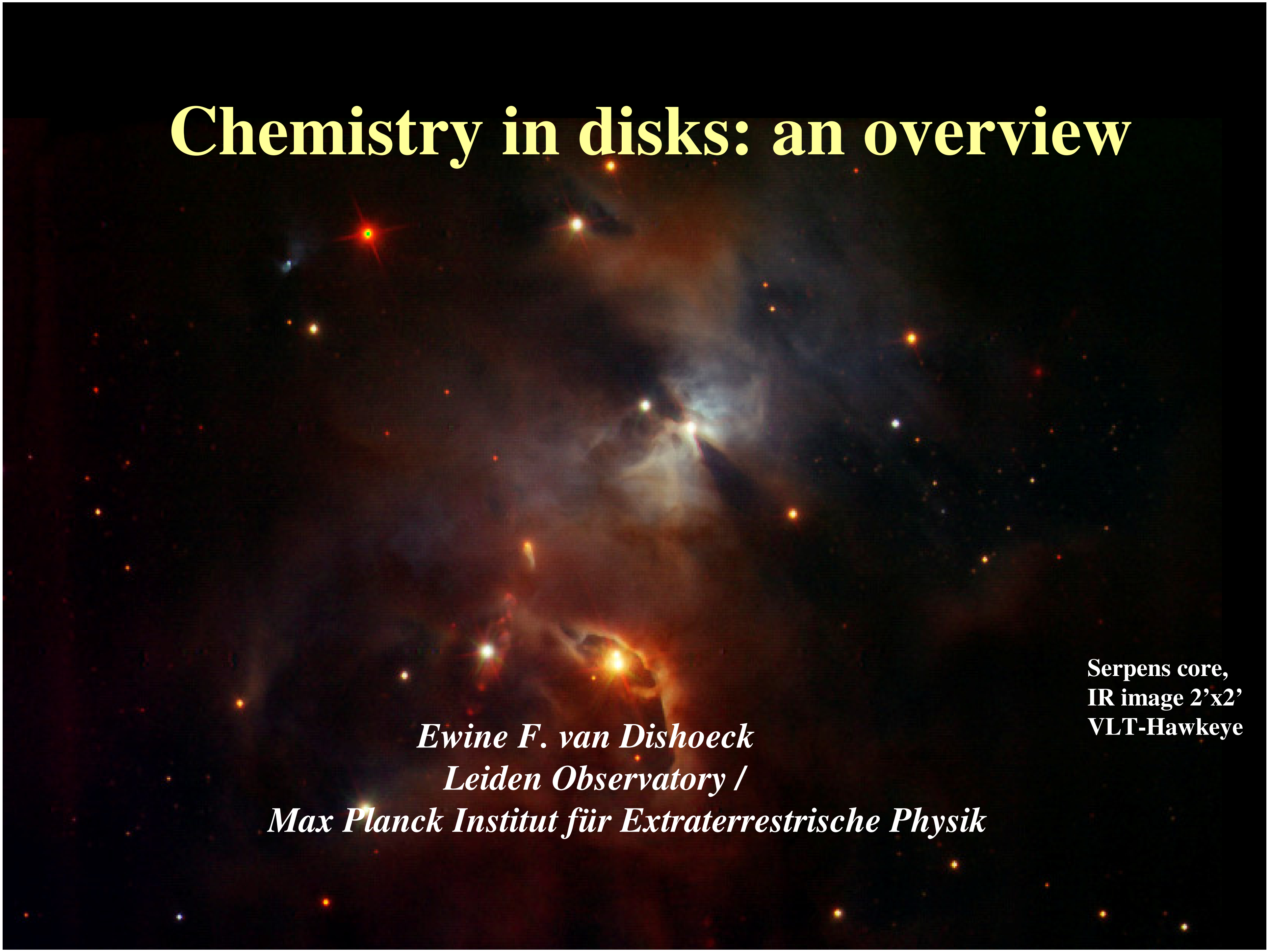
Chemistry in disks: an overview



Serpens core,
IR image 2'x2'
VLT-Hawkeye

Ewine F. van Dishoeck
Leiden Observatory /
Max Planck Institut für Extraterrestrische Physik

Outline

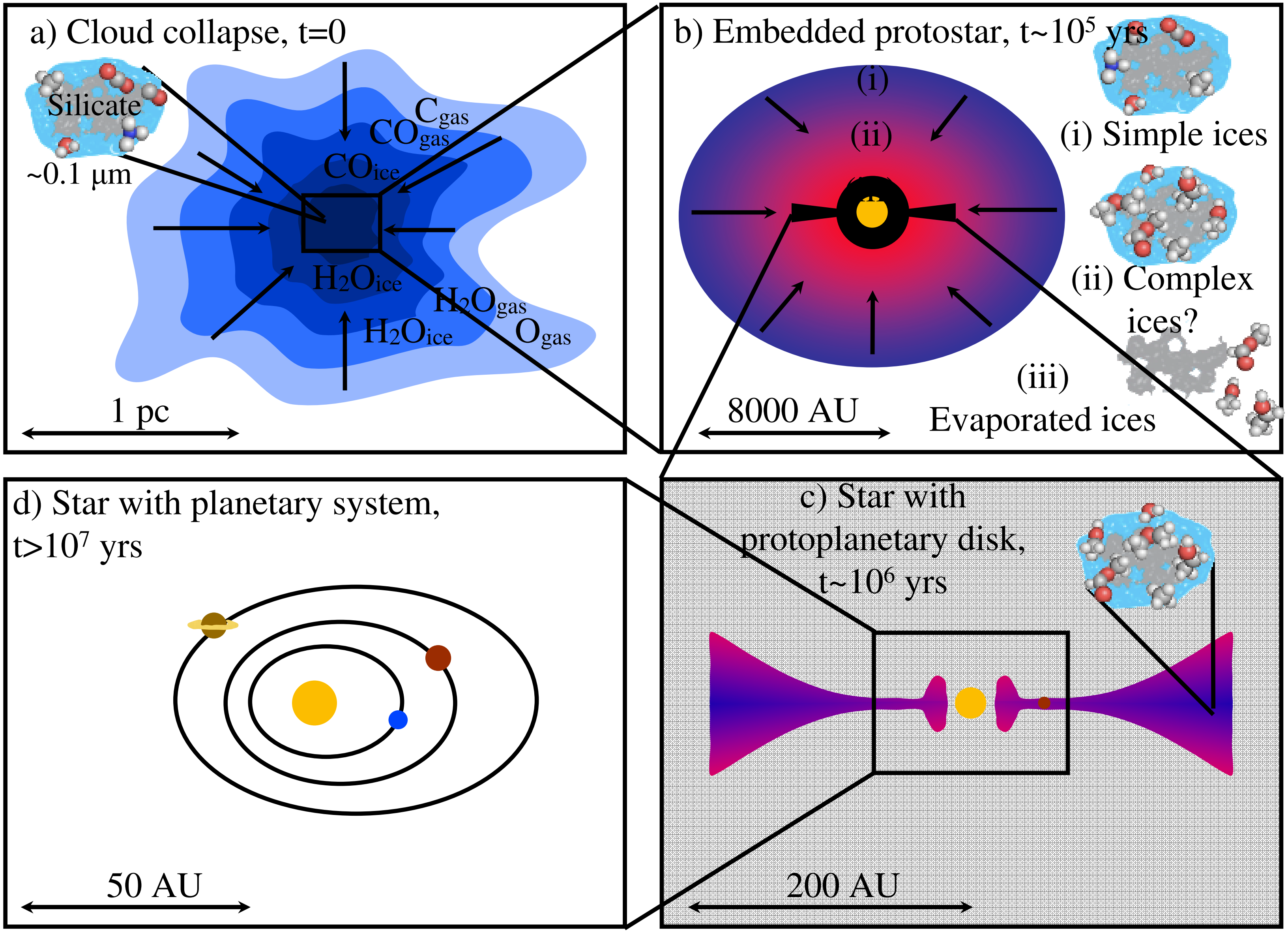
- Introduction
  - Progress in observations and models
- Outer disk: cold-warm chemistry
  - Importance of photoprocesses
  - PAHs
  - Effects of grain growth
  - Inner holes or gaps
- Inner disk: hot chemistry
- Evolution from cloud to disk
- Conclusions

See van Dishoeck 2006 PNAS, Bergin et al. 2007 PPV, Bergin 2009, Semenov 2009 for reviews

Thanks to many collaborators and colleagues

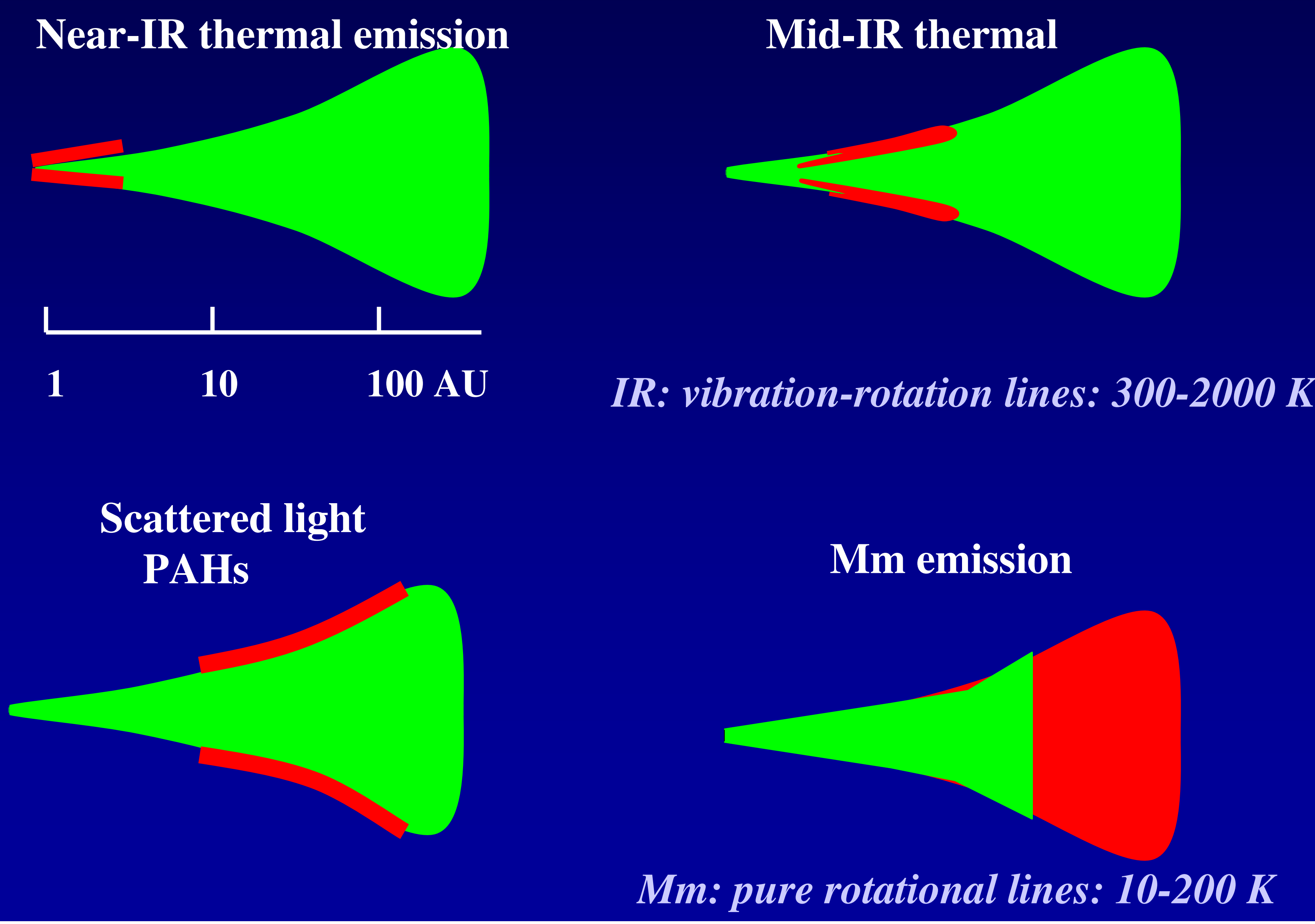
Disk chemistry: from cores to planets

Öberg 2009



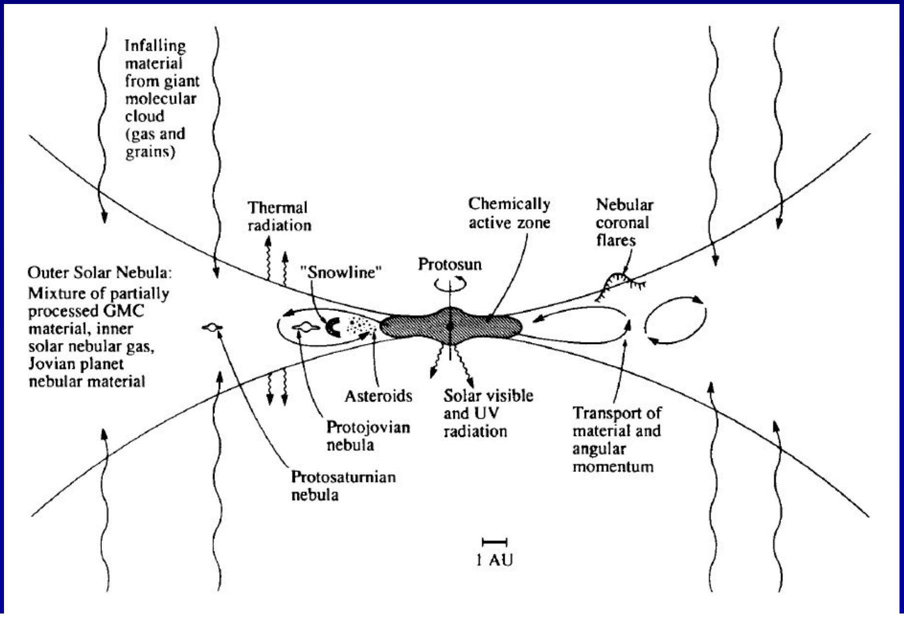
- Inner vs outer disk? Gas vs ices? Preservation pristine cloud material?

Mm vs IR: probing different parts of disks



Some history: solar system community

- Large literature on chemical models of the ‘solar nebula’ (inner 10 AU) since 1970’s
  - E.g., Lewis, Prinn, Fegley, Lunine, ….
- Models applied to large range of solar system observations
  - E.g., CO/CH_4 planetary atmospheres, comet abundances, meteorites
- Chemistry thought to be dominated by thermal equilibrium (3-body) rather than kinetic (2-body) processes



Lunine 1989

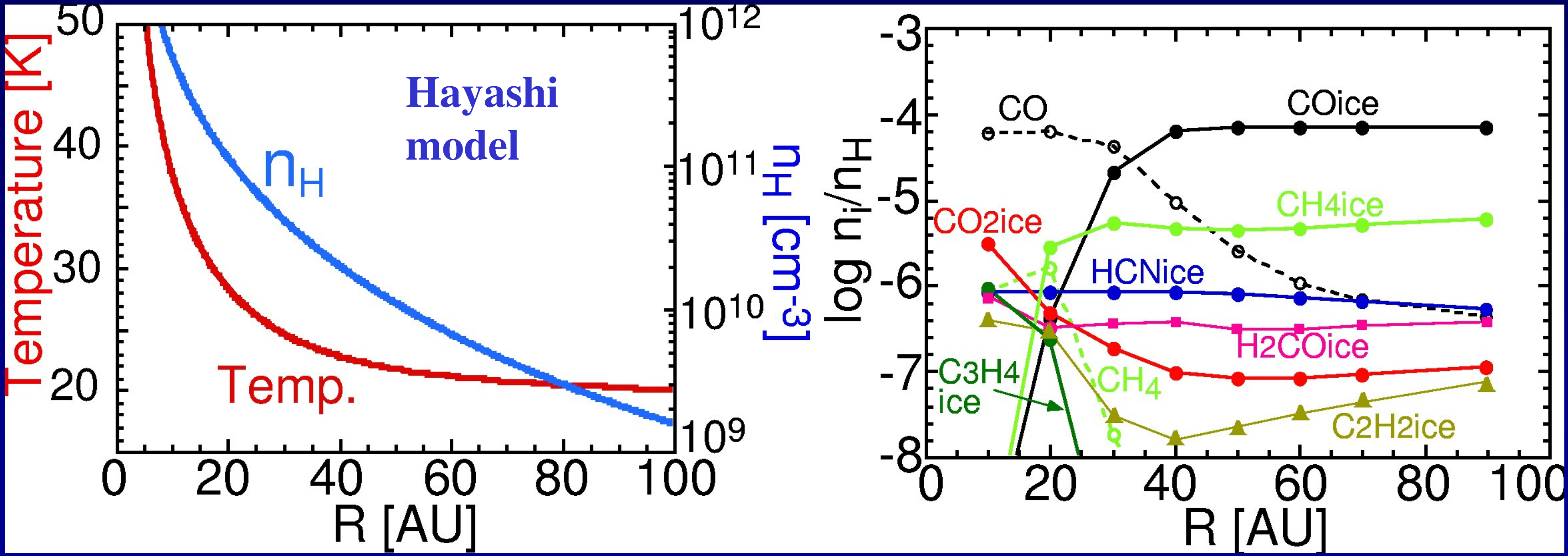
Some history: astrochemistry community

1D Radial transport models

- Consider chemical evolution of parcel of gas as it moves radially from >100 AU to few AU
- Include large gas-phase chemistry network (few hundred species, few thousand reactions) and gas-grain adsorption/desorption processes
- Chemistry dominated by temperature profile: virtually no gas-phase molecules >10 AU (*cold → frozen out*), active gas-phase chemistry <10 AU
  - E.g., Bauer et al. 1997, Finocchi & Gail 1997, Gail 2001-2004, Willacy et al. 1998, Aikawa et al. 1997, 1999

Example

Abundances in midplane after 3x10^6 yr



=> Everything frozen out at >10 AU

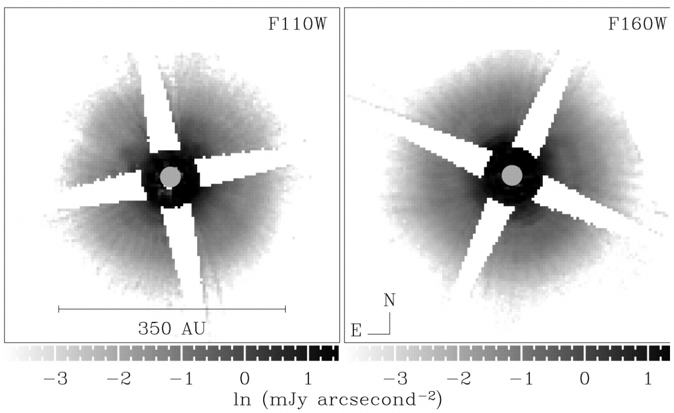
But this is NOT what is observed!

Aikawa et al. 1999

Molecules in disks: single-dish mm

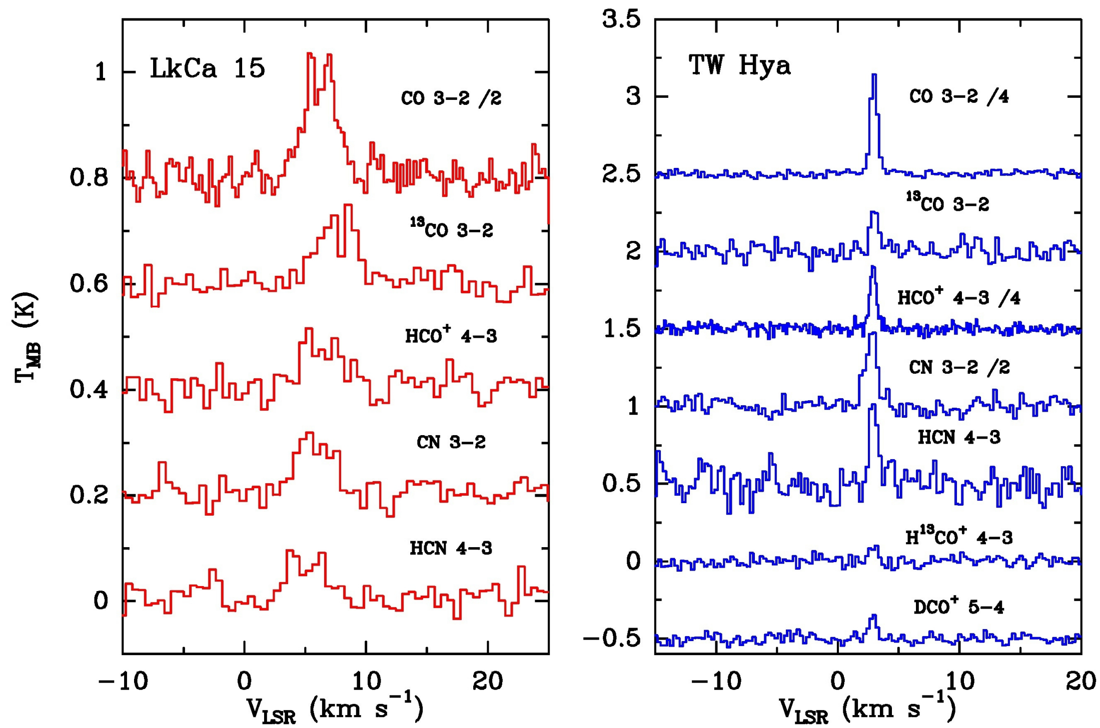
TW Hya face-on disk

1.1 μm **1.6 μm**



Scattered light => radius 200 AU

Weinberger et al. 2002

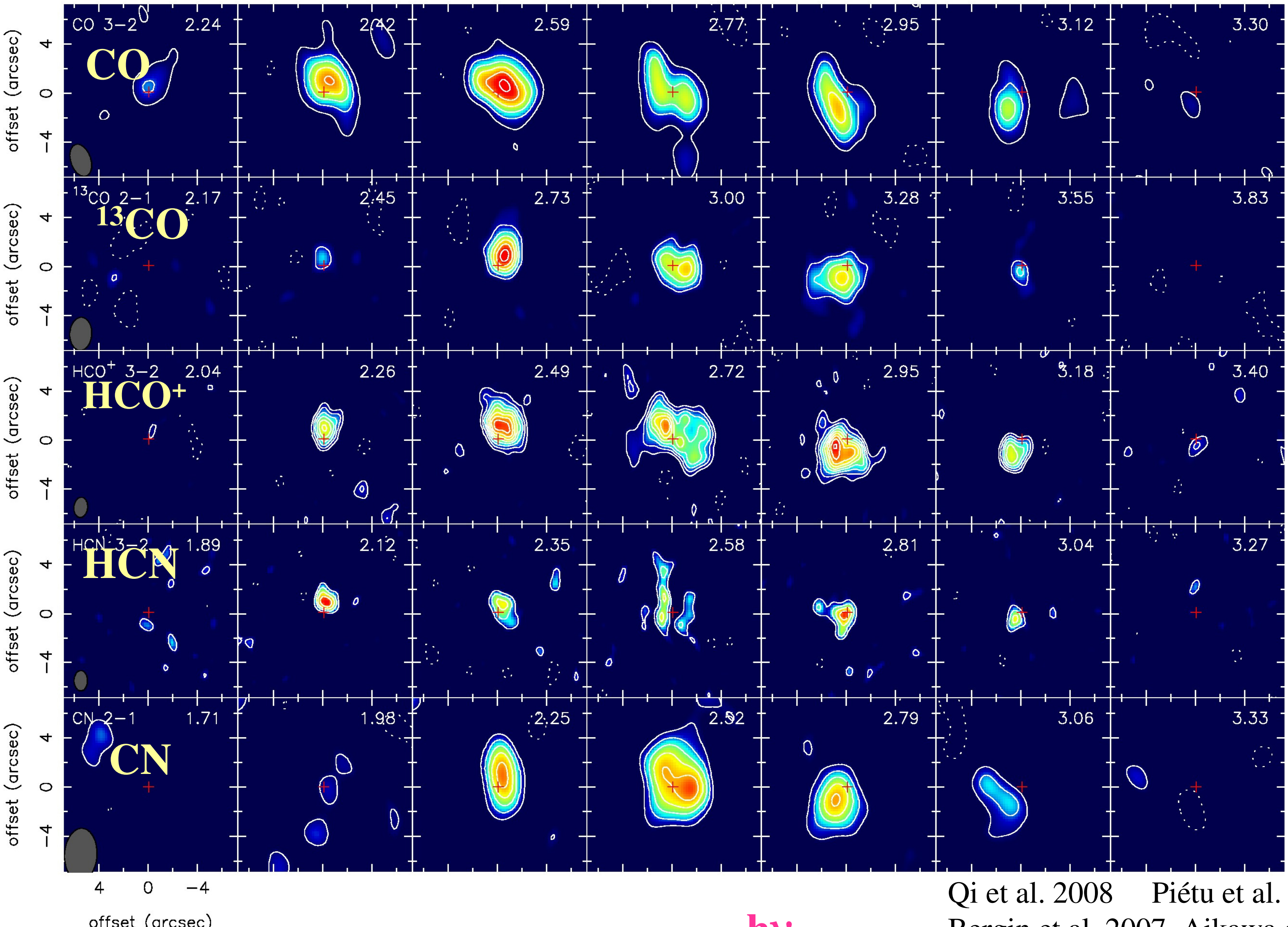


- Simple molecules detected, including deuterated species
- Evidence for ion-molecule chemistry (HCO^+) and photodissociation (CN)
- Instruments do not yet have sensitivity to search for complex molecules

Kastner et al. 1997
Dutrey et al. 1997

van Dishoeck et al. 2003
Thi et al. 2004

Starting to image them



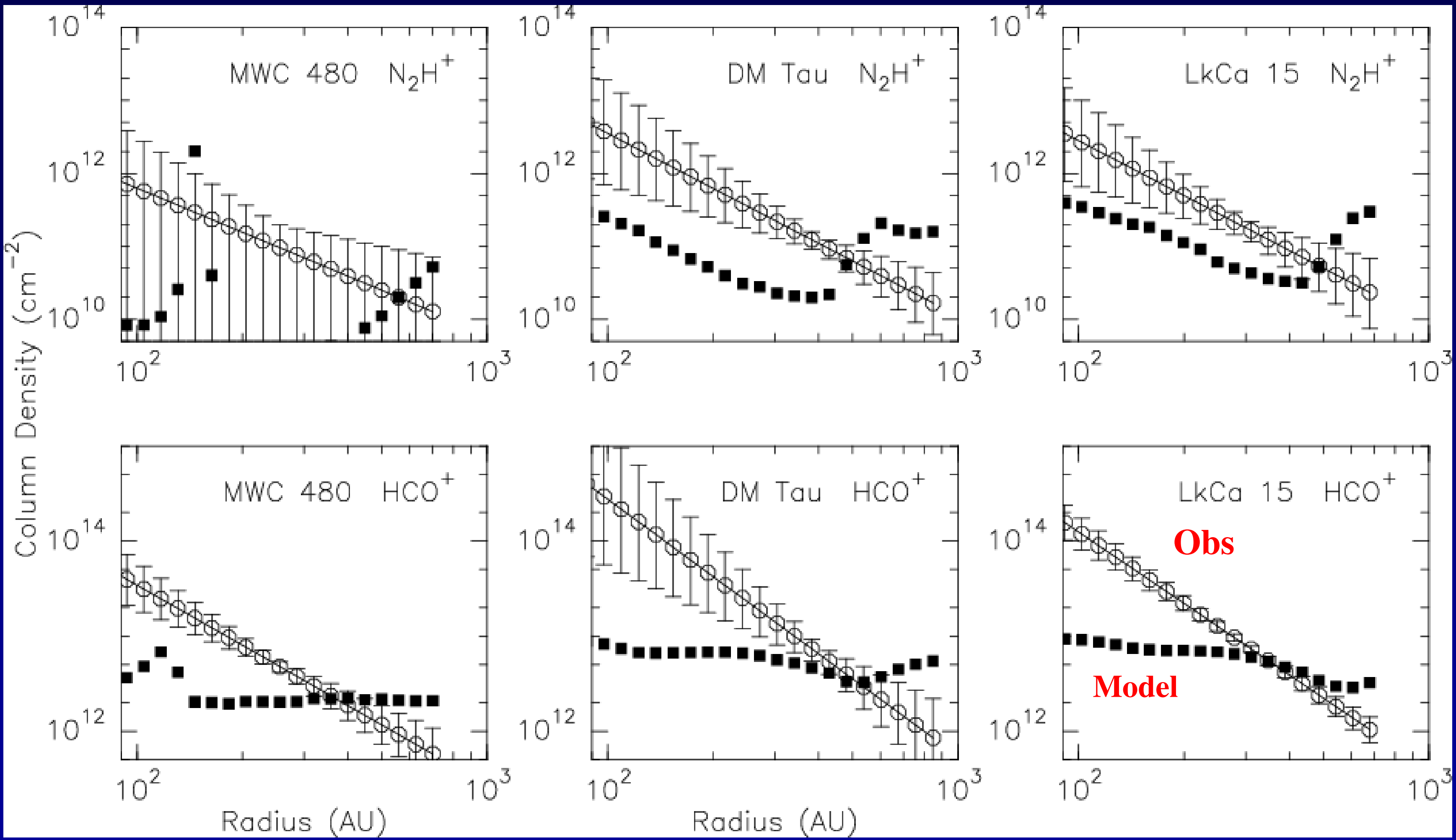
TW Hya

Note CN more extended: HCN $\xrightarrow{h\nu}$ CN

Qi et al. 2008 Piétu et al. 2007
Bergin et al. 2007, Aikawa et al. 2003

Chapillon A16

Radial profiles



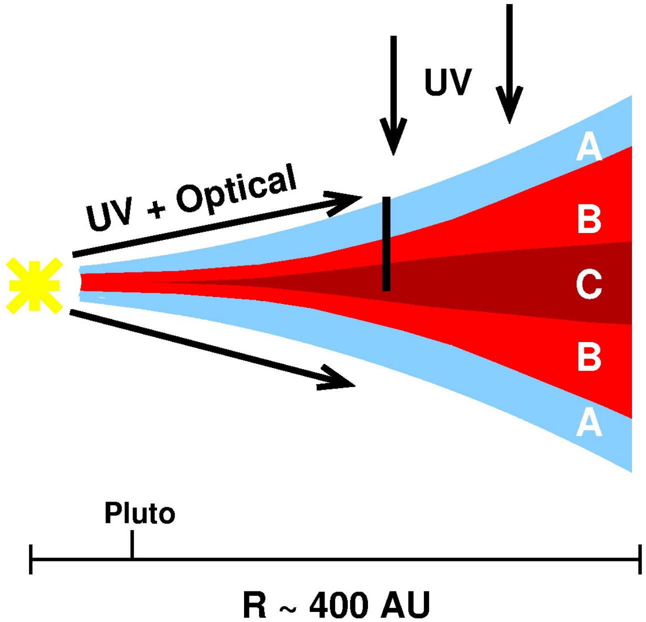
CID project; Dutrey et al. 2007

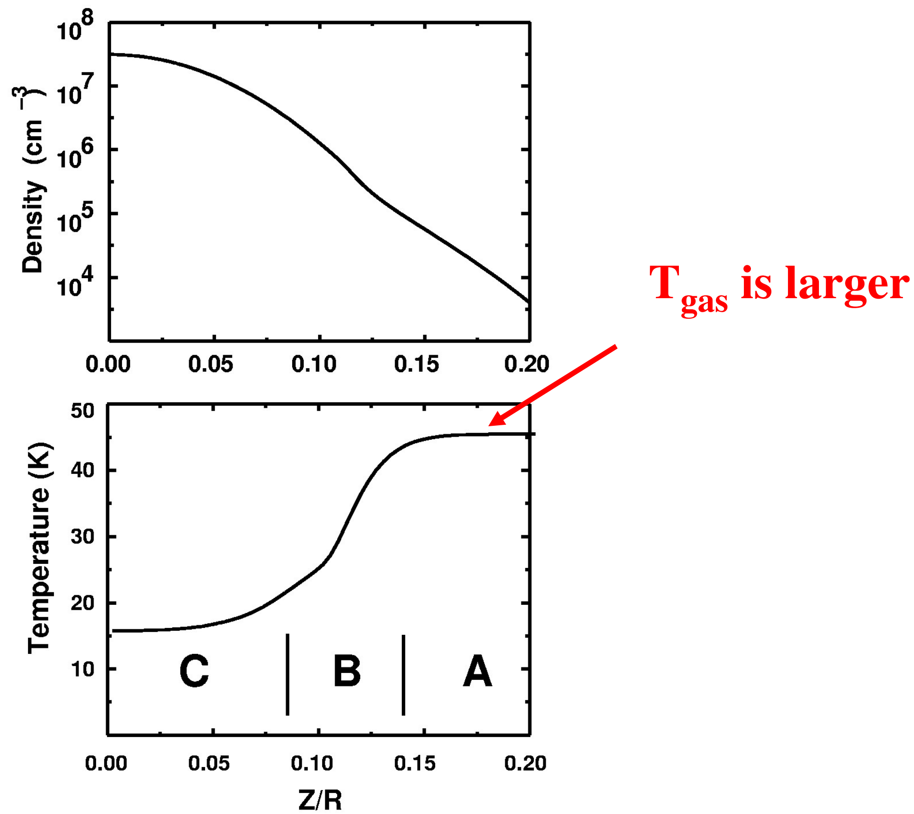
Observed column density profiles steeper than models

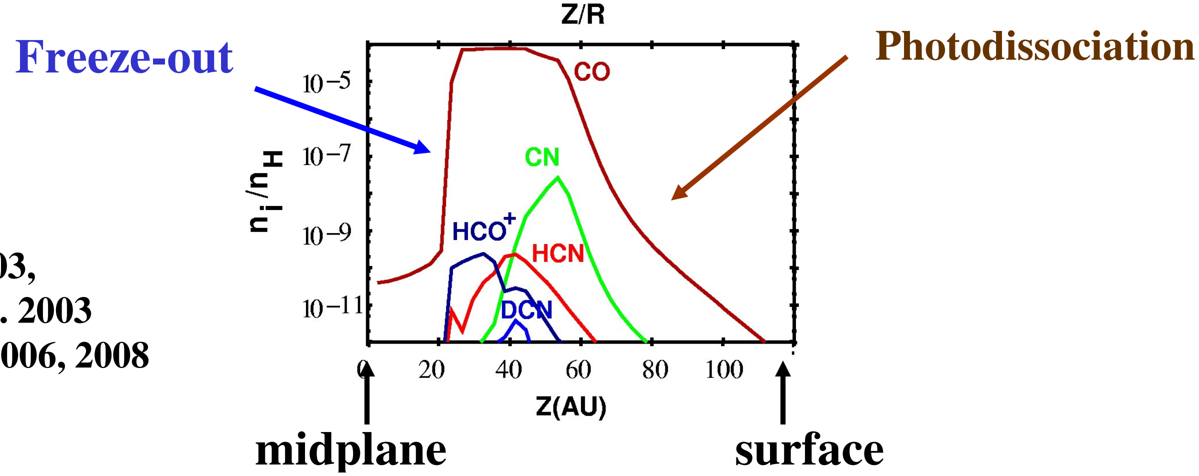
Importance of vertical structure

- **Calculate chemistry in 1+1D static flaring models (>30 AU)**
  - *Aikawa et al. 1999, 2001:*
    - **Kyoto minimum mass solar nebula model**
    - **Low temperatures => needed artifically low sticking coefficient S=0.03 to match observations**
  - *Willacy & Langer 2000*
    - **Two-layer Chiang & Goldreich model**
    - **All molecules photodissociated in warm layer**
    - **All molecules frozen on grains in cold layers => needed high photodesorption rate to match observations**
  - *Aikawa et al. 2002, van Zadelhoff et al. 2003*
    - **D'Alessio et al. models with continuous T,n gradient**
    - **Warm molecular layer where molecules stay off the grains even with S=1**

Three-layer chemical structure



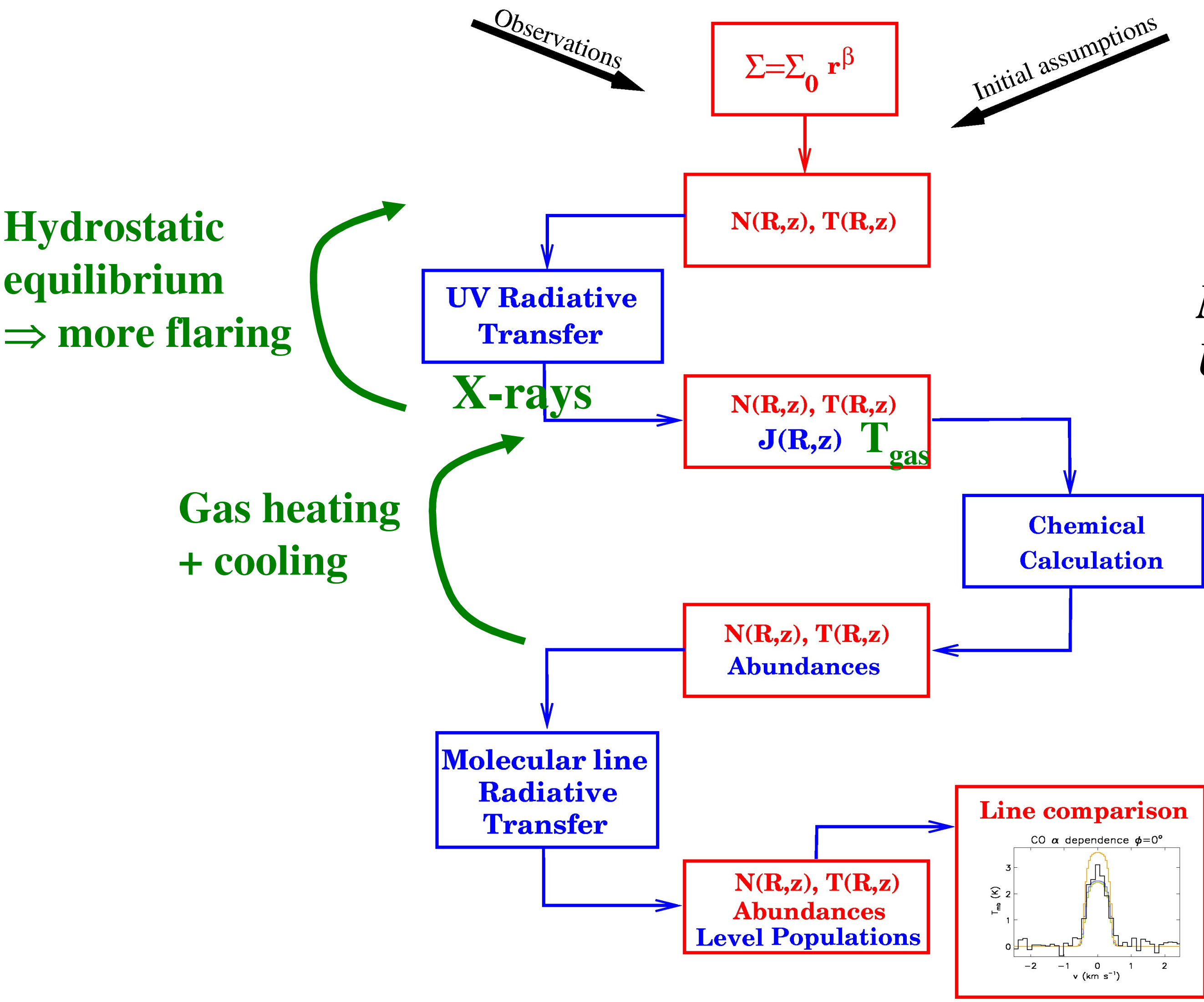




-Most emission comes from warm intermediate molecular layer

Aikawa et al. 2002, Van Zadelhoff et al. 2003,
Markwick et al. 2002, Millar, Nomura et al. 2003
Jonkheid et al. 2004, 2007, Semenov et al. 2006, 2008
Ilgner et al. 2006, ….

Physical-chemical models: flowchart



Need to know T_{dust}, T_{gas}, UV/X-rays for chemistry

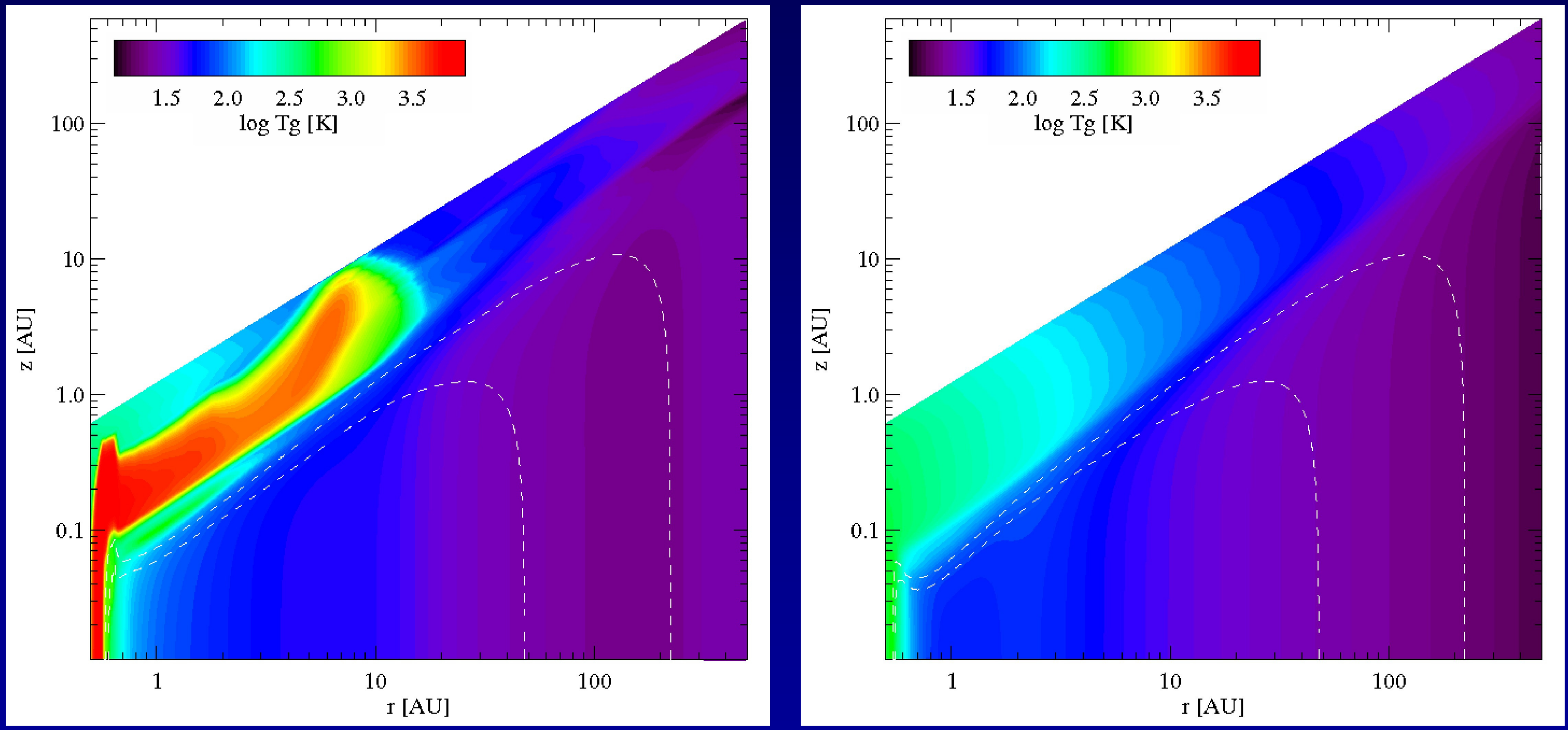
Van Zadelhoff et al. 2003
Jonkheid et al. 2004, 2007
Kamp & Dullemond 2004
Aikawa & Nomura 2006
Gorti & Hollenbach 2004, 2009
Glassgold et al. 2004, 2009
Woitke et al. 2009
….

See Kamp & Bertoldi 2000, Kamp & van Zadelhoff 2001, Kamp et al. 2003 for debris disks

New generation disk models

T-Tauri star+ disk

T gas computed **T gas = T dust**

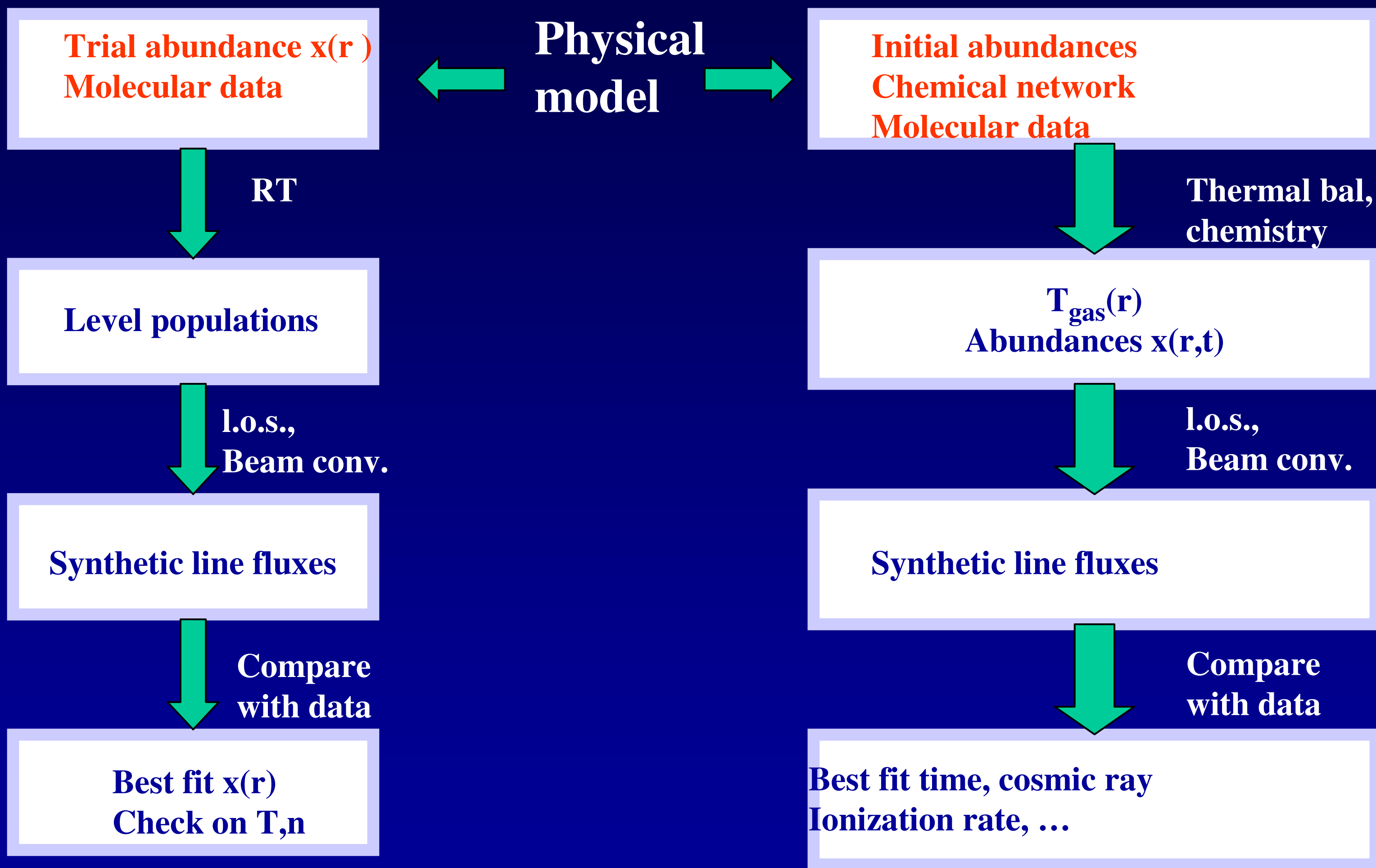


ProDiMo: Woitke, Kamp & Thi 2009

Warm surface layers with *T* up to few thousand K out to 10 AU

Posters: Heinzeller A46, Aresu A3, Chapparo A15, Chapillon A16, Dutrey A28, Fogel A33, Woitke B47

Some thoughts on model philosophies



Empirical or Retrieval method

Full chemical or Forward method

Both need to be done, but initial insight more readily gained from empirical method

A few words about chemistry

Gas-phase chemistry

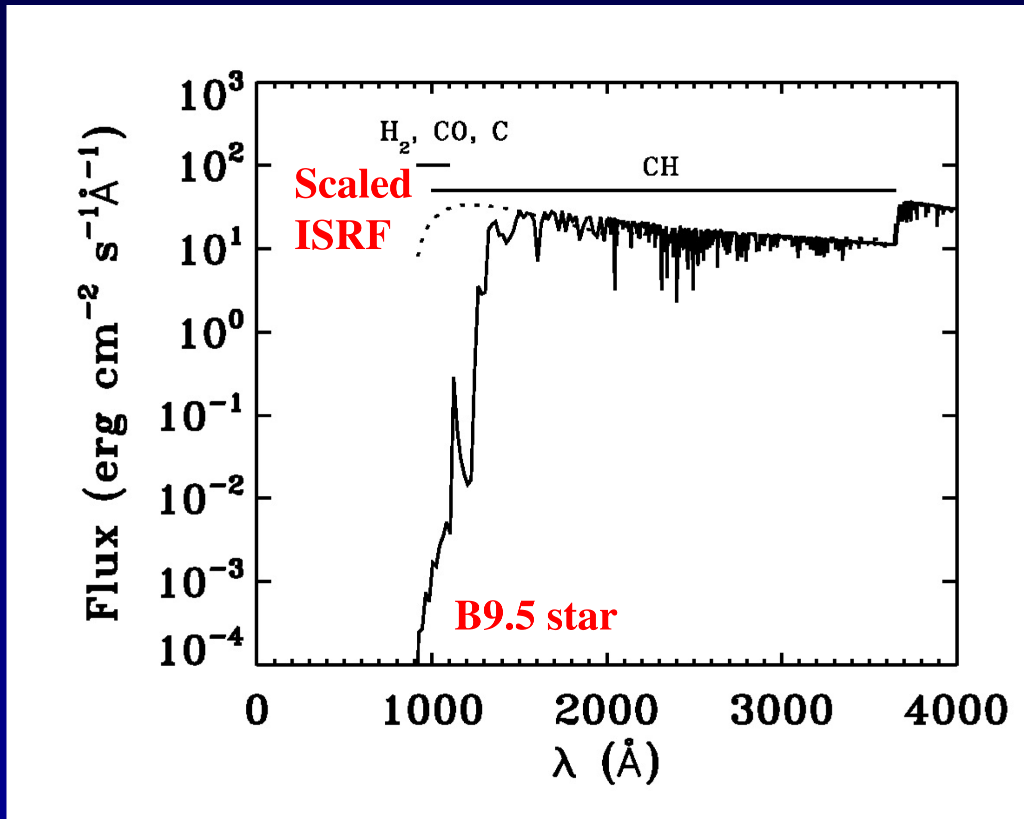
- Elemental abundances (e.g. high vs. low metals) and cosmic ray ionization rate important input parameters
- Gas-phase chemistry not very sensitive to temperature in 10-200 K regime
- Many different chemical networks containing a few hundred to a few thousand reactions => reduction?
  - Wiebe, Semenov et al. 2003, 2004
- Best agreement with well-studied PDRs and dark clouds is a factor of a few – ten => better agreement for disks would be a miracle!

A few words about chemistry

Gas-grain interactions

- **Freeze-out/thermal desorption depend sensitively on dust temperature profile**
  - **Species dependent: CO T>20 K, H_2O T>100 K; binding energies not well known for all species and depend on type of ice or surface**
- **Fundamental issues with formulation grain surface reactions (diffusion-limited vs. accretion-limited)**
- **Timescales: t_{ads}~$2x10^9/n_H$ yr => strongly dependent on density**

Importance of shape radiation field

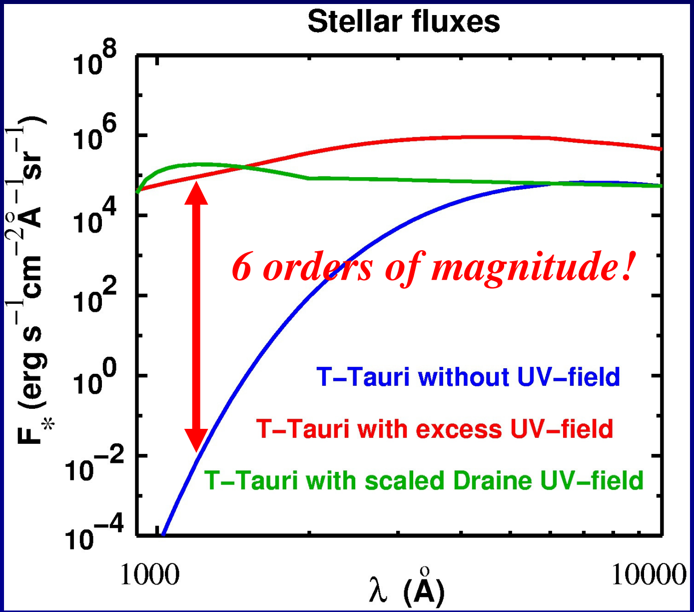


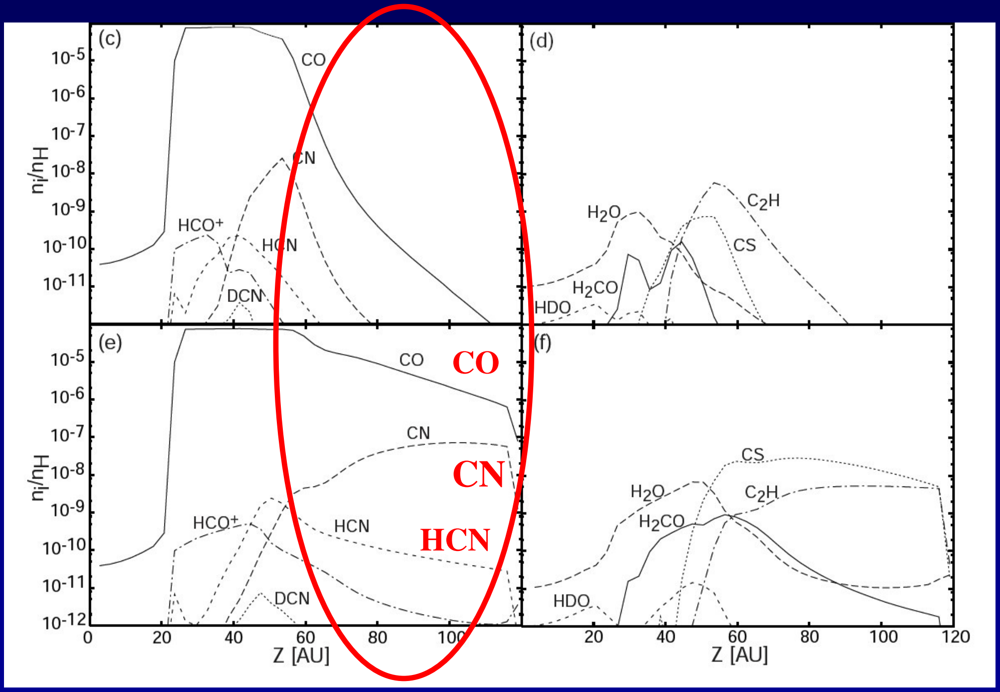
- Photodissociation rate $k_{pd} = \int \sigma(\lambda) I(\lambda) d\lambda$
- Results sensitive to adopted UV field, especially <1100 Å
- Affects H→ H_2 and C^+ → CO transition, just as in PDRs
- Some molecules are dissociated by Lyα (e.g., H_2O, HCN), others are not (e.g. CN, CO, H_2)

www.strw.leidenuniv.nl/~ewine/photo

Van Dishoeck et al. 1987, 2006
Bergin et al. 2003

Effect of stellar UV





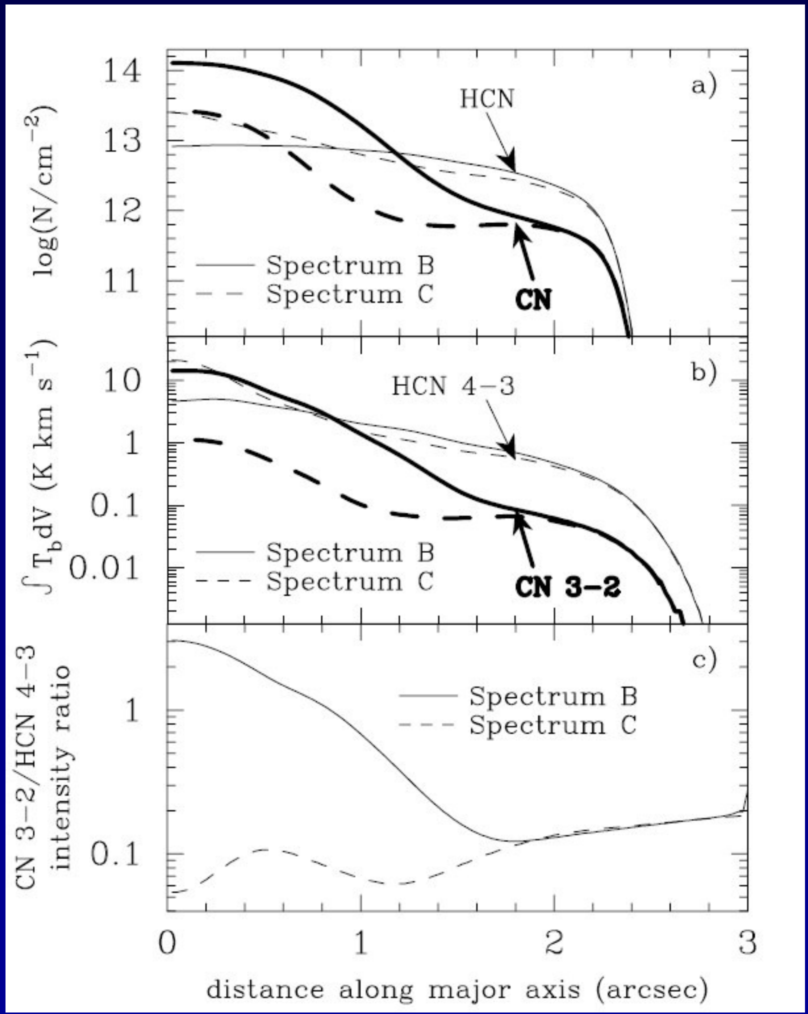
With UV

No UV

=> Molecules extended to greater height if no far-UV

Van Zadelhoff et al. 2003

Lines: with or without excess UV

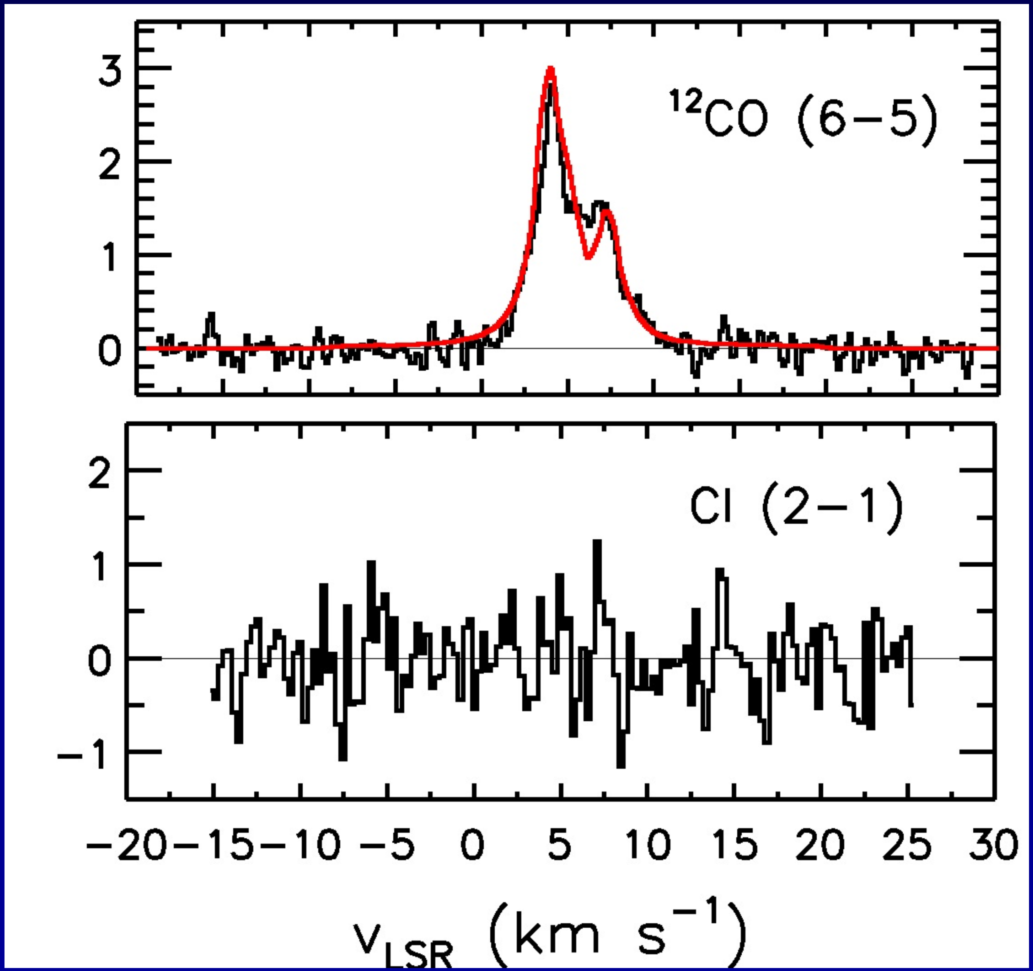


CN/HCN ratio

Van Zadelhoff et al. 2003

- **Difficult to disentangle with single-dish data**
- **Need ALMA resolution to probe variations**

Lack of [C I] from disks



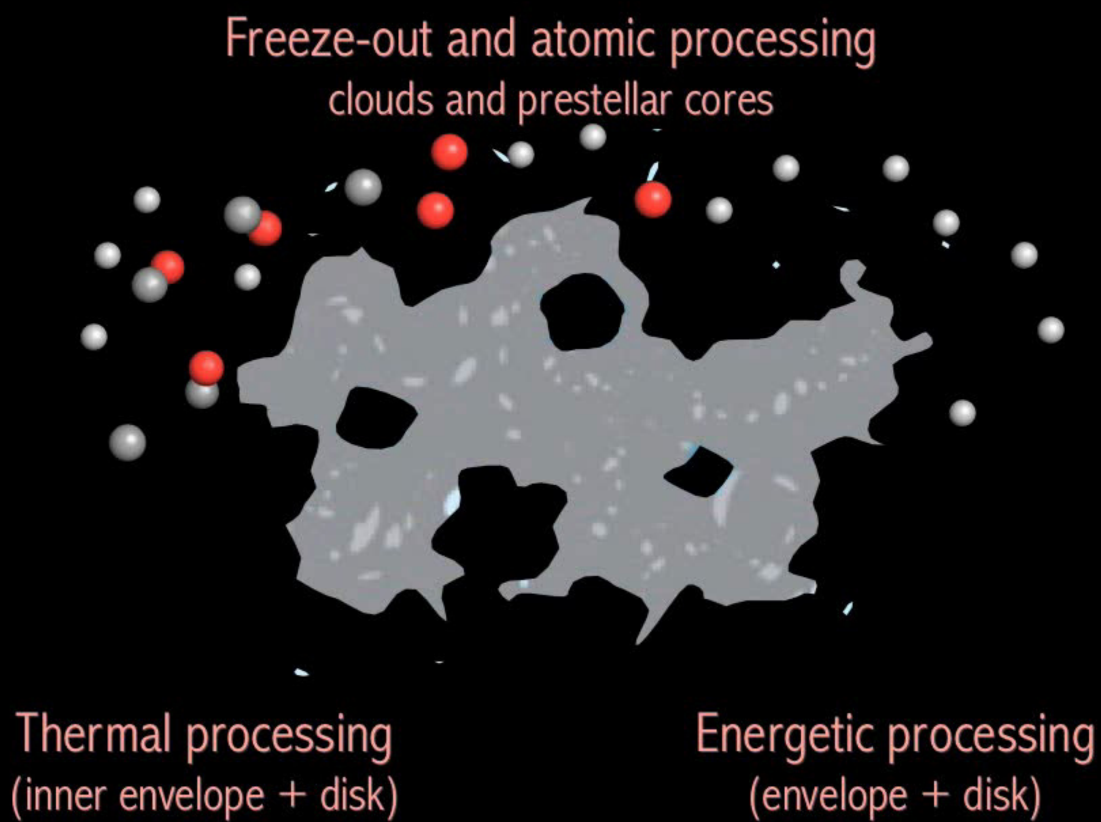
HD 100546 disk

APEX-CHAMP$^+$
Panić et al. 2010

Factor >5 weaker than predicted by Jonkheid et al. 2007

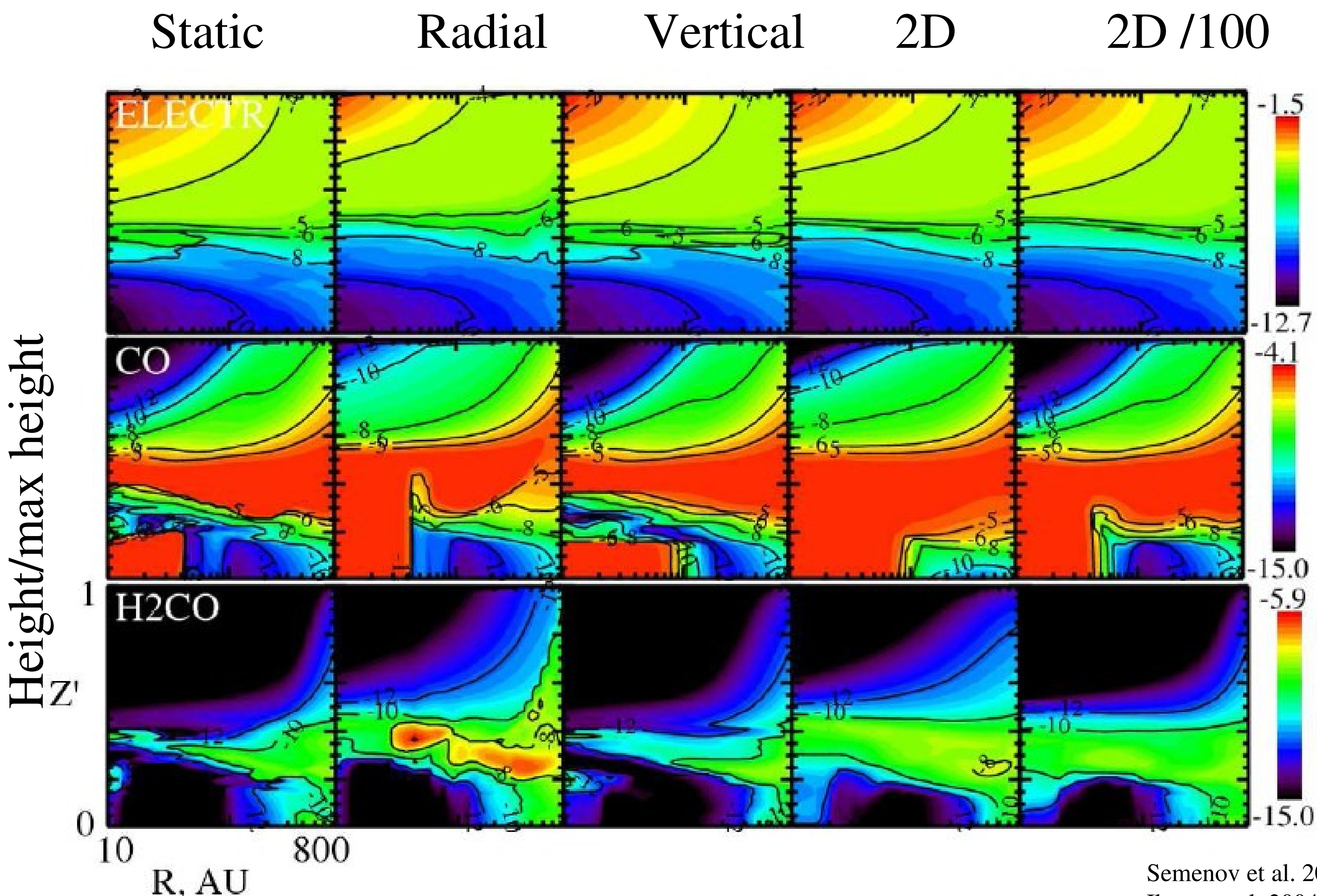
Lack of [C I] suggests more carbon-ionizing photons

Importance of gas-grain chemistry



K. Öberg 2009

Effect of mixing

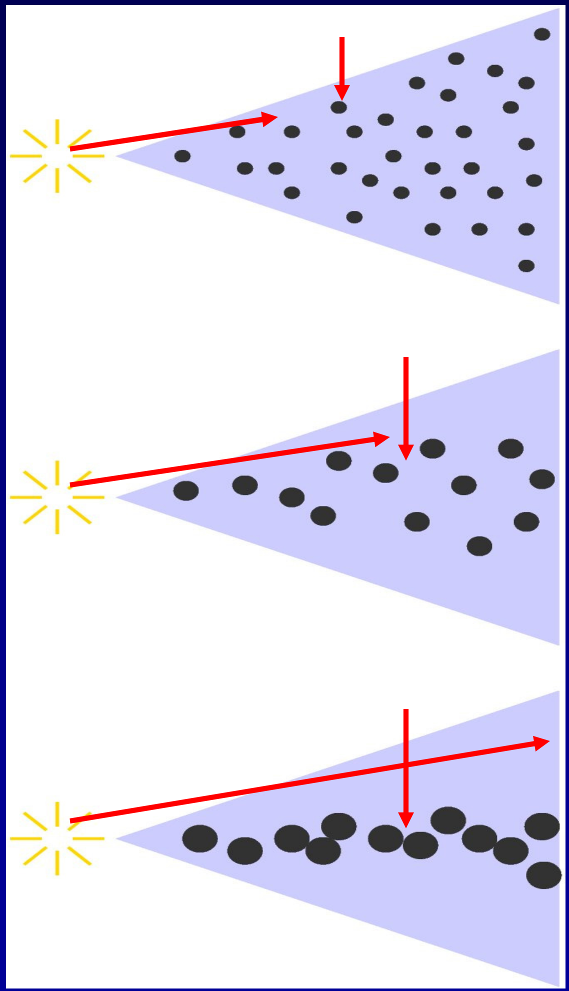


Largest effects for molecules formed on grains

Semenov et al. 2006
Ilgner et al. 2004
Willacy et al. 2006
Aikawa & Nomura 2006

Importance of grain growth + settling

- Disk evolution
  - Grain growth + settling
  - Mass loss
- Much deeper penetration of UV
  - Enhances photodissociation and photodesorption
  - Heats disk to deeper layers

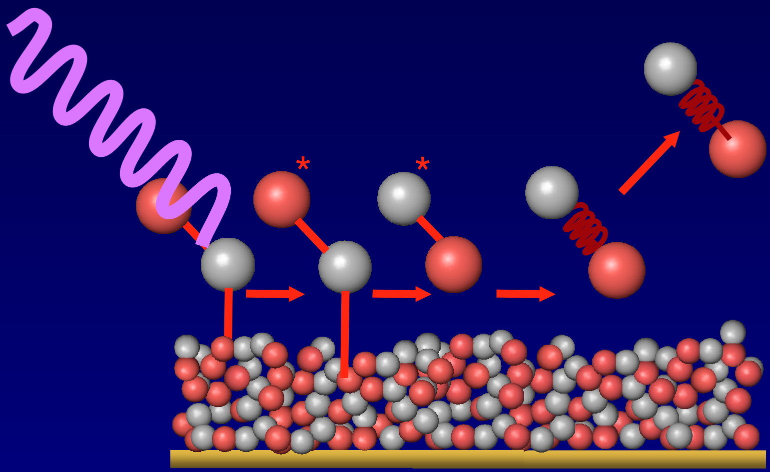


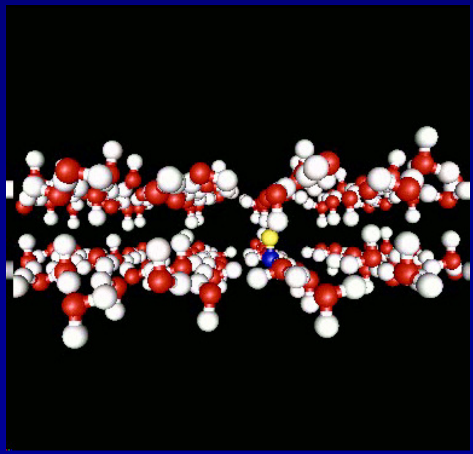
Fogel A33

Jonkheid et al. 2004, 2007
Aikawa & Nomura 2006
Bethell & Bergin 2009

Importance of photodesorption

- **Needed to explain observations of cold CO (<20 K)**
  - Dartois et al. 2003, Hersant et al. 2009
  - Alt: turbulent mixing: Semenov et al. 2006, Aikawa 2007
- **Desorption yields per incident UV photon measured in lab under UHV conditions**





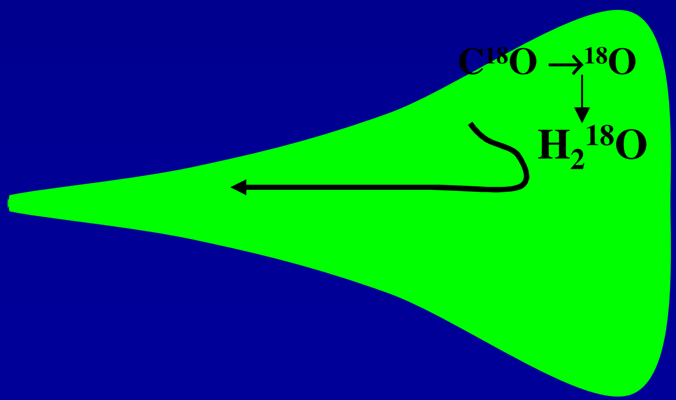
$$Y_{CO} = 2.7 \times 10^{-3} - 1.7 \times 10^{-4}\,(T - 15)$$

Two orders of magnitude more efficient than thought before!

Öberg et al. 2007, 2009
Andersson et al. 2006
Takahashi & van Hemert in prep.

Isotope selective photodissociation of CO

- Isotope-selective photodissociation leads to fractionation, i.p. enhancement of ^{18}O,^{17}O with respect to ^{16}O
- Enhanced ^{18}O,^{17}O can be incorporated into H_2O
- Invoked to explain mass-independent oxygen isotope fractionation found in meteorites
  - Clayton et al. 1973; Clayton 1993; Lyons & Young 2005
- New model with updated molecular data
- Effects enhanced for large grains

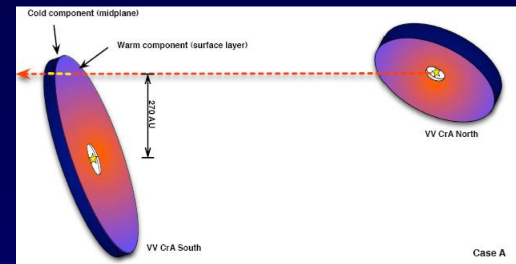


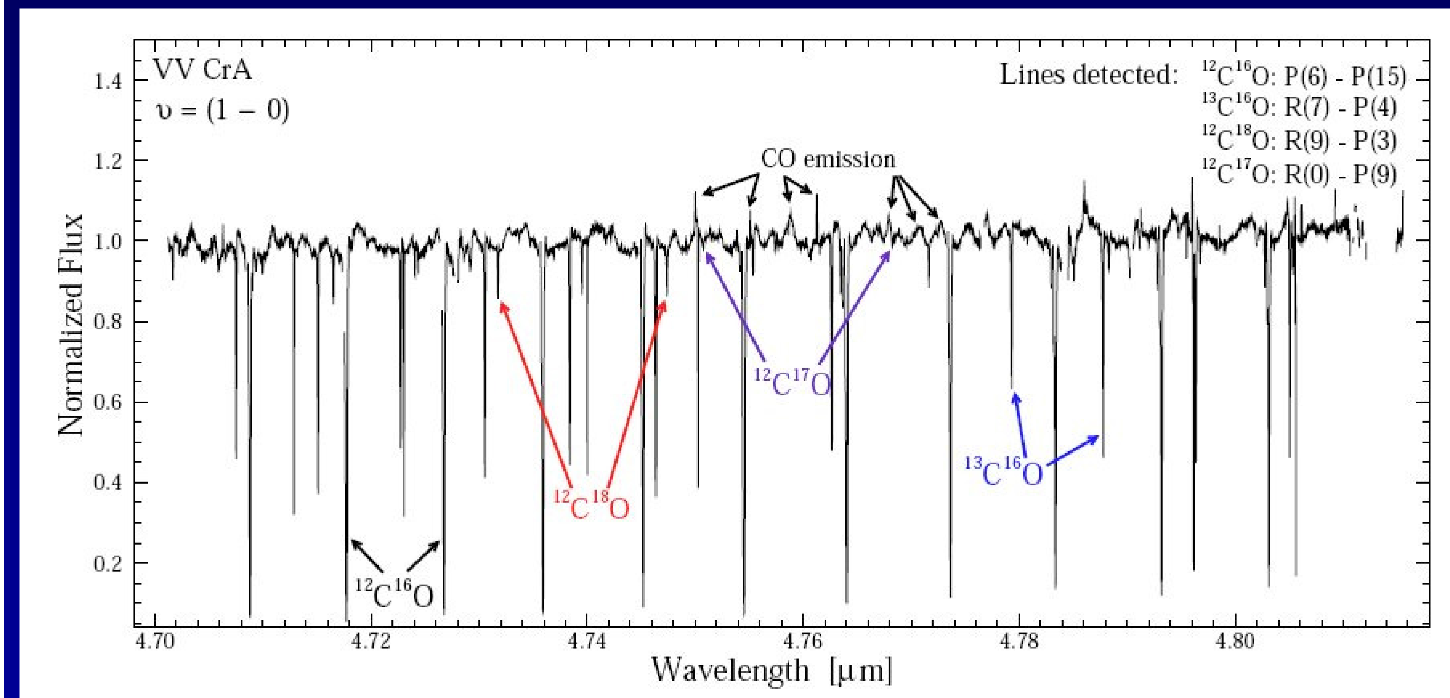
Van Dishoeck & Black 1988, Eidelsberg et al. 1988, **Visser et al. 2009**

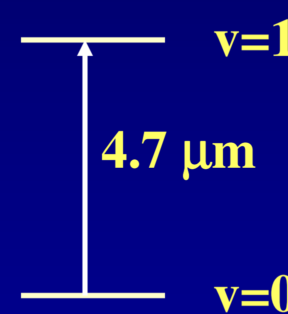
Willacy & Wood 2009 for $^{12}C/^{13}C$

Gas-phase CO isotopologues in disks

VLT CRIRES R=10^5







Smith, Pontoppidan et al. 2009

Smith B35

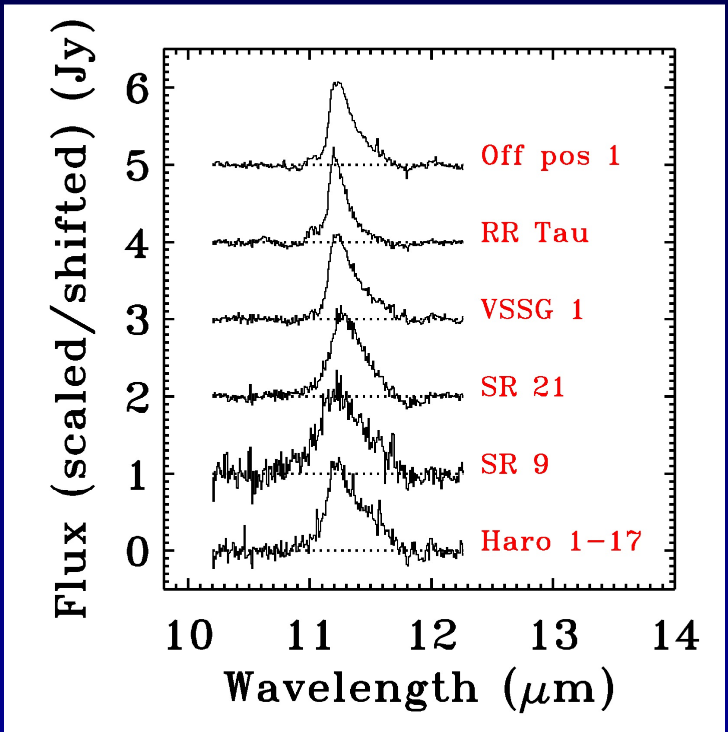
- **Even $C^{17}O$ detected!**
- **Isotope ratios indicate isotope selective photodissociation of ^{17}O, ^{18}O**

Importance of PAHs with grain growth

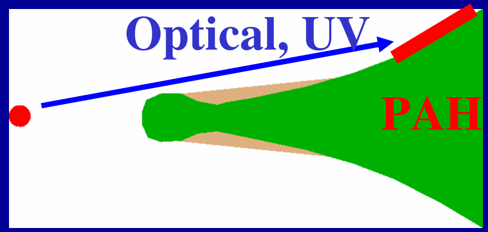
- Absorbers of UV ⇒ shielding
- Heating of gas
- Formation of H_2
- Formation of CH, CH^+

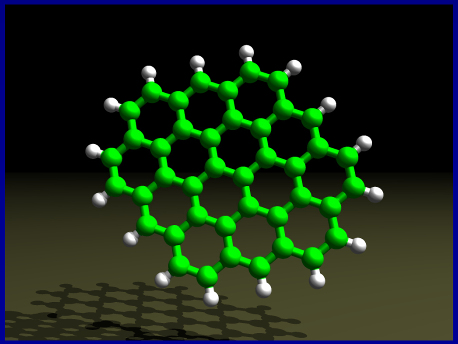
  ⇒ precursors of CO
- Charge transfer
  - $C^+ + PAH/PAH^- \Rightarrow C + PAH^+/PAH$

Lack of PAH emission from disks



- ~50% of Herbig Ae stars show PAHs, but only 11% or less of T Tauri stars
  - Only G stars detected, not K, M
- Absence in majority of T Tau disks due to low PAH abundance (0.1 x ISM)
  - Coagulation and/or freeze-out in embedded phase
- Observed out to 100 AU => probe of UV
- Only larger (N_C>100) PAHs can survive in planet-forming zones

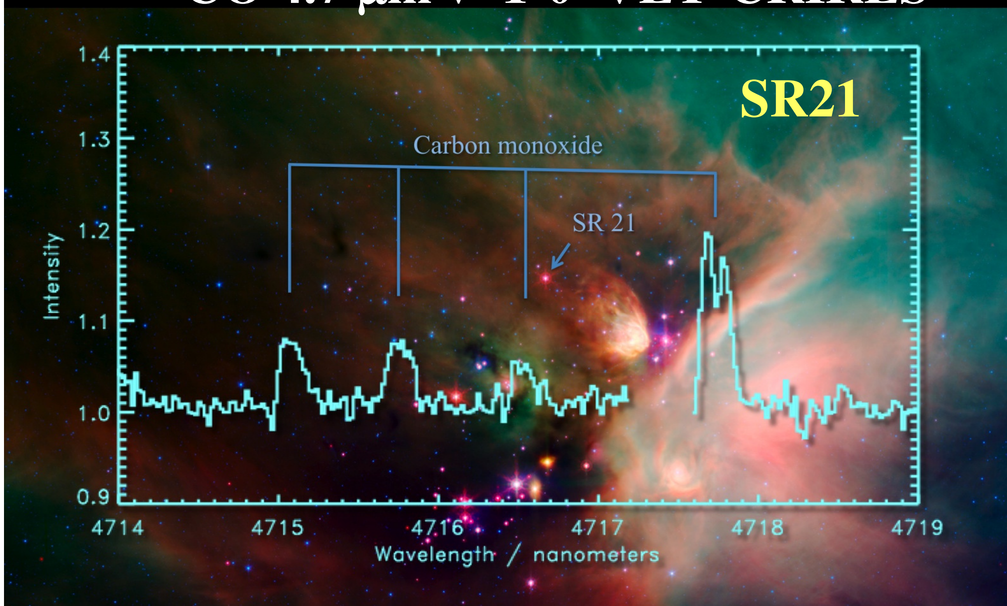




Acke & van den Ancker 2004: obs Herbig Ae
Geers et al. 2006, 2007, 2009: obs T Tau
Habart et al. 2006, Visser et al. 2007: models

Molecular gas in gaps: observations

CO 4.7 μm v=1-0 VLT-CRIRES

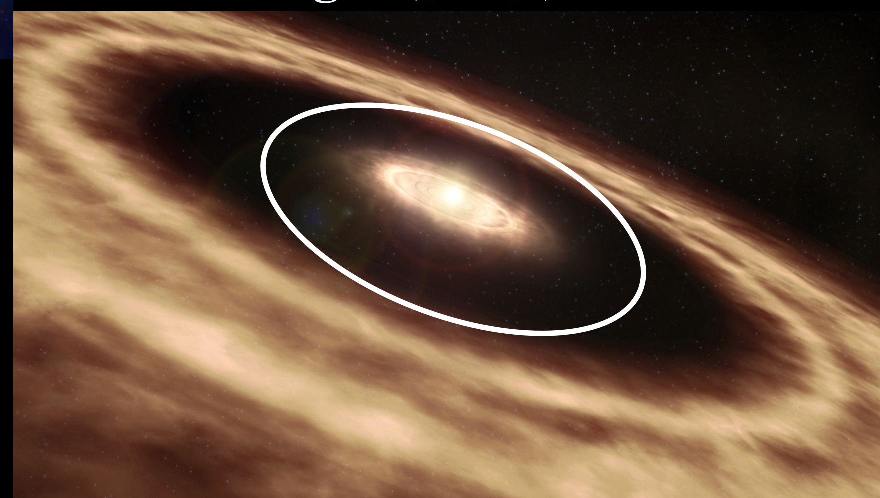


Pontoppidan et al. 2008

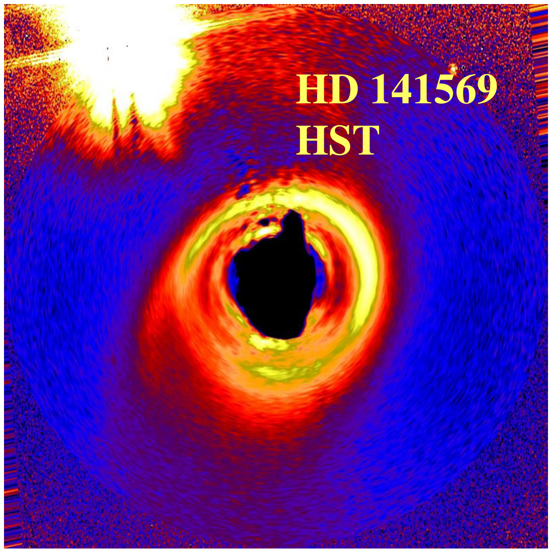
- SR 21 has dust gap of ~20 AU as imaged with SMA

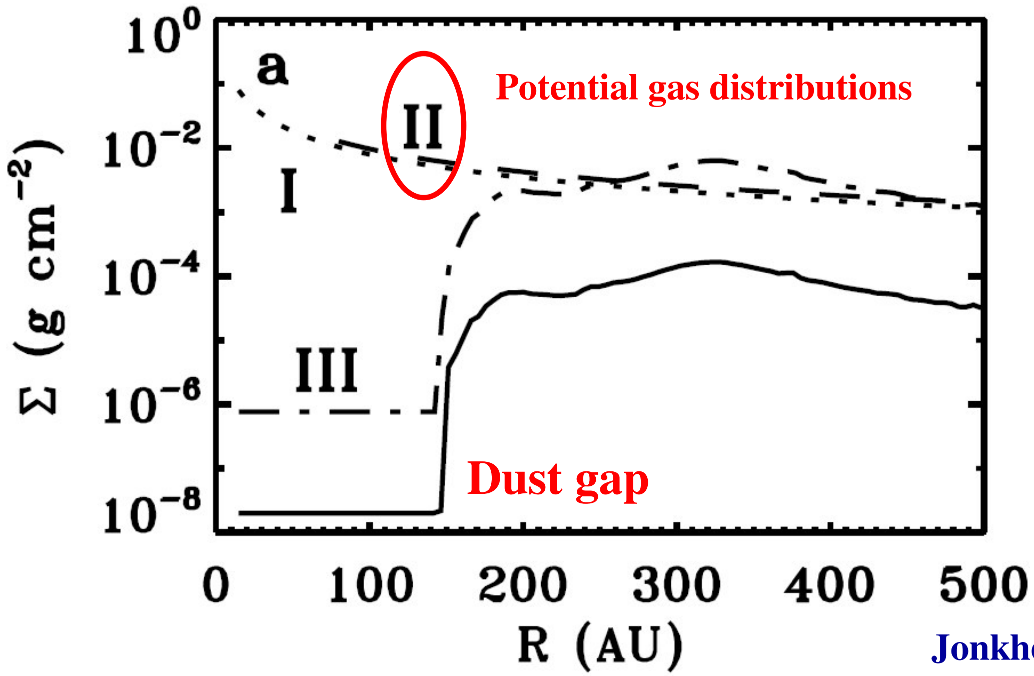
- Spectroastrometry of near-IR lines allows to pinpoint location to 7±1 AU ⇒ well inside gap!

-ALMA can detect/image molecular *and* atomic gas ([C I]!)



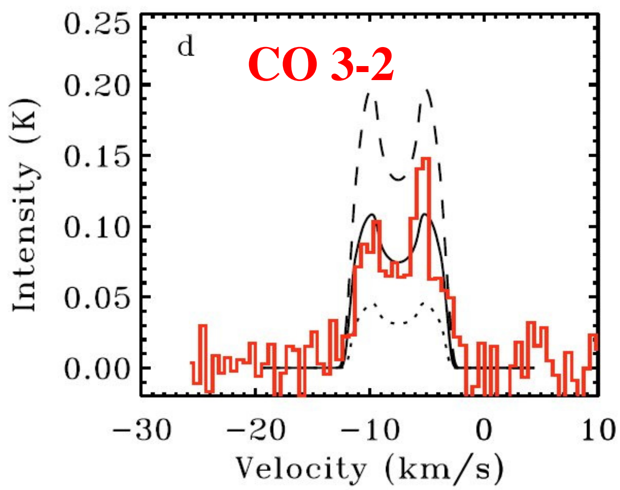
Chemistry in dust gaps





Jonkheid, Kamp et al. 2006

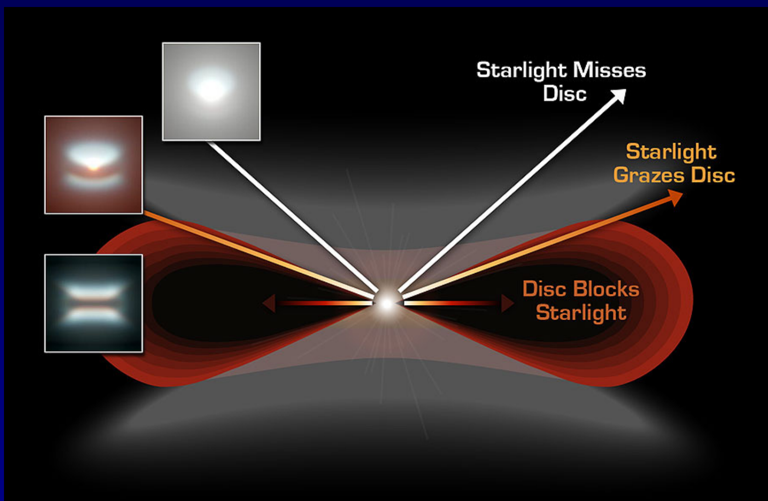
- H_2 and CO can survive inside dust gap if ~0.1 M_{Jup} of gas; presence of PAHs helps

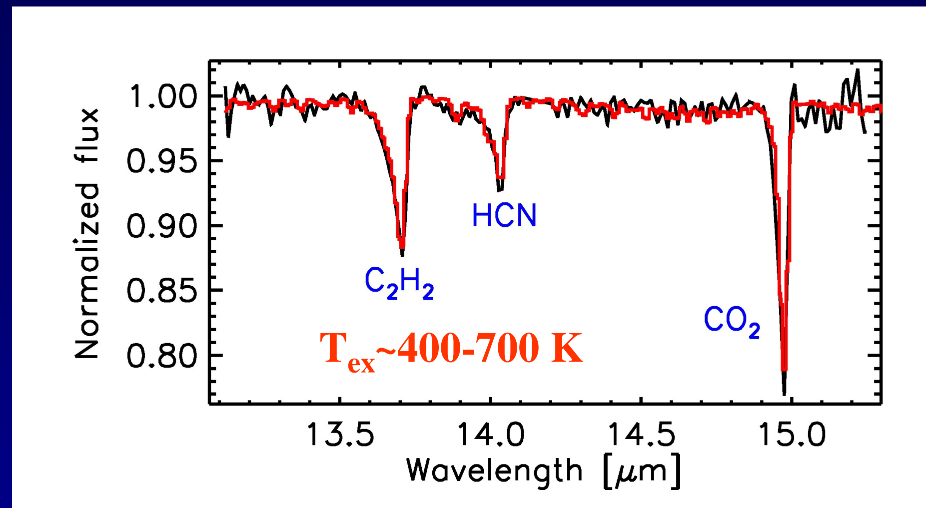


See also Kamp & Bertoldi 2000

Hot organic chemistry in inner disk

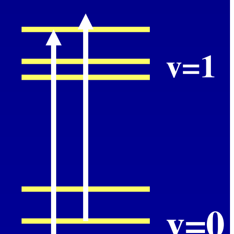
Low-mass: IRS46





Pontoppidan et al. 2005

Lahuis et al. 2006

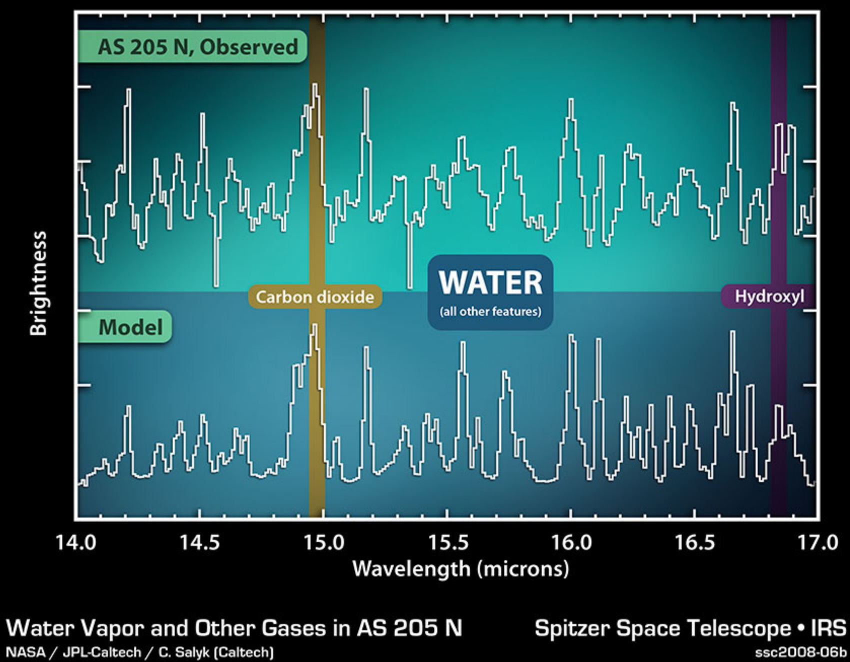


- **Abundances factor 1000 larger than in cold clouds**
- **No mm emission ⇒ must arise within inner 11 AU ⇒ inner disk**
- **Absorption variable on timescales of ~yr: disk structure**
  - **Also seen for GV Tau (Gibb et al. 2007)**

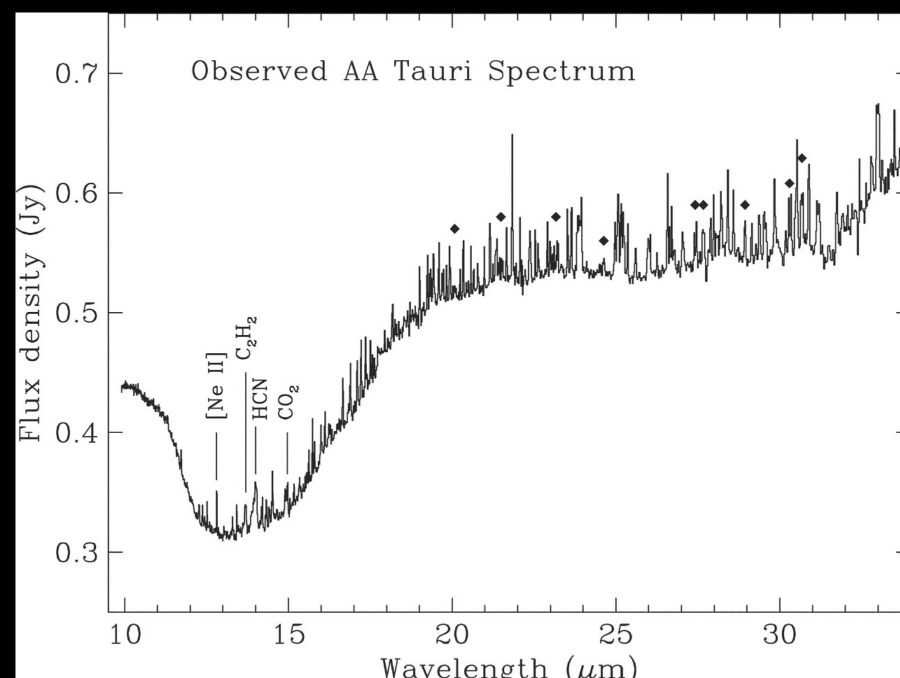
Lahuis B5

First probe of organic chemistry in planet-forming zones

Hot water and organics in the planet-forming zones of disks



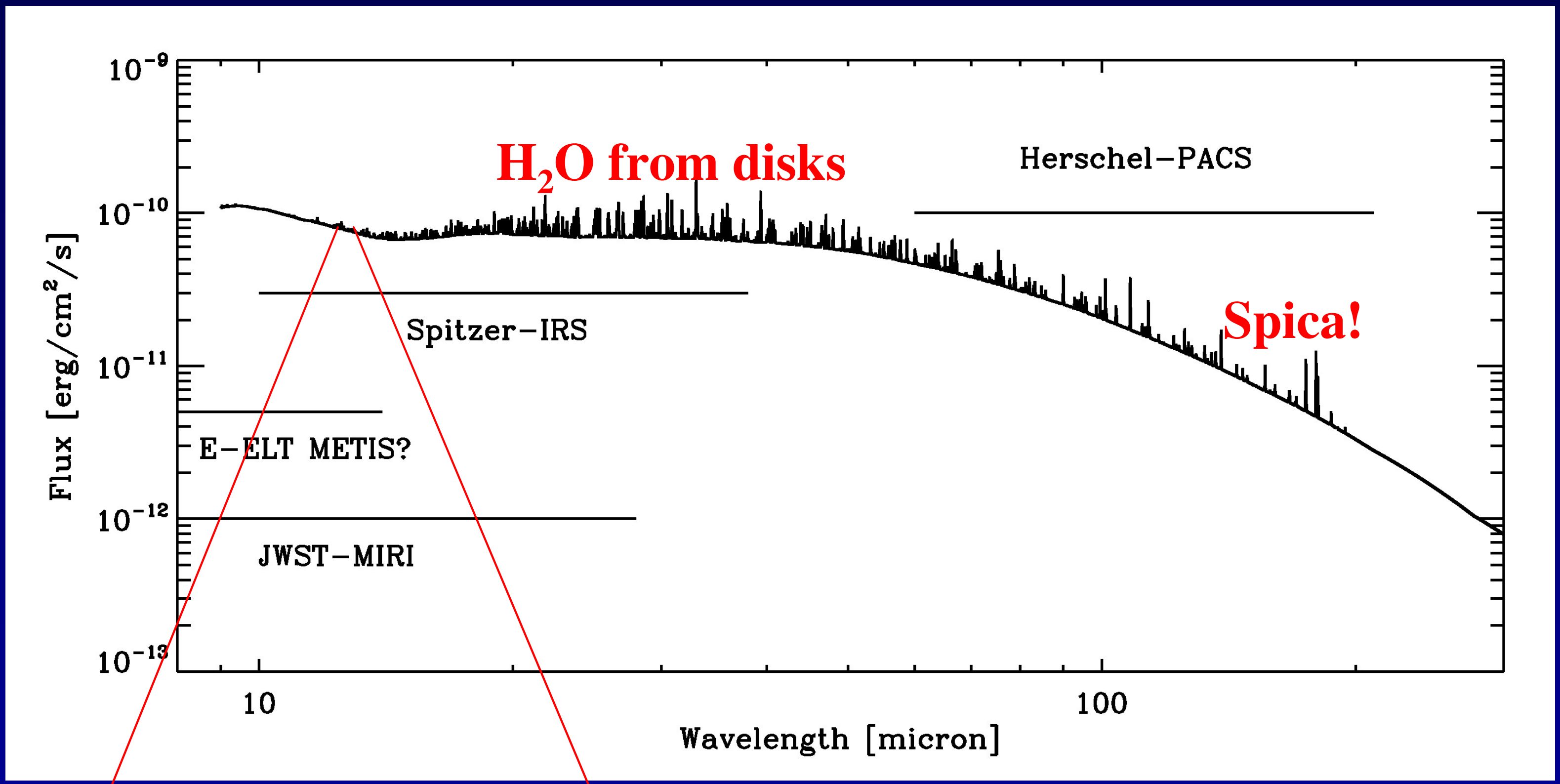
Salyk, Pontoppidan, Blake et al. 2008

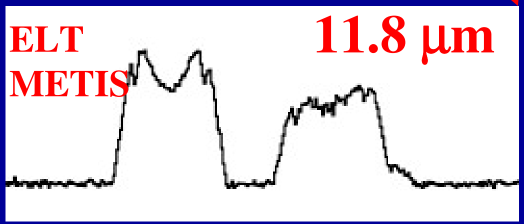


Carr & Najita 2008, Pascucci et al. 2008

See next 2 – 3 talks

Future mid/far-IR





Pontoppidan & Meijerink 2009

These instruments will be important complement to ALMA to study + image inner disk chemistry (<1-10 AU)!

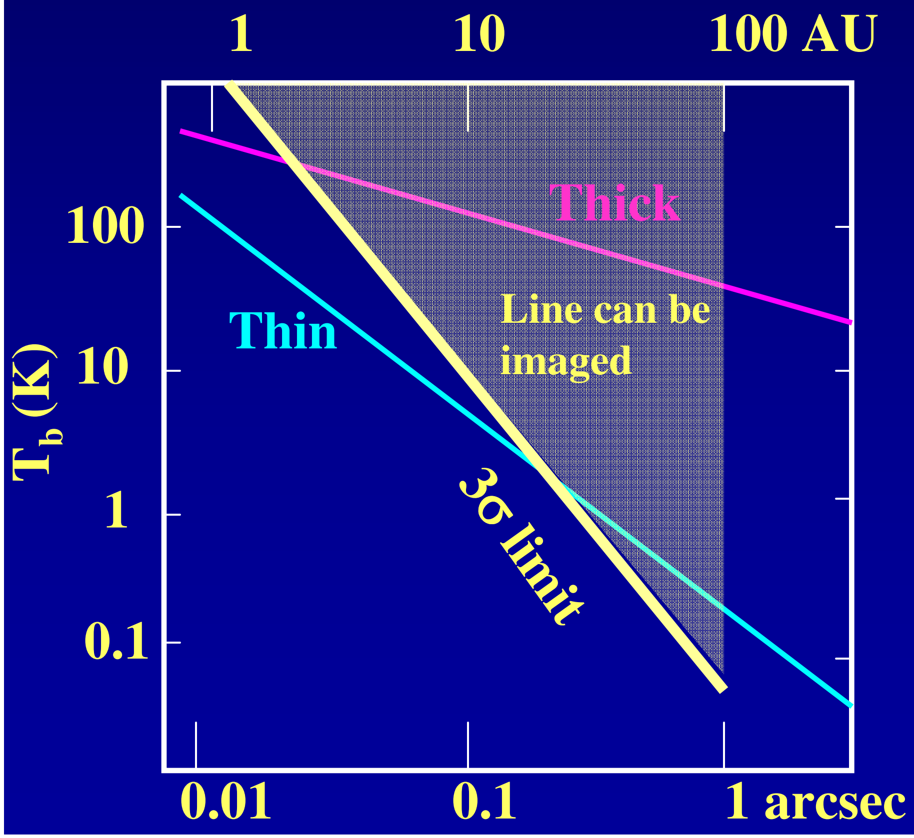
Can ALMA probe this region?

- **Take HCN as example**
- **IR data: line width, T_{ex} ⇒ emission comes from inner 1 AU**
- **Typical column ~10^{17} cm^{-2} ⇒ mm lines optically thick ⇒ T_R~T_{ex}~800 K if no beam dilution**
- **ALMA time estimator: 1 AU (0.01''), 0.5 km/s bin ⇒ T_b~200 K rms**

- ALMA can detect these molecules, but not image them on 1 AU scales, only at ~few AU scales in optically thick lines
- Need optically thin lines to probe midplane

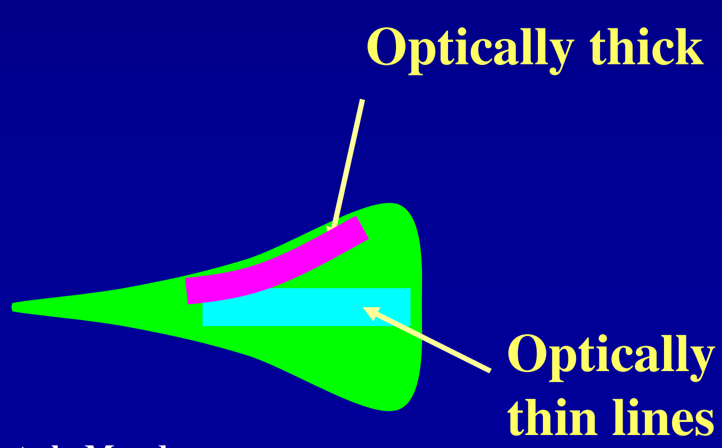
Prospects for ALMA

- Optically thick lines probe *intermediate* warm layer
  - ALMA can image down to few AU in ~8 hr
- Optically thin lines probe *midplane*
  - ALMA can image down to ~15 AU in ~8 hr



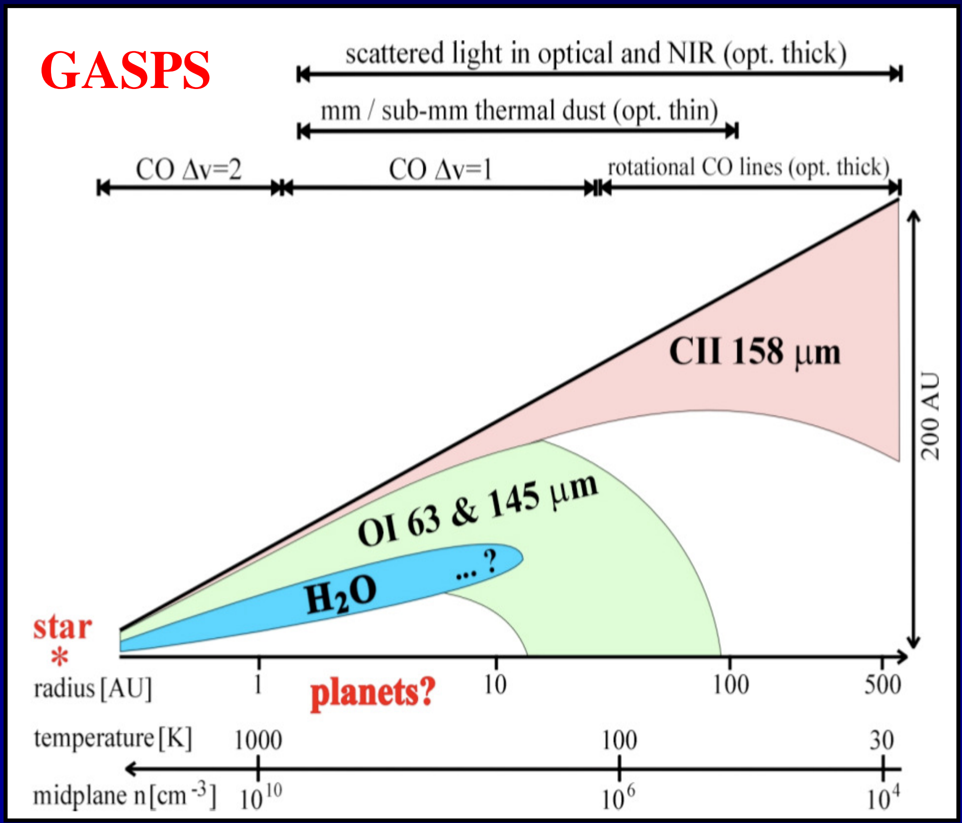
230-345 GHz
0.5 km/s
resolution

Disk at
100 AU



Dutrey et al., Mundy

Prospects for Herschel

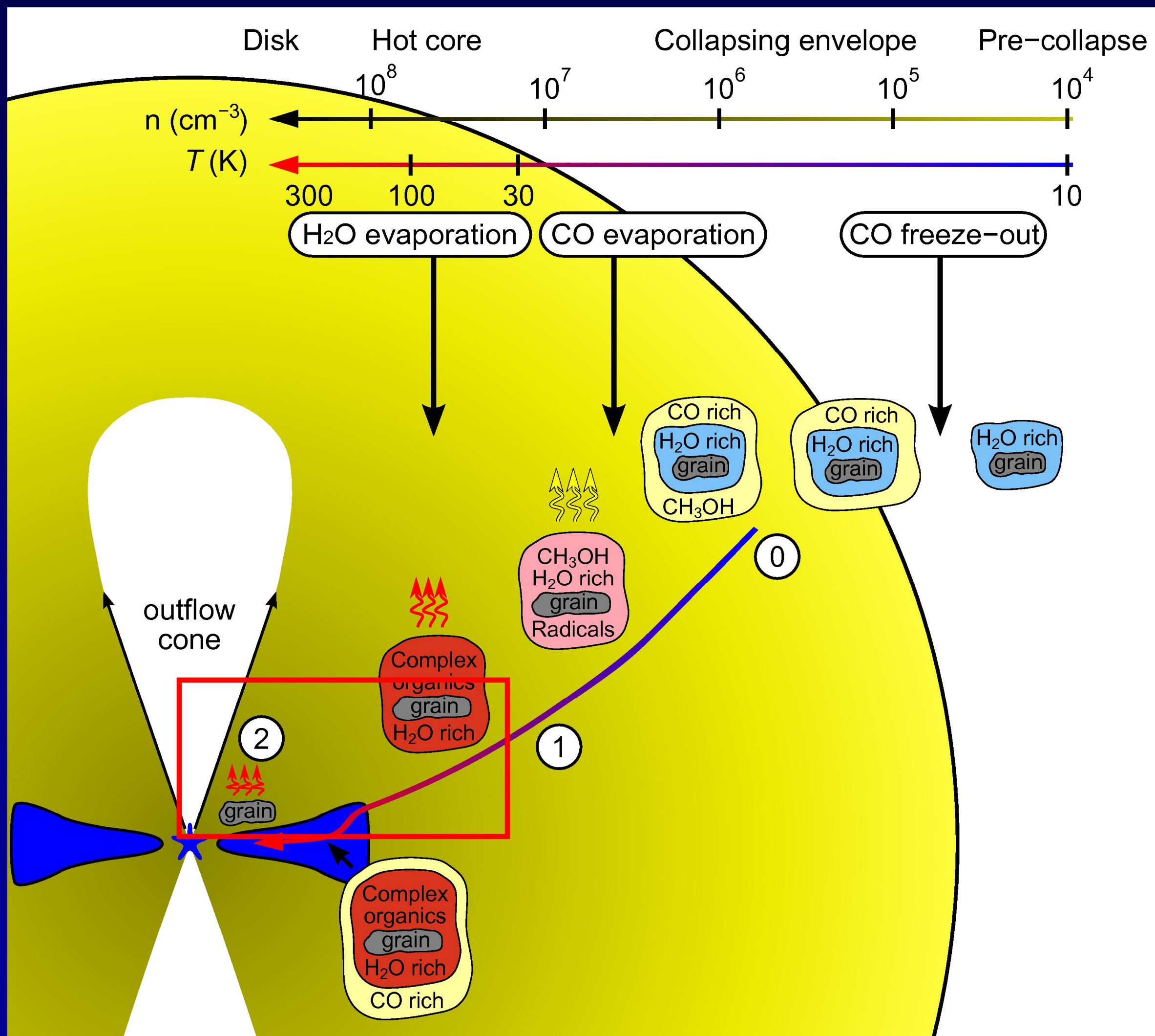


GASPS figure

- WISH: deep HIFI observations of H_2O of ~12 sources
- GASPS: ~200 disks distributed over spectral type, age, and disk mass: [CII], [OI], CO and H_2O lines
- DIGIT: full spectral scans of Herbig Ae disks

Prospects for JWST/ELT: see Meijerink talk

History of molecules in disks

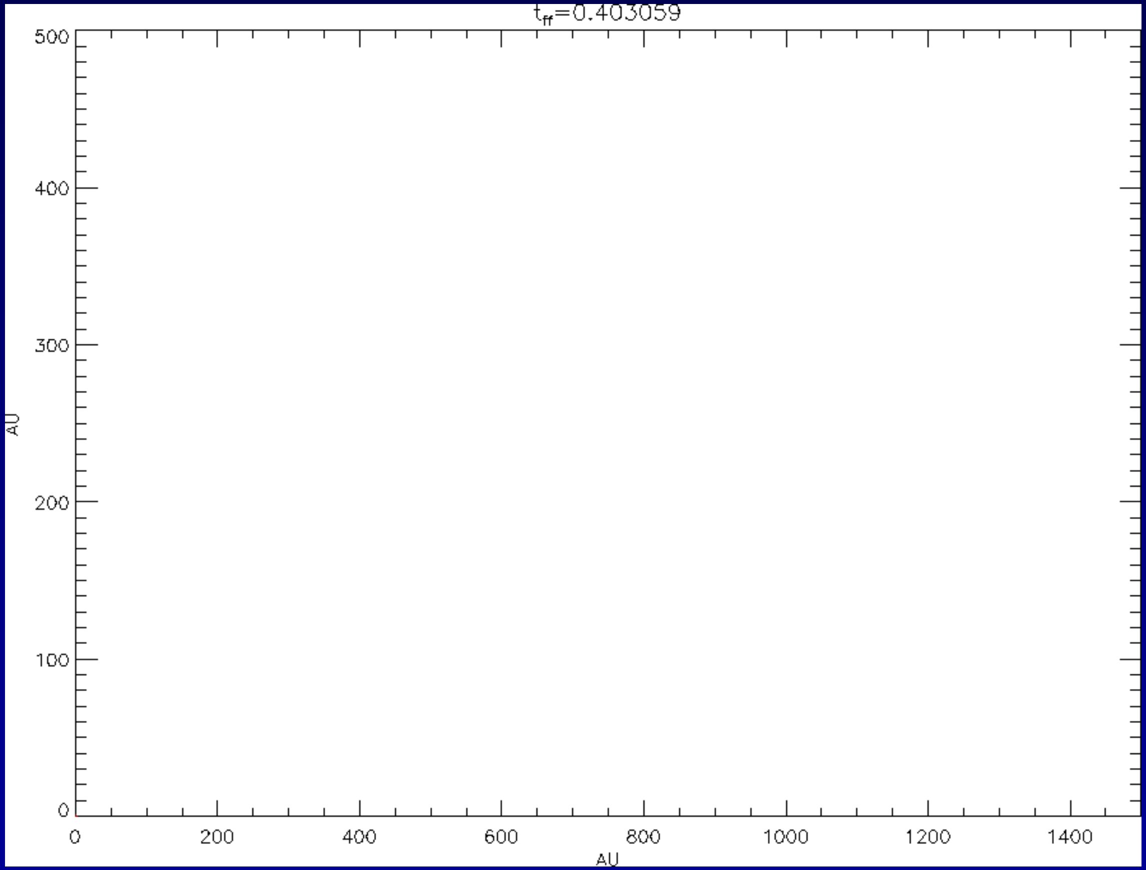


Visser et al. 2009

Herbst & vD ARA&A 2009

To what extent are abundances in disks determined in pre/protostellar phase?

2D Disk formation



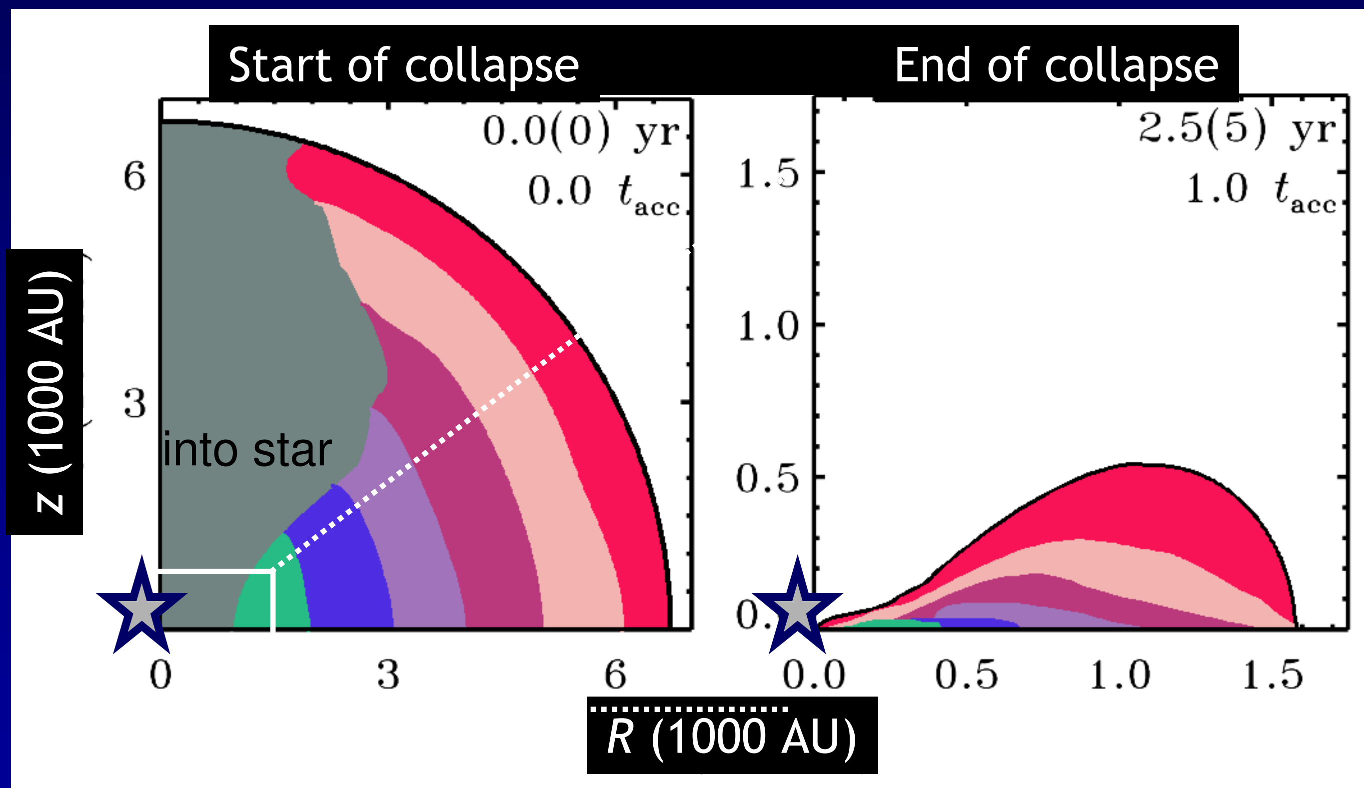
Numerical:
Van Weeren , Brinch & Hogerheijde 2008

Semi-analytic:
Visser et al. 2009

- **Accretion onto 2D disk fundamentally different from 1D**
- **More material enters disk on back side, far from star**
- **Layered accretion: Outer envelope parcels end up in surface layer disk**

Where does material go to?

Inside-out collapse gives a layered disk



Strongly bound ices (H_2O, …) partly survive,
Weakly bound ices (CO, …) not

Visser et al. 2009

Summary

- Disk chemistry rapidly evolving field
- Outer disk: 3-layer ‘sandwich’ structure
- Inner disks: new Spitzer results and ground-based data open up study of inner AU
- Next generation physical-chemical models
  - Importance of T_{gas}, UV, X-rays, gas-grain
- Some abundances may be set in pre- and protostellar phase

ALMA, Herschel, JWST, ELTs critical to test these!