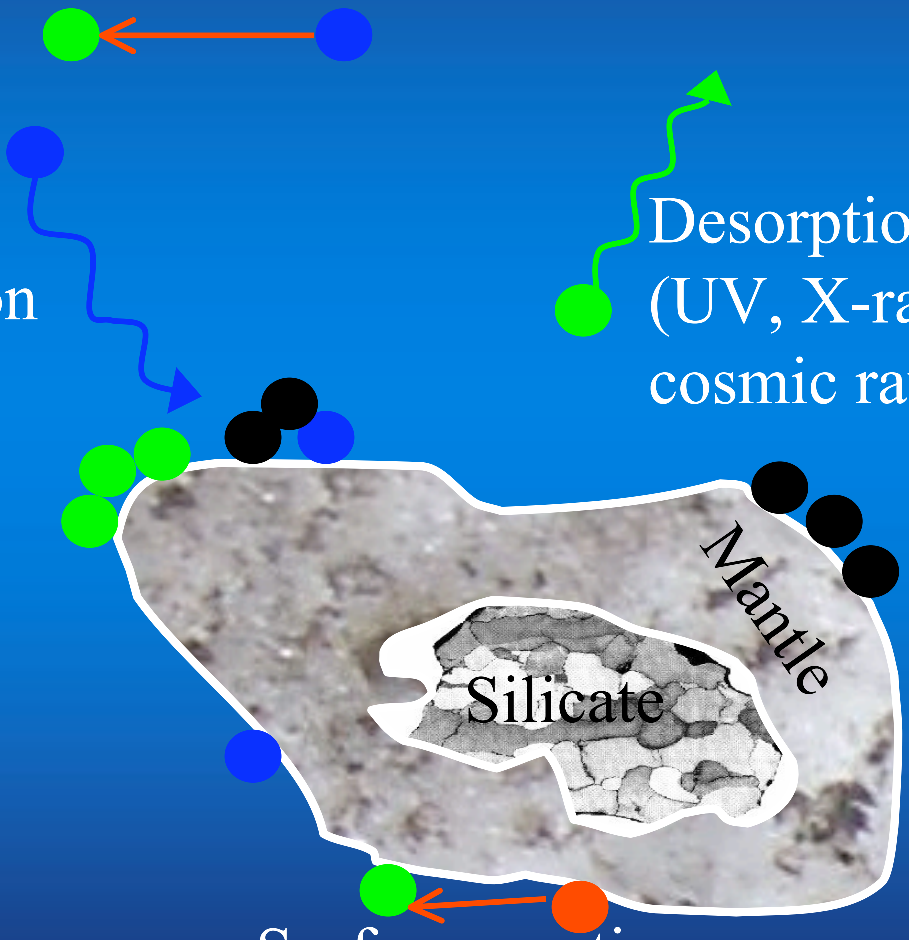
Formation and Destruction of Molecules

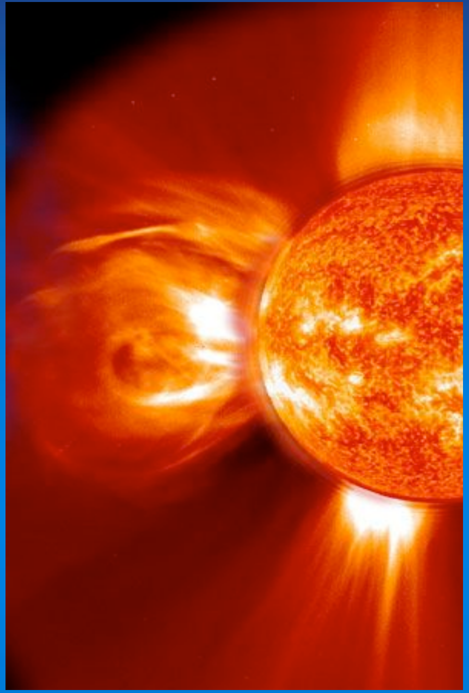


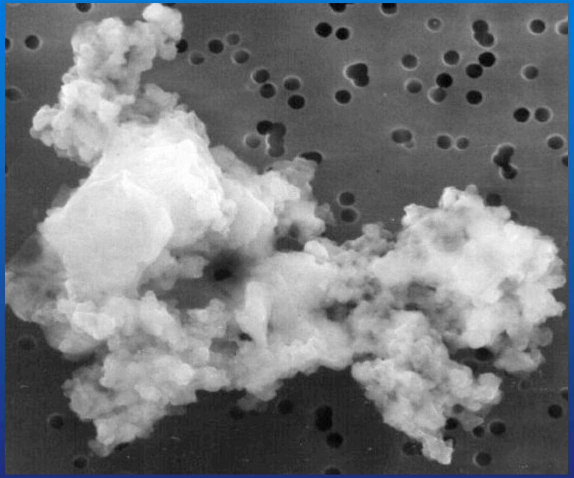
Collisions in gas phase

Accretion

Desorption
(UV, X-ray,
cosmic rays)

Surface reaction
(thermal hopping)





Important Reactions

- Ionization: $H + h\nu, X, CRP \Rightarrow H^+ + e^-$
- Photodissociation: $CH \Rightarrow C + H$
- Charge exchange: $H^+ + O \Rightarrow H + O^+$
- Atom exchange: $O^+ + H_2 \Rightarrow OH^+ + H$
- Radiative association: $H + C \Rightarrow CH + h\nu$
- Neutral-neutral: $CH + NO \Rightarrow HCN + O$
- Ion-molecule: $H_3^+ + CO \Rightarrow H_2 + HCO^+$
- Dissociative rec.: $H_3O^+ + e^- \Rightarrow H_2O + H$
- Surface reactions: $H + O \Rightarrow OH$

(yellow – effective at low temperatures)

Chemical Reaction Databases

- Ohio State University (OSU): 4300 reactions, 430 species, 12 elements
- Manchester University (UMIST):
  - Rate95: 4000 reactions, 400 species, 12 elements
  - Rate07: 4600 reactions, 420 species, 12 elements

  (www.udfa.net)
- NIST Chemical Kinetics Database: ~30,000 neutral-neutral reactions, theory and experiment, generate best fit
- JPL (Anicich): Compilation of all ion-molecule reactions with references

Courtesy of Eric Herbst

Chemical Reaction Databases

- About 10-20% of all reactions have accurately determined rates
- Extrapolation of rates on low T
- Many neutral-neutral reaction rates were “guessed”
- Branching ratios are not well constrained
- Photorates are based on 1D plane-parallel UV model
- Scarse X-ray chemistry
- Unknown surface chemistry / desorption energies

> *“Errors using inadequate data are much less than those using no data at all.”*
>
> Charles Babbage (1792-1871)

Time-Dependent Chemistry Modeling

$$\frac{\partial n_i}{\partial t} = \sum_{j,k\neq i} k_{jk} n_j n_k - n_i \sum_l k_l n_l + \nabla D n_{\mathrm{H2}} \nabla n_i / n_{\mathrm{H2}} - \nabla U n_i$$

Evolution = Formation - Destruction + Diffusion + Advection

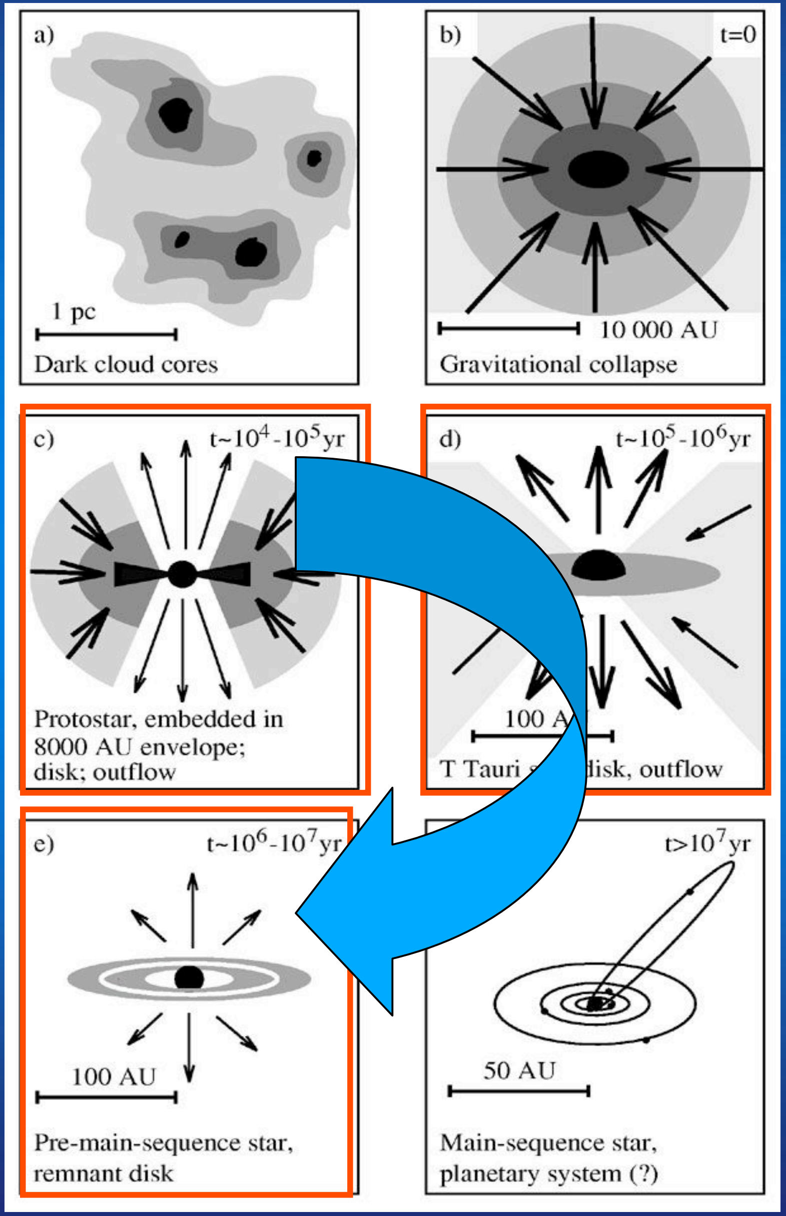
[Chemistry] [Dynamics]

Input information:

- Physical conditions, diffusion coefficient & flow data
- Initial abundances of species
- Chemical network
- Numerical solver
- Benchmarking

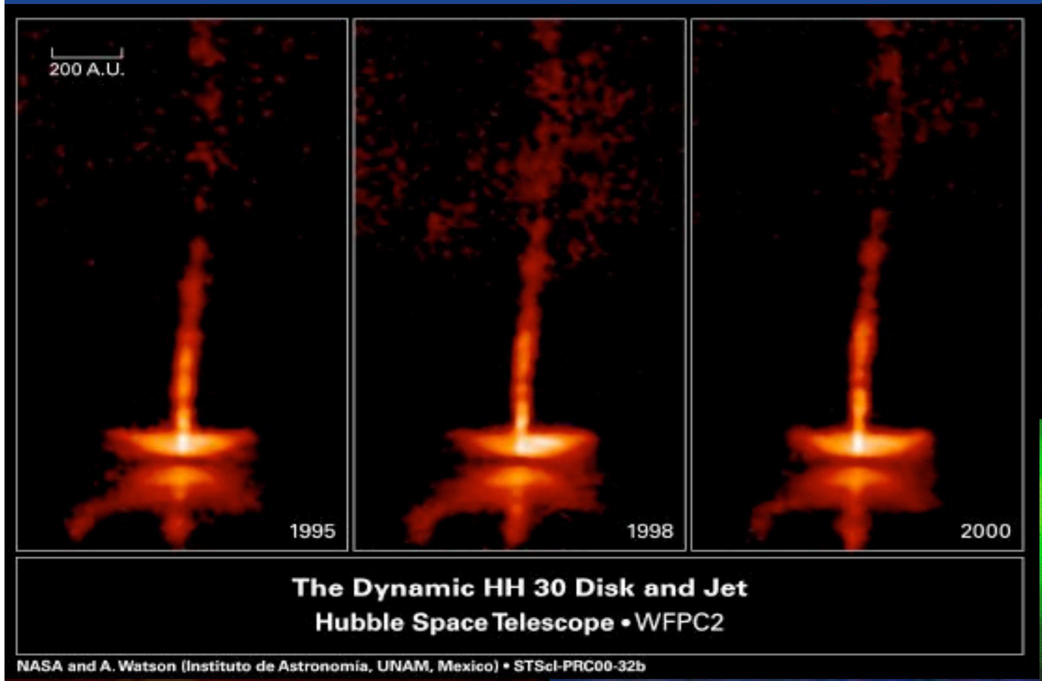
Motivation to Study Protoplanetary Disks

- Initial conditions for planet formation
- Composition of primitive bodies in the solar system
- Gas depletion and dissipation in disks – Molecules as tracers of disk evolutionary history
- Chemistry – Physical state of the disk (temperature, density, radiation, ionization, transport)



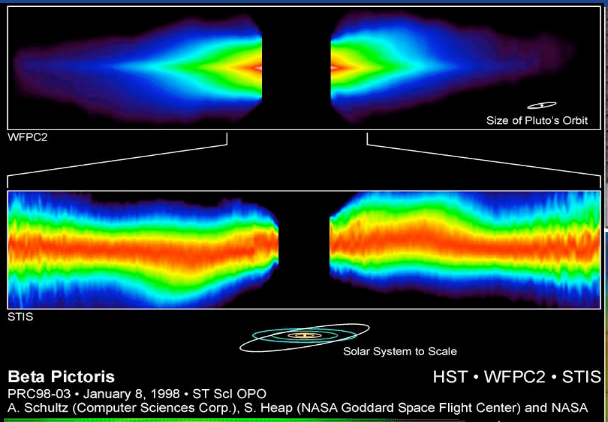
Hogerheijde (1999)

Disk Bestiary

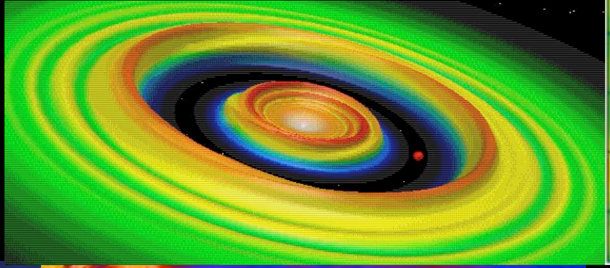


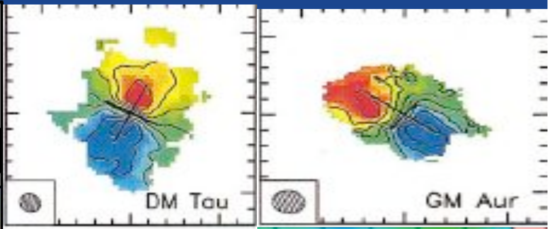
The Dynamic HH 30 Disk and Jet
Hubble Space Telescope • WFPC2

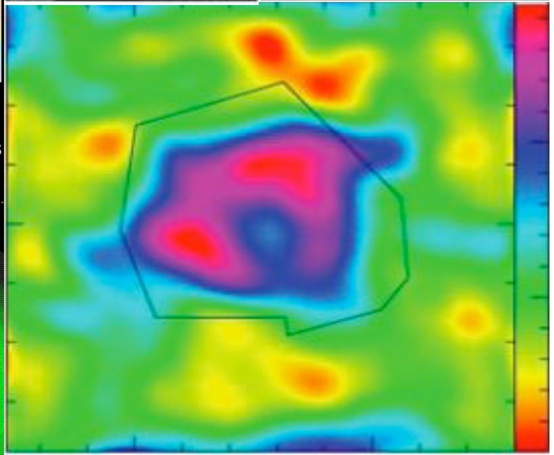
NASA and A. Watson (Instituto de Astronomía, UNAM, Mexico) • STScI-PRC00-32b

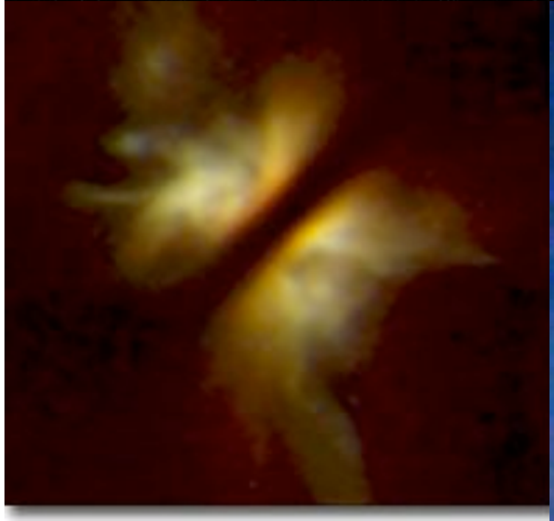


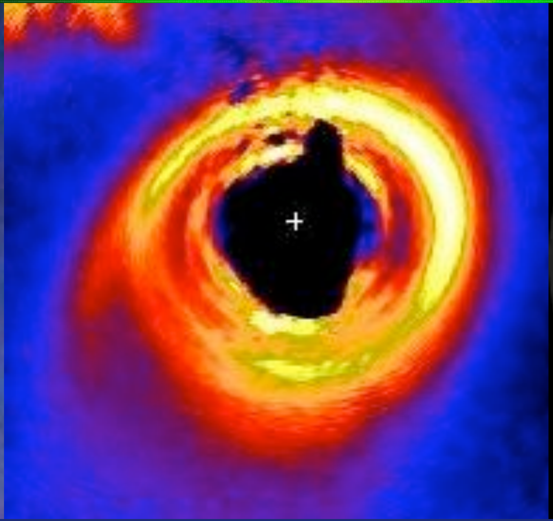
Beta Pictoris HST • WFPC2 • STIS
PRC98-03 • January 8, 1998 • ST ScI OPO
A. Schultz (Computer Sciences Corp.), S. Heap (NASA Goddard Space Flight Center) and NASA

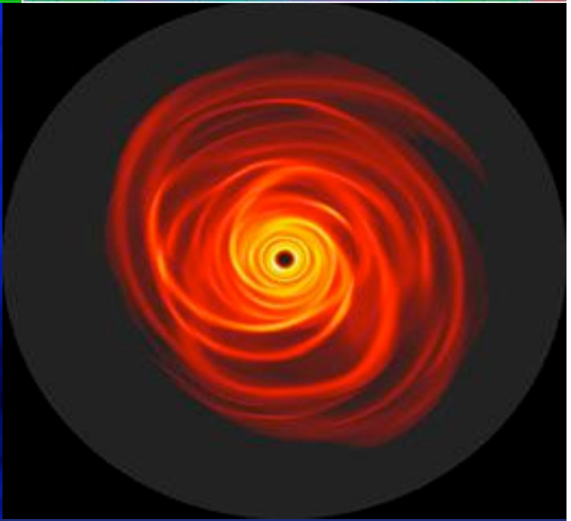






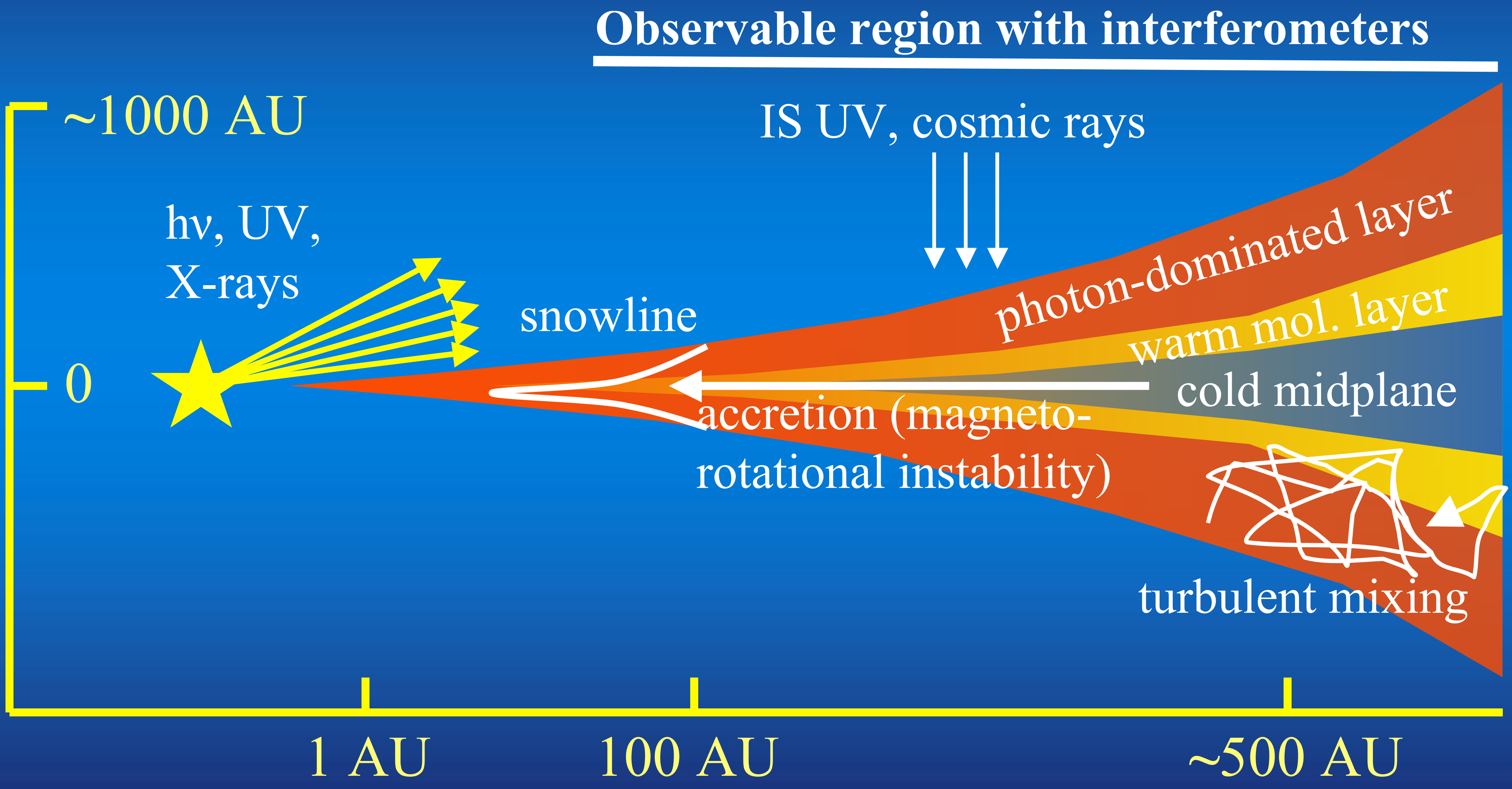






Courtesy of NASA, NRAO, Cornell Univ., IRAM, etc.

Disk Structure

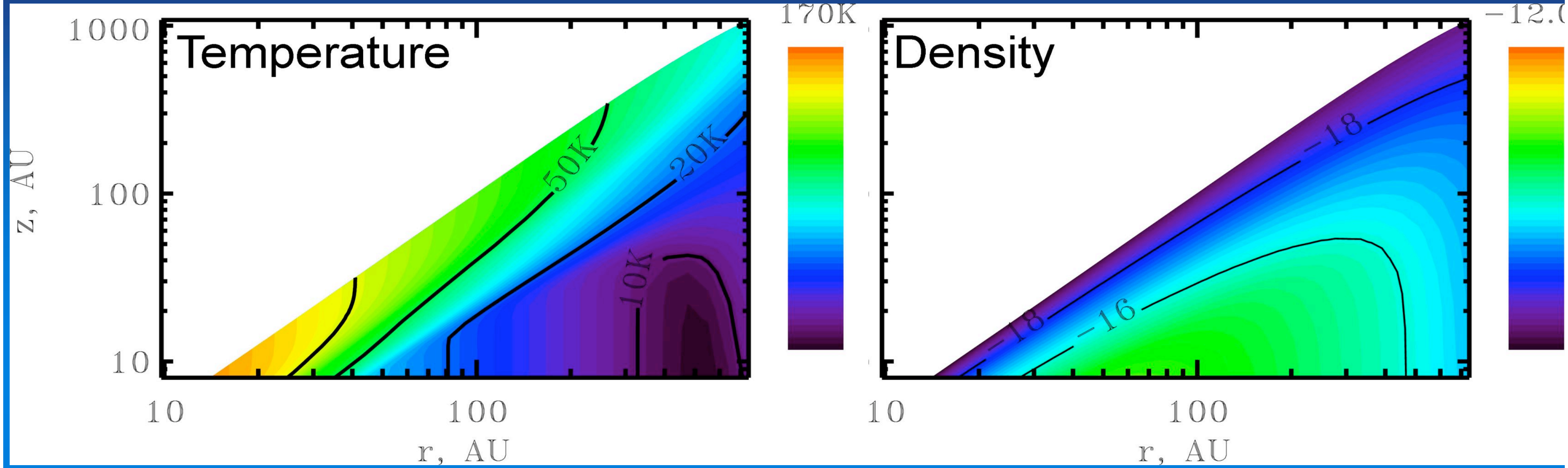


Results: I. Ionization Degree in Disks

- Angular momentum transport via MHD turbulence (Balbus & Hawley 1991)
- Low ionization implies non-ideal MHD regime but often simple chemical equilibrium is used
- “Dead” zone size and location

(Semenov, Wiebe, Henning, 2004, A&A, 417, 93)

Disk Physical Model



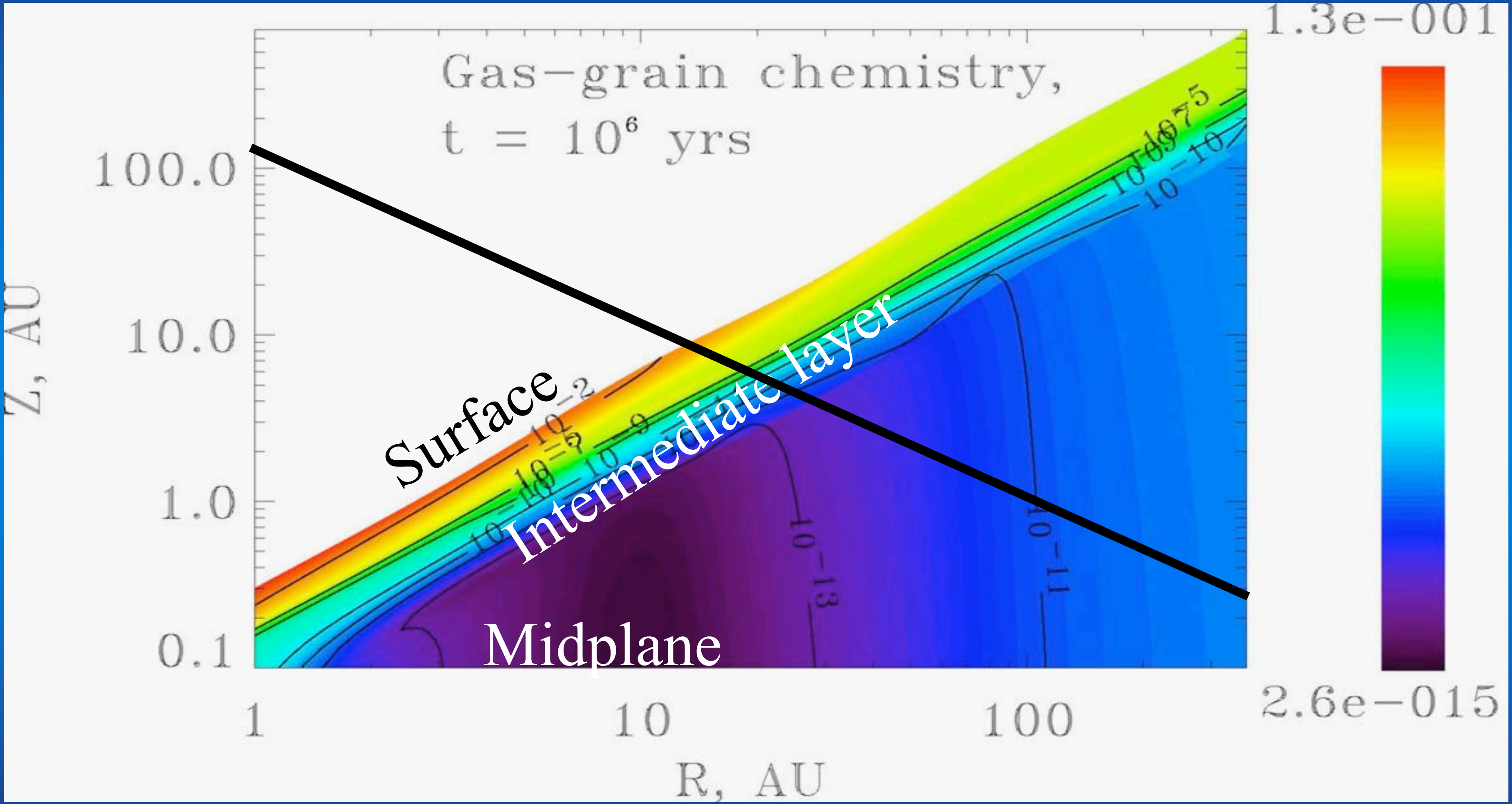
- Steady-state flared disk of D‘Alessio et al. (1999)
- Mass: 0.05-0.5M_{sun}, radius: 200-800 AU, α=0.01-01
- Grain size distribution (mostly sub-micron particles)

Disk Chemical Model

- Updated UMIST’95 network
- Limited deuterium chemistry
- High-energy sources: X-ray, UV, cosmic ray particles
- Gas-grain interactions: accretion, desorption
- Surface chemistry
- Atomic/Molecular initial abundances
- Evolution over a few Myr

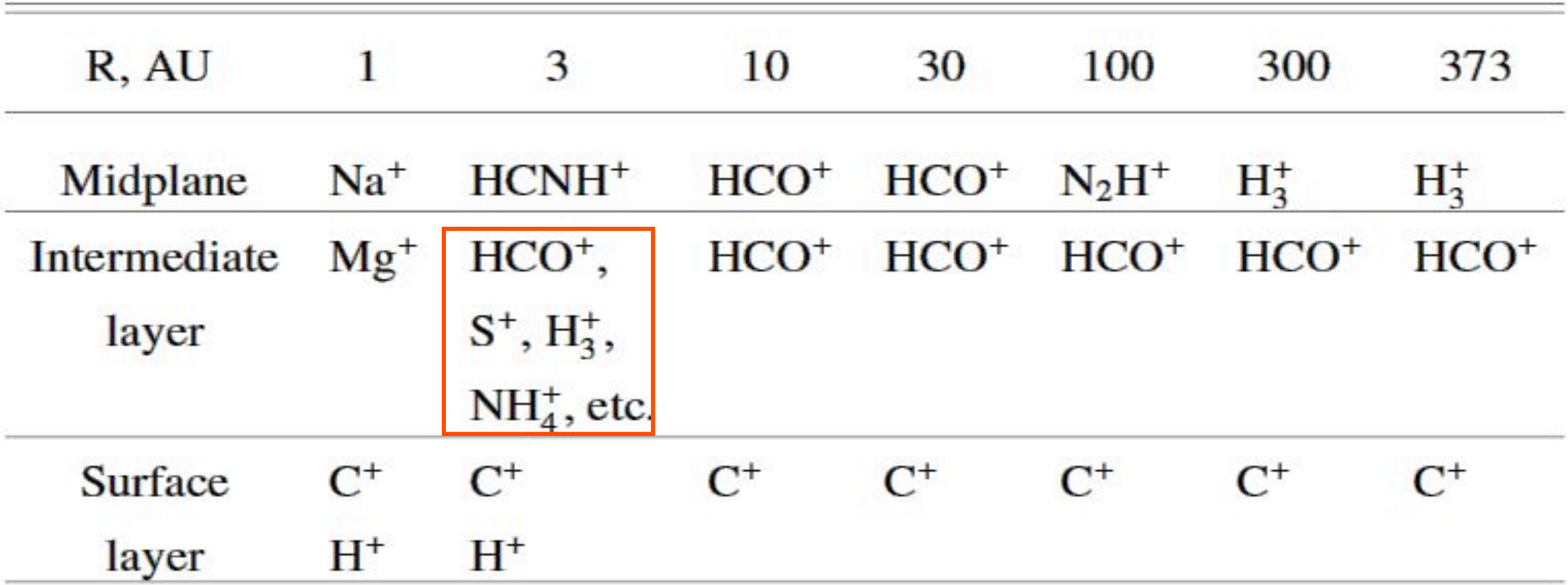
(Semenov et al., 2004-06)

Ionization Structure at 1 Myr



„Layered“ vertical structure

Dominant Ions at 1 Myr

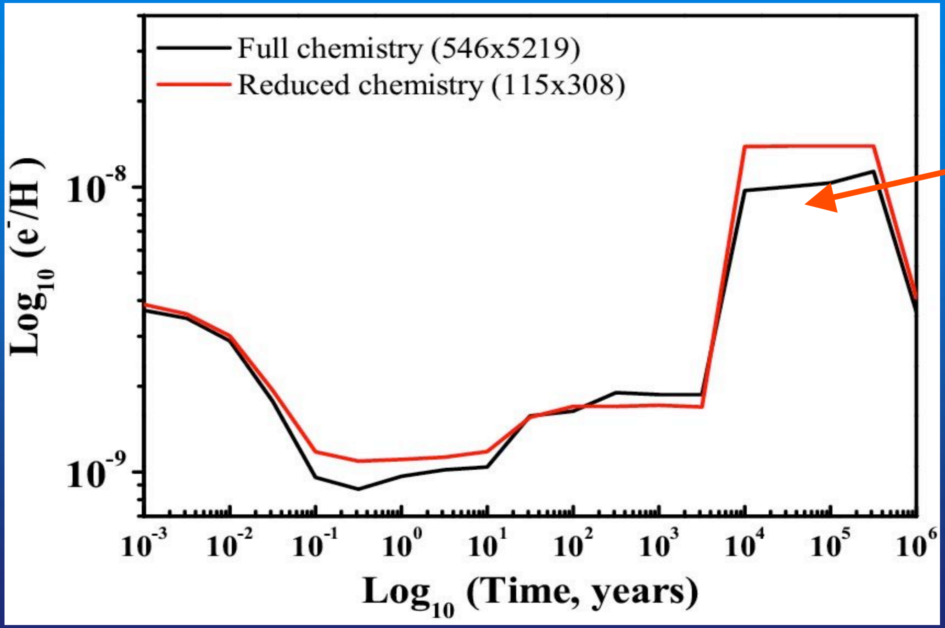


R, AU	1	3	10	30	100	300	373
Midplane	Na^+	$HCNH^+$	HCO^+	HCO^+	N_2H^+	H_3^+	H_3^+
Intermediate layer	Mg^+	HCO^+, S^+, H_3^+, NH_4^+, etc.	HCO^+	HCO^+	HCO^+	HCO^+	HCO^+
Surface layer	C^+ H^+	C^+ H^+	C^+	C^+	C^+	C^+	C^+

C^+ is the most abundant ion,
HCO^+ is the most abundant observable ion

Chemical Stratification

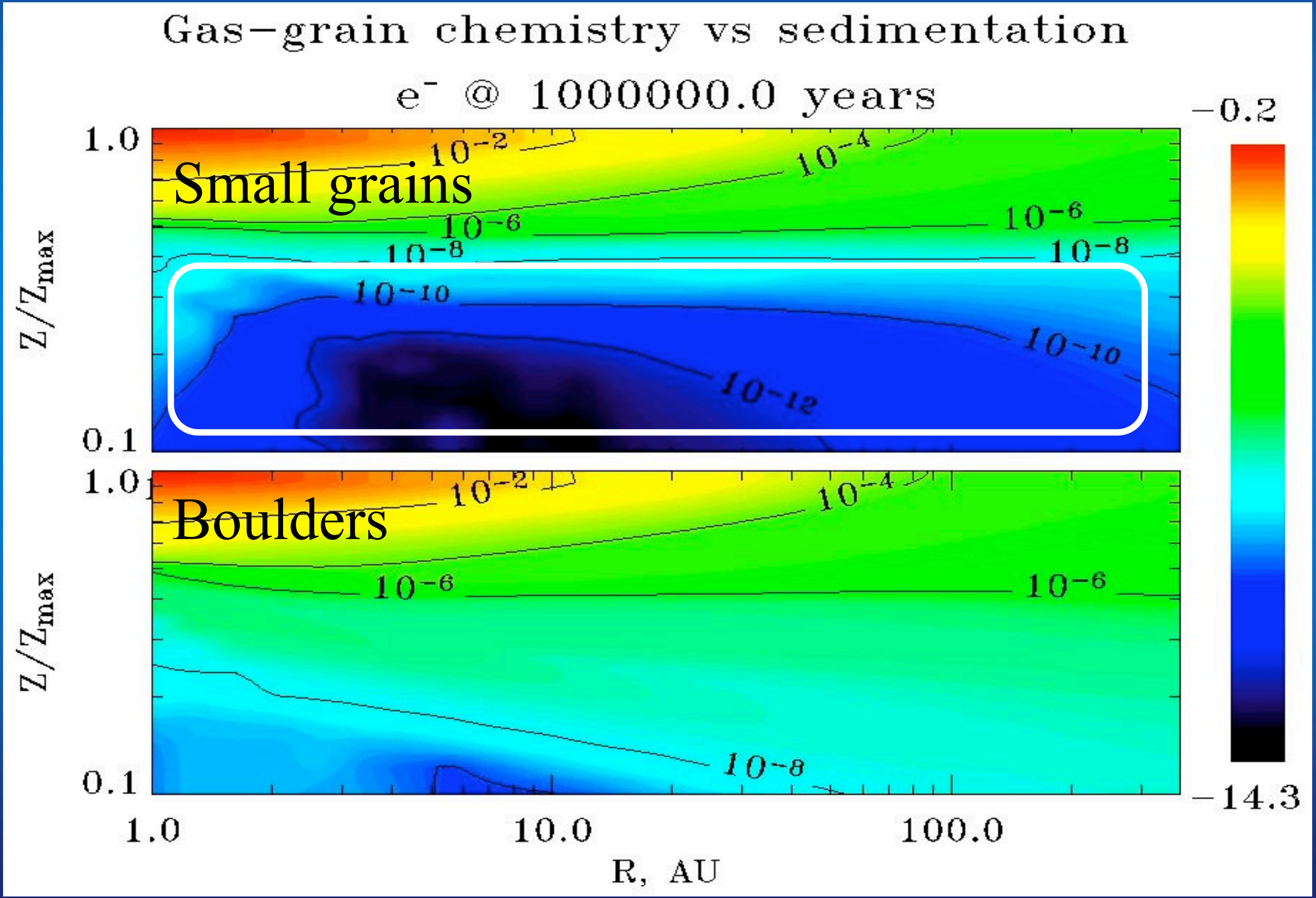
- Surface (~10 species, 20 reactions, ~1,000 yrs):
  Photochemistry driven by stellar X-rays and UV
- Midplane (~20 species, 50 reactions, ~10,000 yrs):
  “Dark” chemistry (cosmic rays, RN) with freeze out
- Intermediate layer (~100 species, 300 reactions):
  “Rich” molecular chemistry (X-rays), no equilibrium!



Surface reactions!

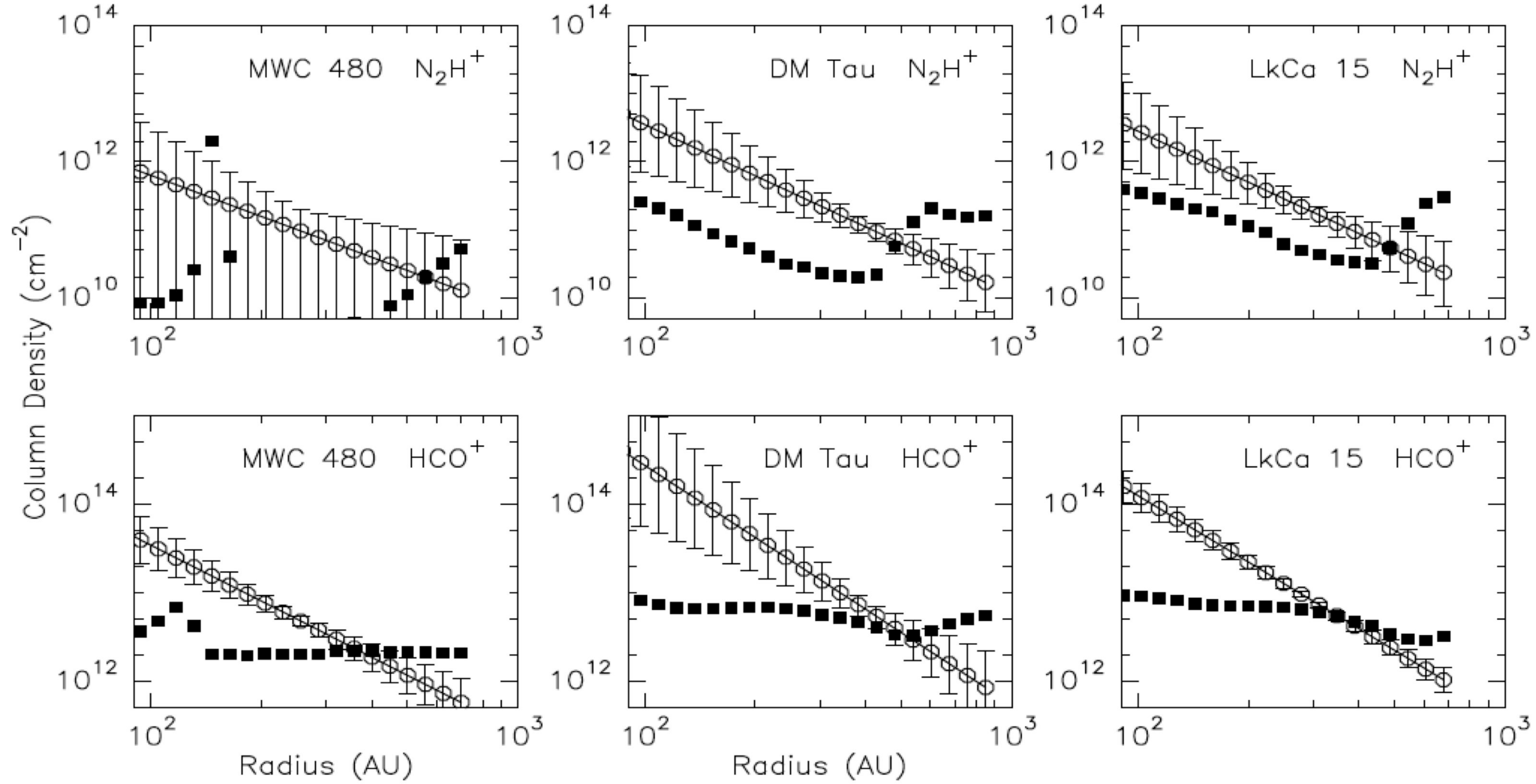
Chemical equlibrium is not reached in the inner disk zone

Ionization Structure: Effect of Grain Evolution



Observed N_2H^+ and HCO^+:

(„CID“: Bordeaux – Heidelberg – Jena – Grenoble - Paris)



(Dutrey, Henning et al. 2007, A&A, arXiv:astro-ph/0612534)

II. Turbulence in Disks

Theoretical Milestones:

- Anomalous viscosity (von Weizsäcker, early 40s)
- Alpha-model of disks (Shakura & Sunyaev 1973)
- Magnetorotational instability (Balbus & Hawley 1991)

Observational Hints:

- Non-thermal line broadening (~100 m/s)
- Crystalline silicates in comets and outer disk regions (van Boeckel et al. 2005, Wooden et al. 2005)
- Gas-phase CO at T<20K in DM Tau (Dartois et al. 2003)

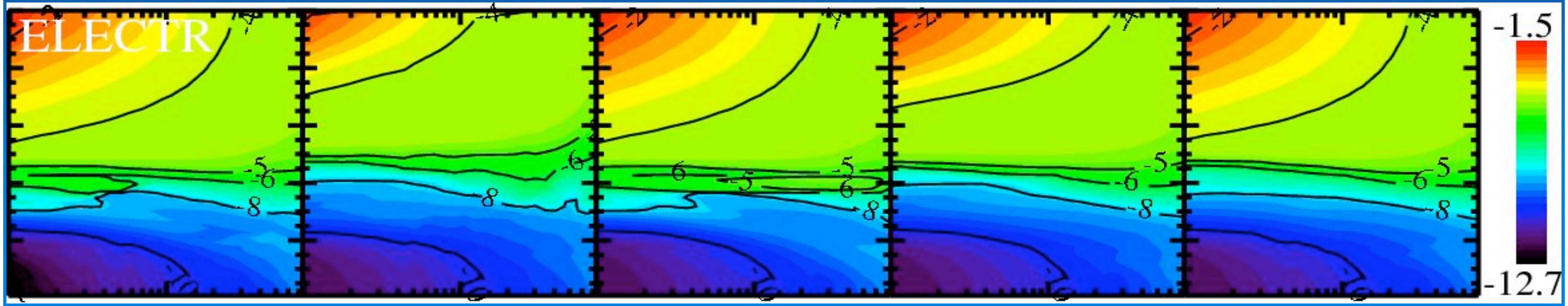
Previous Results

- Layered disk structure is preserved
- Ionization degree is not affected
- Many species abundances are increased
- CO_2 formation in inner zone (<10 AU)
- Oxygen isotopic anomaly in Solar Nebula
- Better agreement with observations (1D-model)

Gail & Tscharnuter (>2000), Ilgner et al. (2004, 2006),
Lyons & Young (2005), Willacy et al. (2006)

New: Disk Ionization Degree

Static 1D-Vertical 1D-Radial 2D-Mixing 2D-Mixing/100



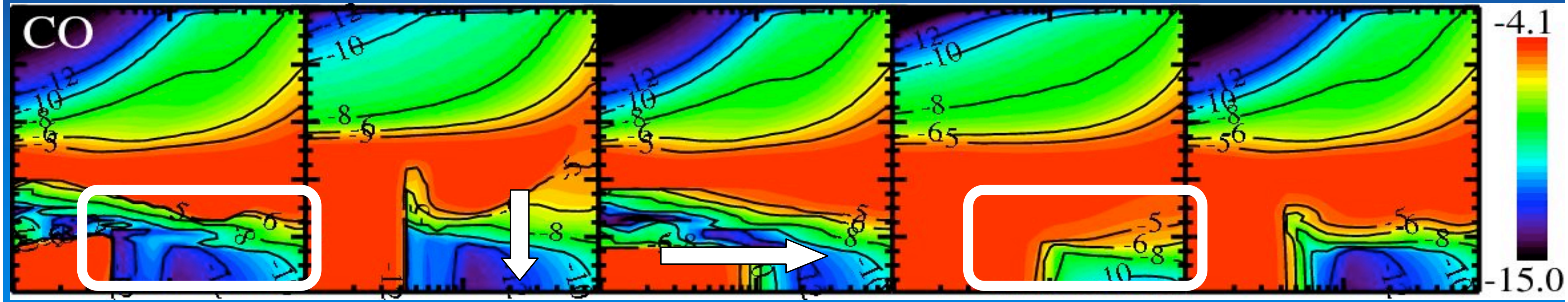
10 AU 800 AU

Comp: 2h 48h 24h 7days

Chemical equilibrium is faster then dynamics
(~1,000 vs 10,000 years)

New: Cold CO Gas

Static 1D-Vertical 1D-Radial 2D-Mixing 2D-Mixing/100

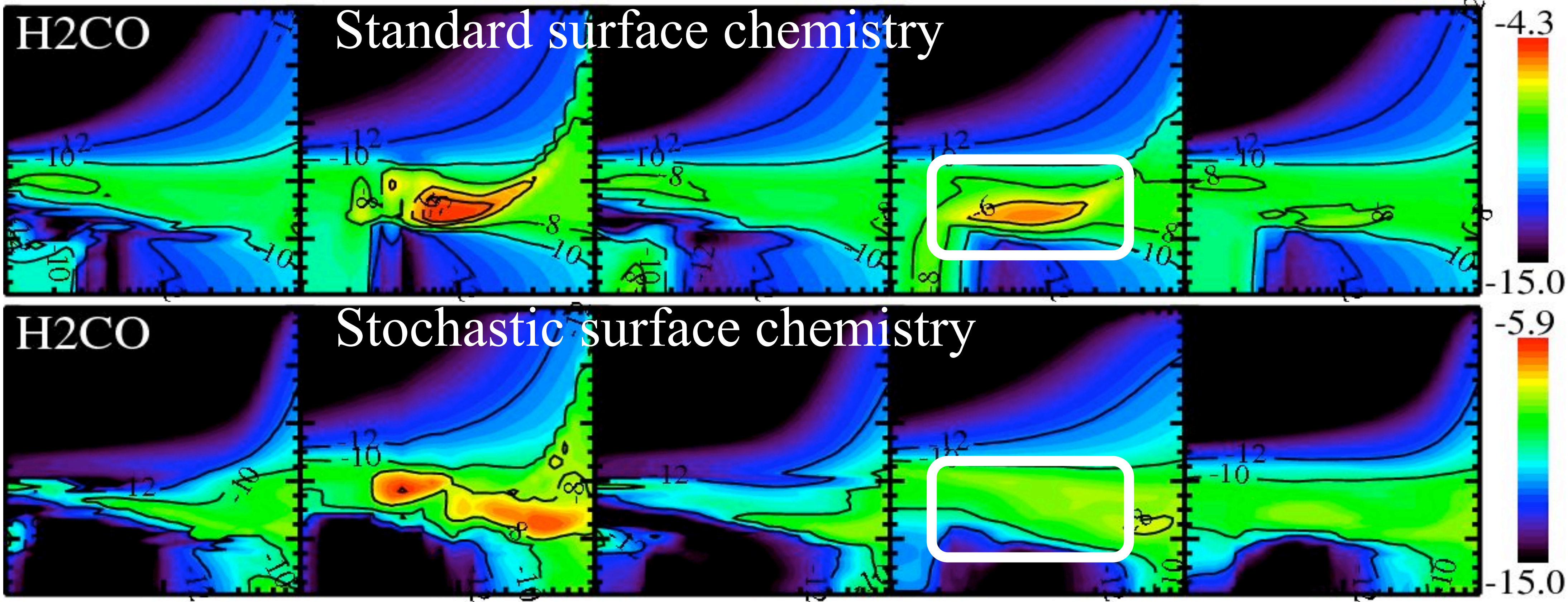


10 AU 800 AU

Effective transport of CO (2D-model)
supports the observations of Dartois et al. (2003)

New: Gas-phase H_2CO

Static 1D-Vertical 1D-Radial 2D-Mixing 2D-Mixing/100



Standard surface chemistry

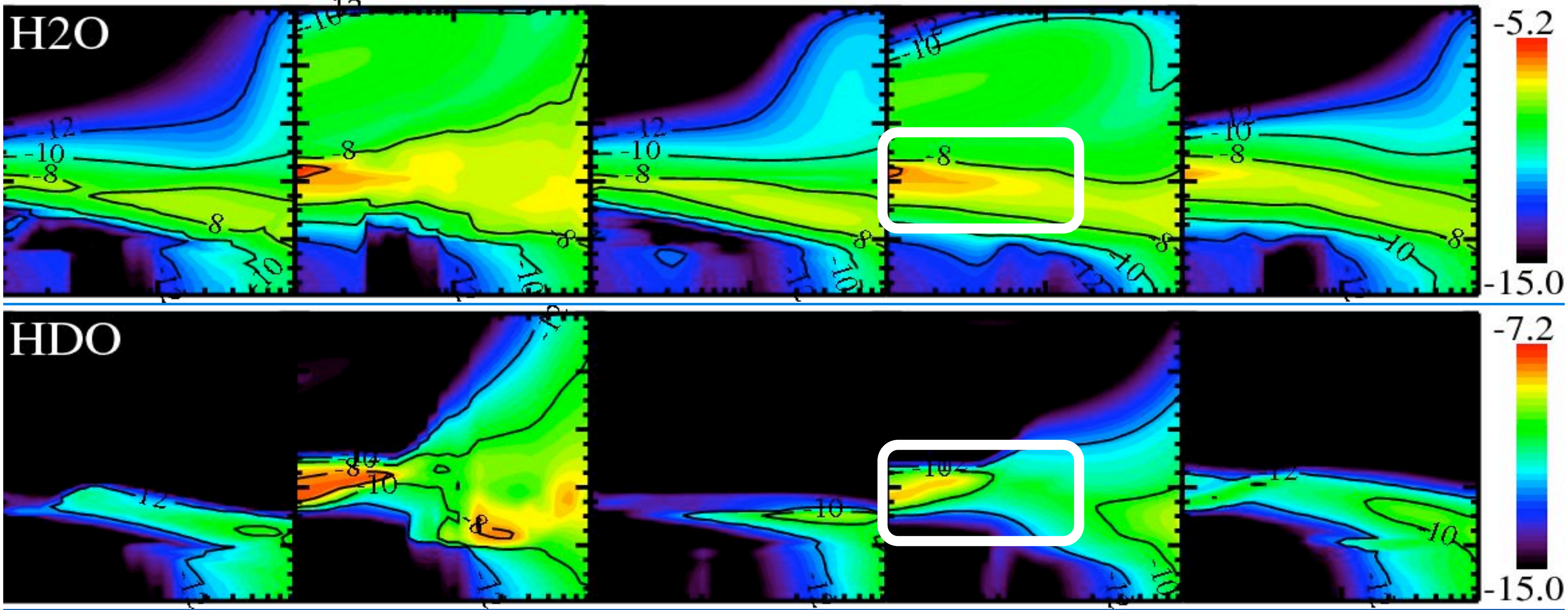
Stochastic surface chemistry

10 AU 800 AU

H_2CO abundances are sensitive to the details of surface chemistry

New: Gas-phase H_2O and HDO

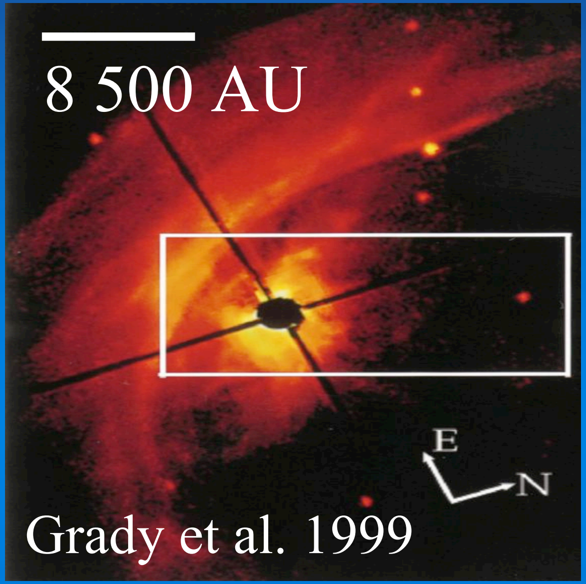
Static 1D-Vertical 1D-Radial 2D-Mixing 2D-Mixing/100



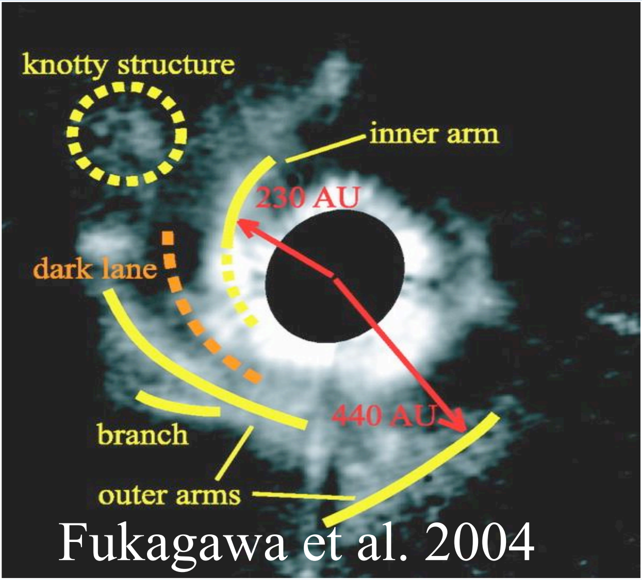
10 AU 800 AU

More gas-phase water in planet-forming zone

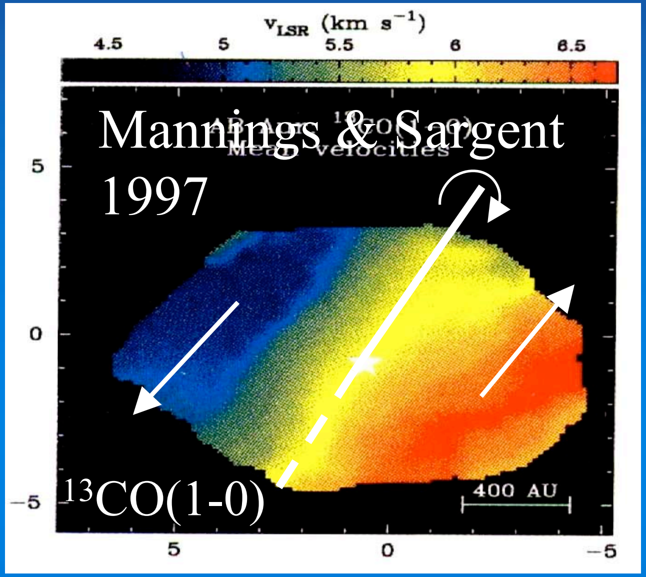
III. Observations and Modeling of AB Aur



Grady et al. 1999



Fukagawa et al. 2004



Mannings & Sargent 1997

Star: Herbig Ae, 140pc, 10 000K, $\approx 2.5 M_{\rm Sun}$, $\sim$ 2Myr

Rotating disk: $\sim$ 400 AU, $\sim 0.01 M_{\rm Sun}$

Envelope: diffuse, $\sim$ 35000 AU, $\sim 1 M_{\rm Sun}$

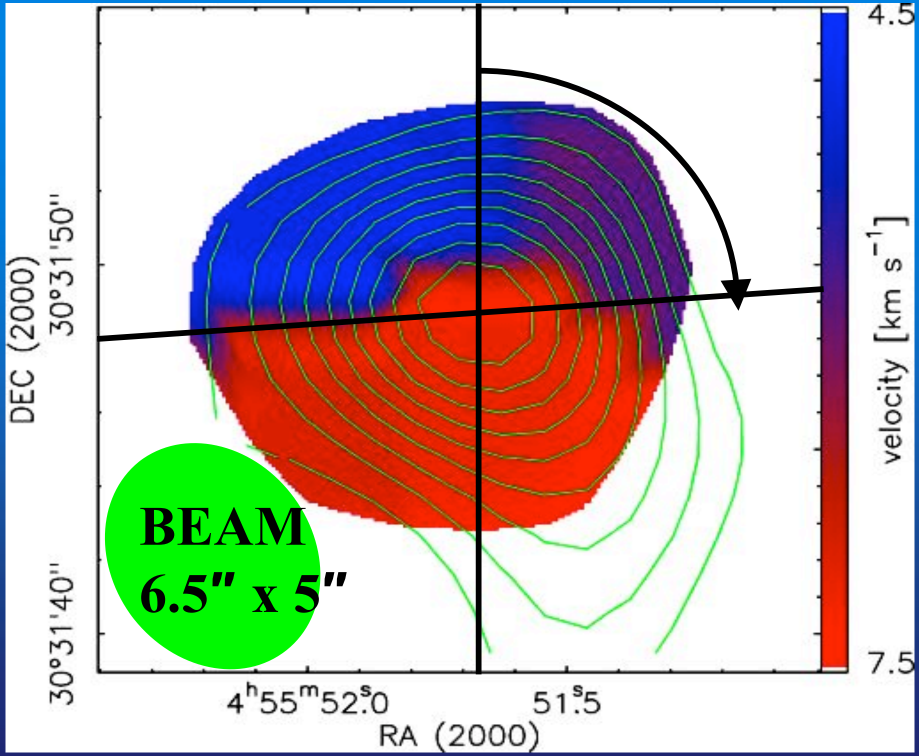
Sub-millimeter Observations

IRAM 30-m antenna: HCO^+, DCO^+, CO, $C^{18}O$, HCN, HNC, CN, H_2CO, SiO, CS @ 10"–30"

(~ 1500 – 4500 AU)

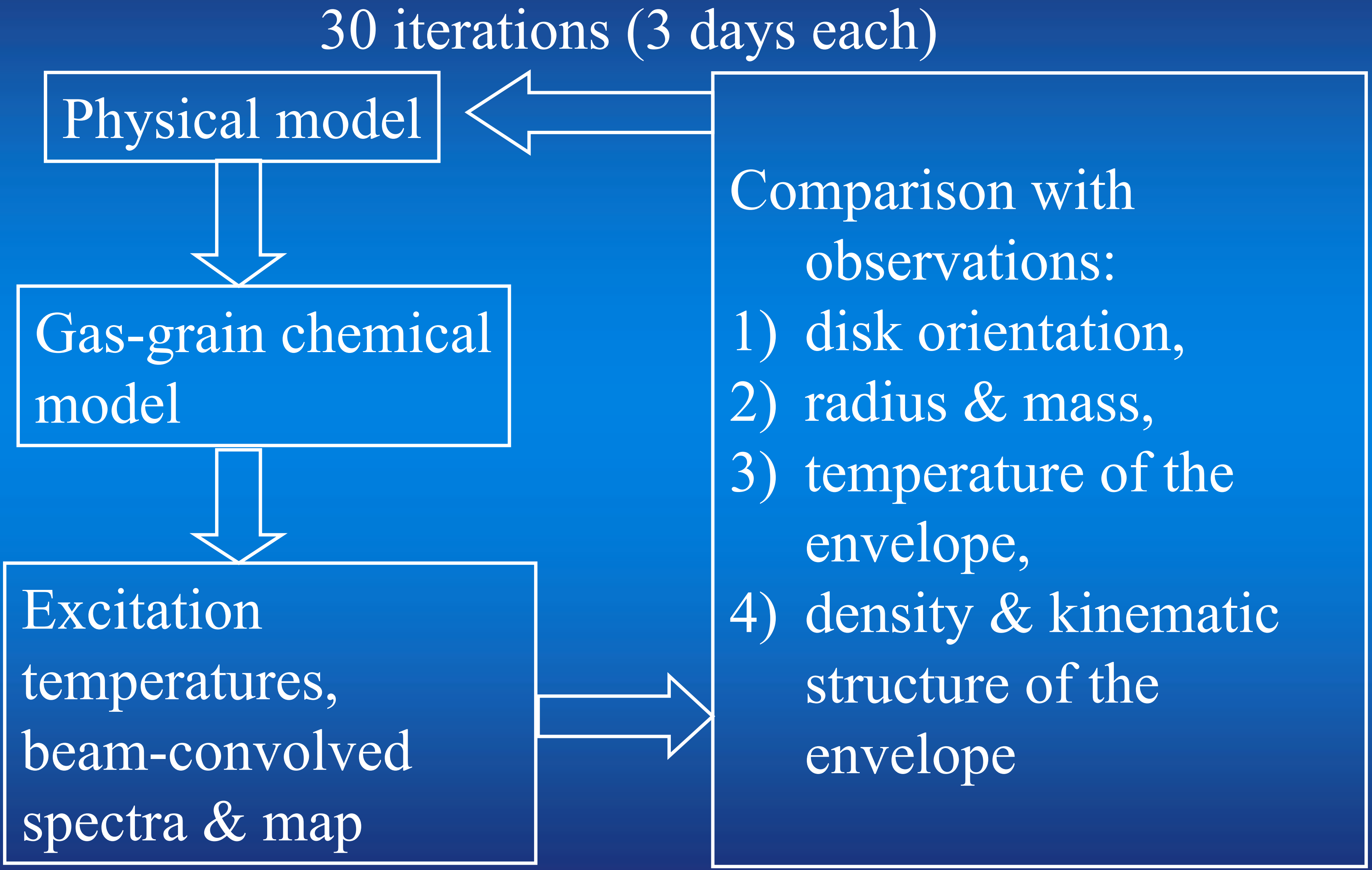
Plateau de Bure interferometer (5x15-m antennas):

HCO^+ (1-0) @ 5.1" x 6.8" (~ 850 AU)



Face-on rotating disk ($r \leq$ 1000 AU), positional angle ~ 80°

„Step-by-step“ Modeling Scheme



30 iterations (3 days each)

Physical model

Gas-grain chemical model

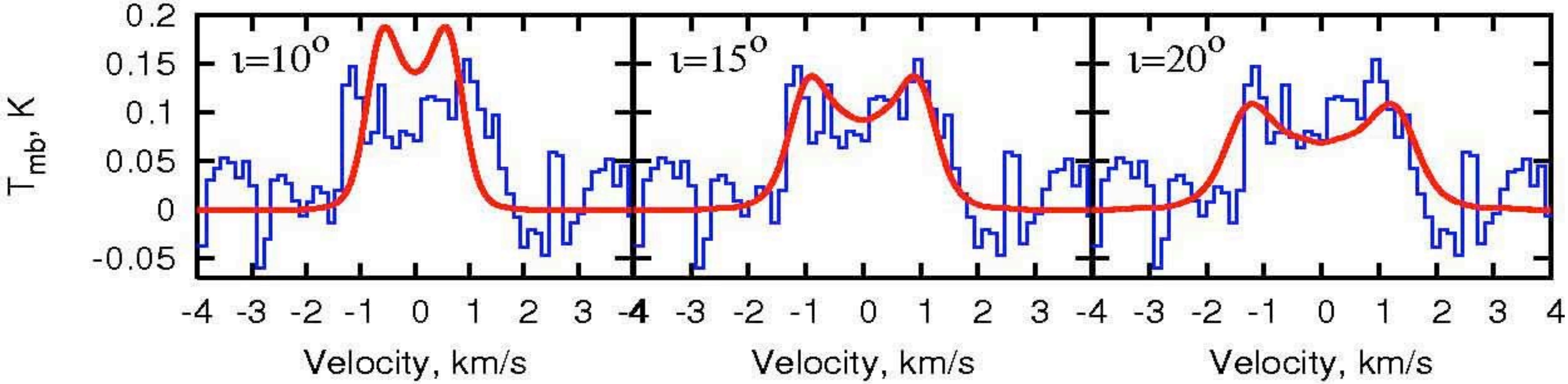
Excitation temperatures, beam-convolved spectra & map

Comparison with observations:

1) disk orientation,
2) radius & mass,
3) temperature of the envelope,
4) density & kinematic structure of the envelope

Orientation

(Semenov et al., 2005, ApJ, 621, 853)

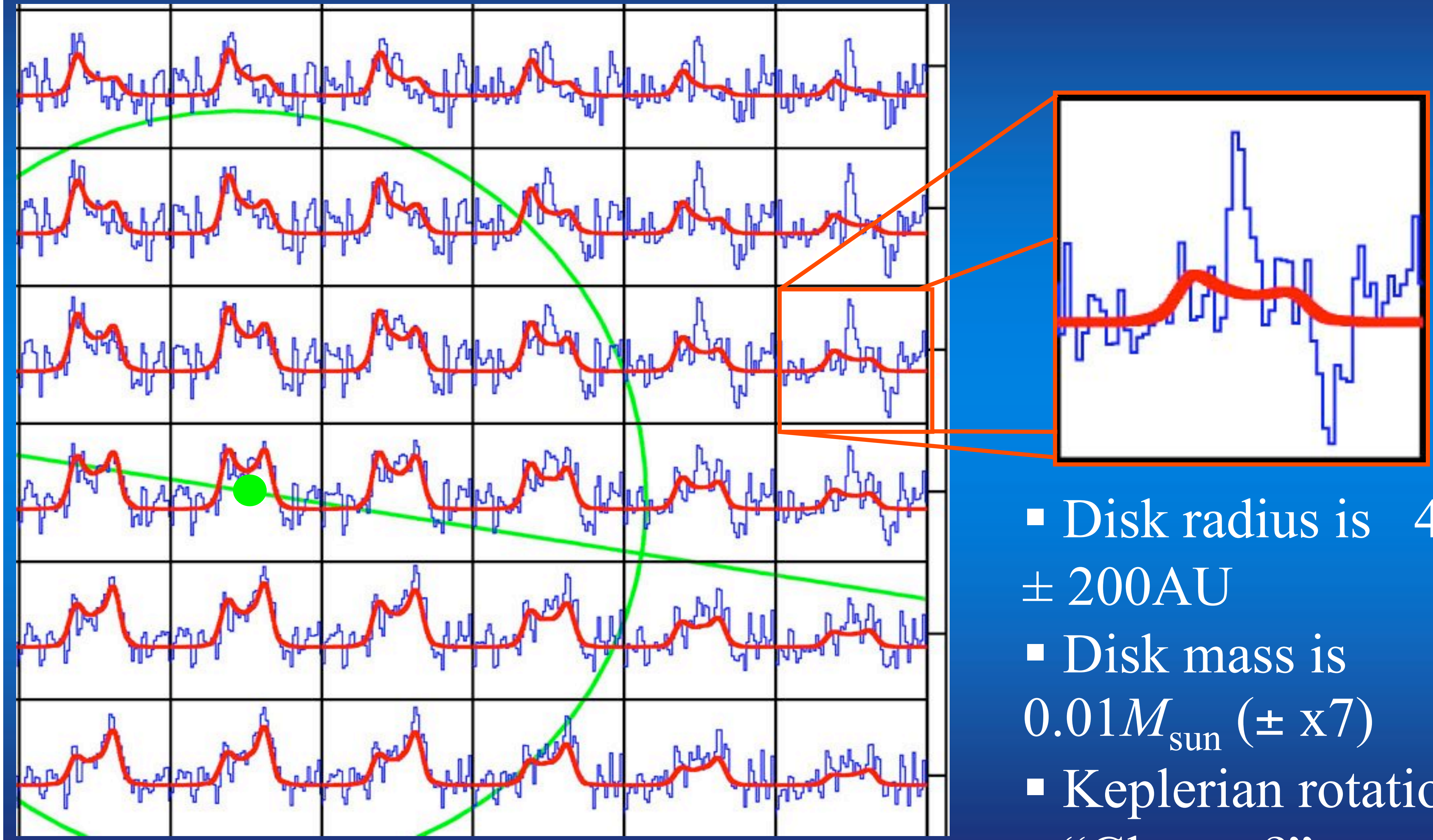


(depends on the stellar mass and disk density gradient)

Inclination angle (width): $i = 17^{+6°}_{-3}$

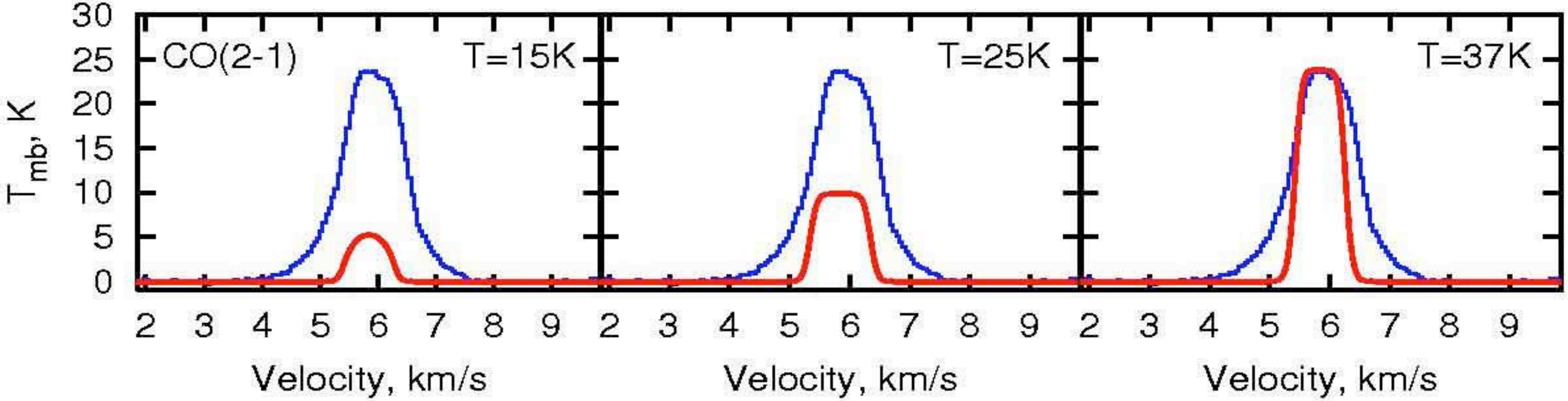
Positional angle (shape): $\varphi = 80° \pm 30°$

HCO^+(1-0) Interferometric Map



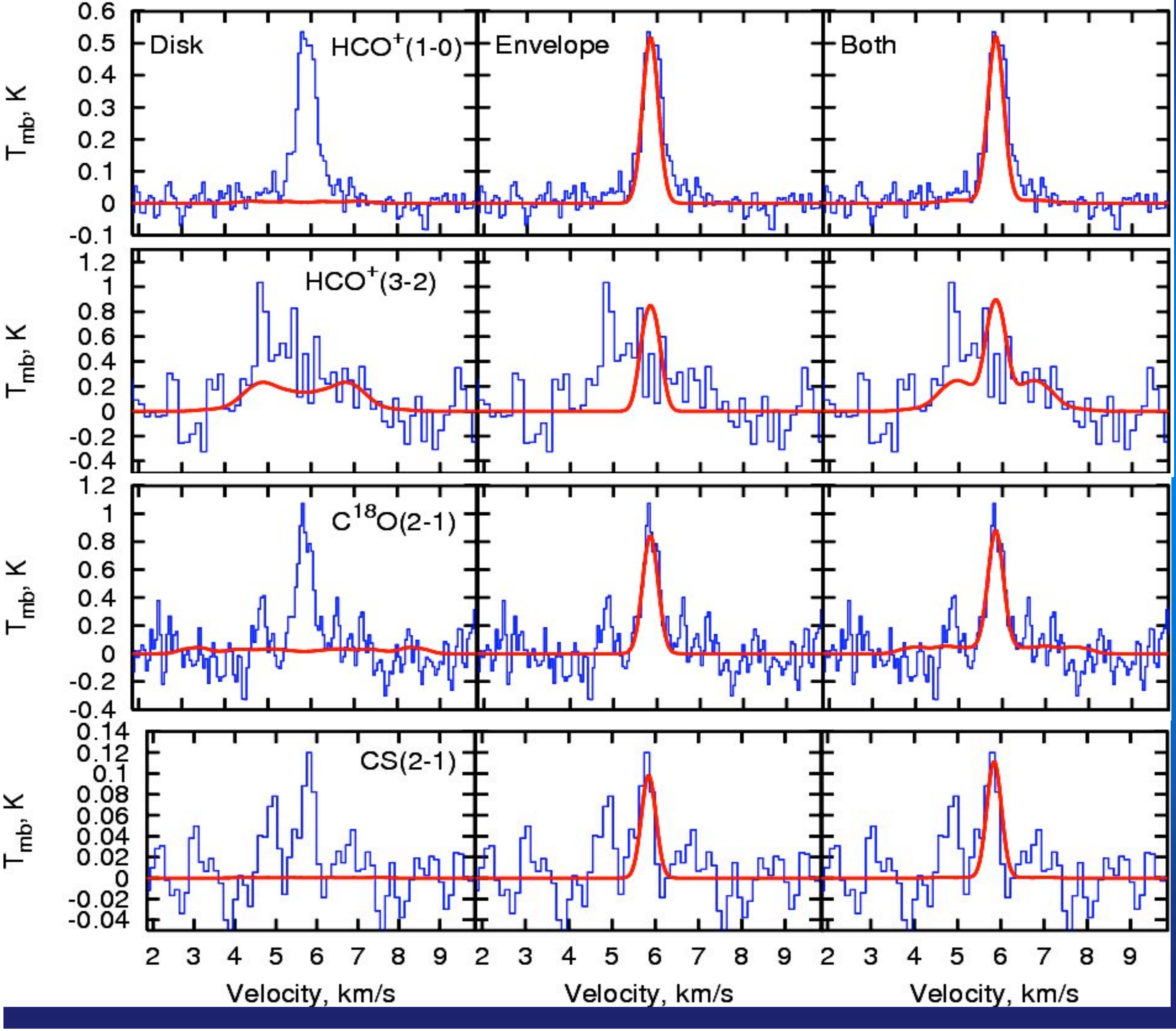
- Disk radius is   400 ± 200AU
- Disk mass is $0.01M_{sun}$ (± x7)
- Keplerian rotation
- “Clumps?”

Temperature in Envelope: CO(2-1)



Temperature ≈ 35±14K ($r \leq 800$ AU)

Density of Envelope



HCO$^+$(1-0): n_0=4·10 (5) cm^{-3}

(3-2)/ (1-0): p=−1±0.3, infall profile

Total mass: about 1 M_{sun}

Accretion rate: 4·10(-8) M_{sun} /yr

Disk dispersal: about 0.3Myr

Envelope age: < 25 Myr

Conclusions

- Mostly equilibrium chemistry for ionization degree
- HCO^+ is the dominant observable ion (radio)
- Stochastic surface chemistry in disks
- Mixing works as non-thermal desorption
- Both radial and vertical mixings are crucial
- Mixing model agrees better with observations
- Consistent chemical and LRT modeling provides a wealth of information about disks
- Envelopes can be crucial for disk evolution

Collaborators

- CID collaboration (A. Dutrey, S. Guilloteau, V. Pietu, A. Bacmann, J. Pety, V. Wakelam)
- D. Wiebe (Moscow): Chemistry with mixing
- Ya. Pavlyuchenkov (MPIA): Line Radiative Transfer
- K. Schreyer (Jena): Disk observations
- C. Dullemond (MPIA): Disk dynamics