Modelling of protoplanetary disks

A "cookbook" for observationally-motivated disk physico-chemical models

Catherine Walsh
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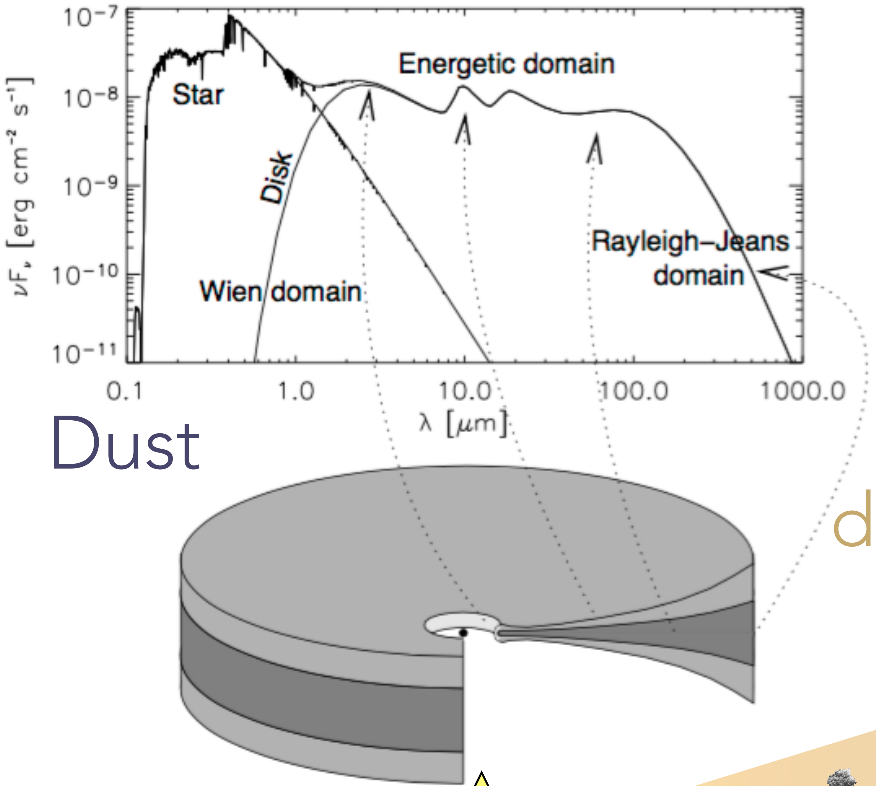
Leiden Observatory

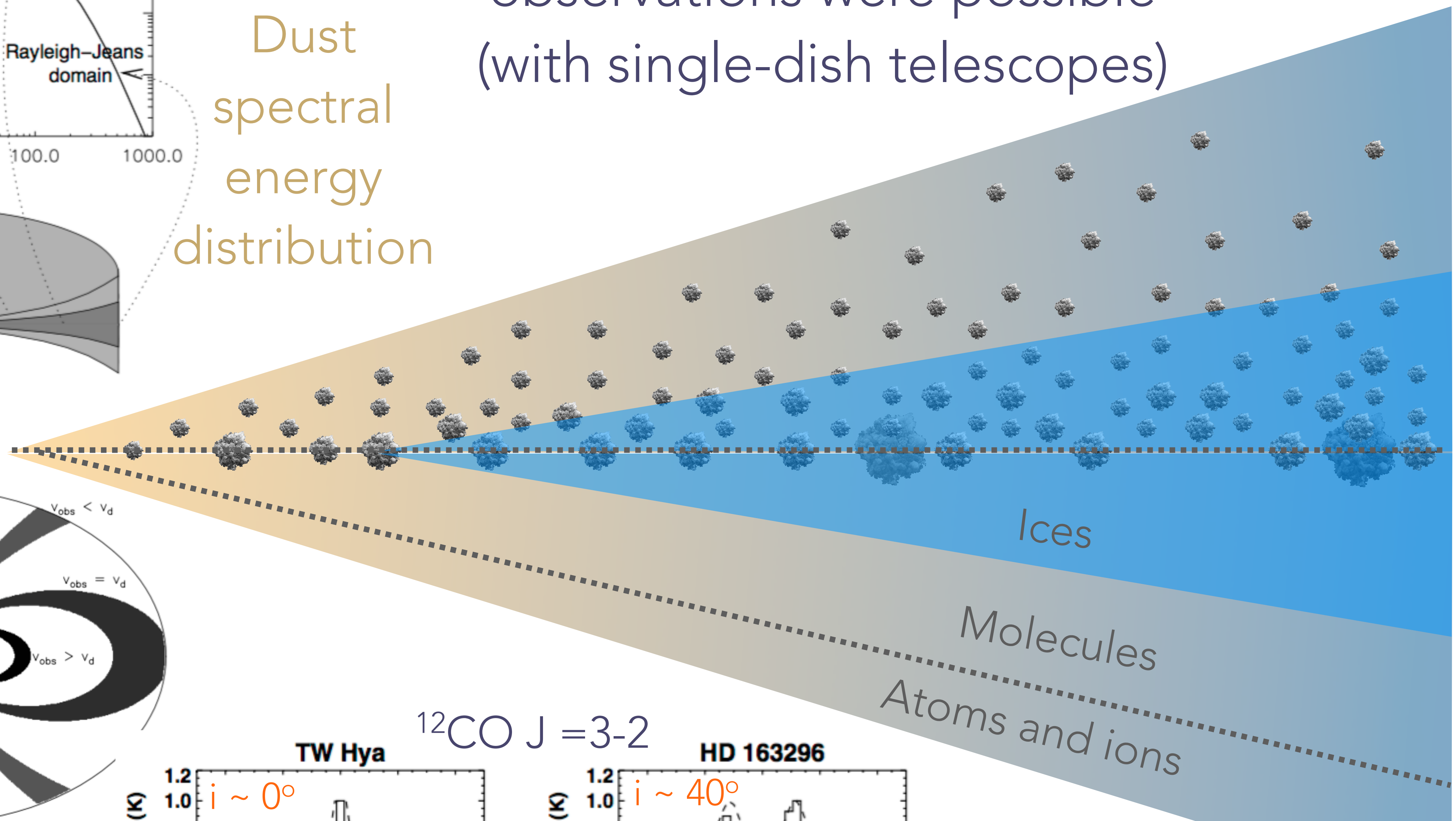
Observations of protoplanetary disks

Until recently: only spatially-unresolved observations were possible (with single-dish telescopes)

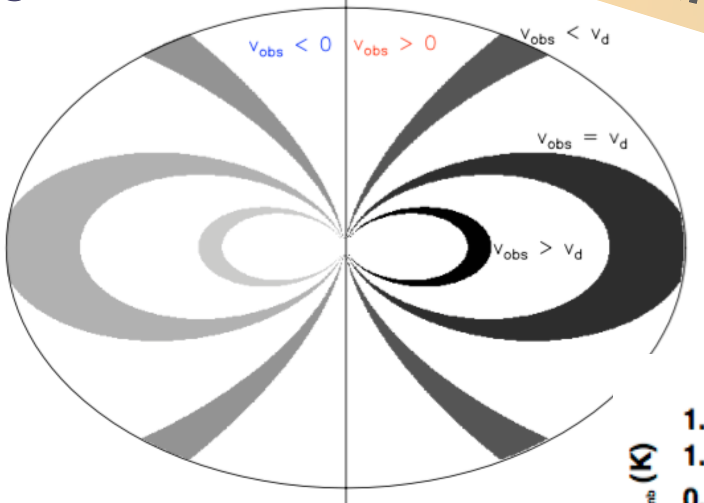
Dust



Dust spectral energy distribution

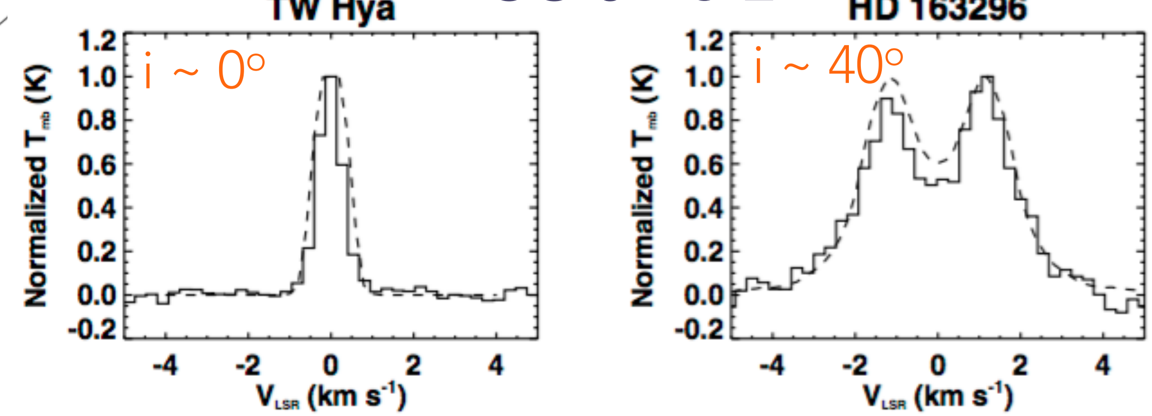


Gas



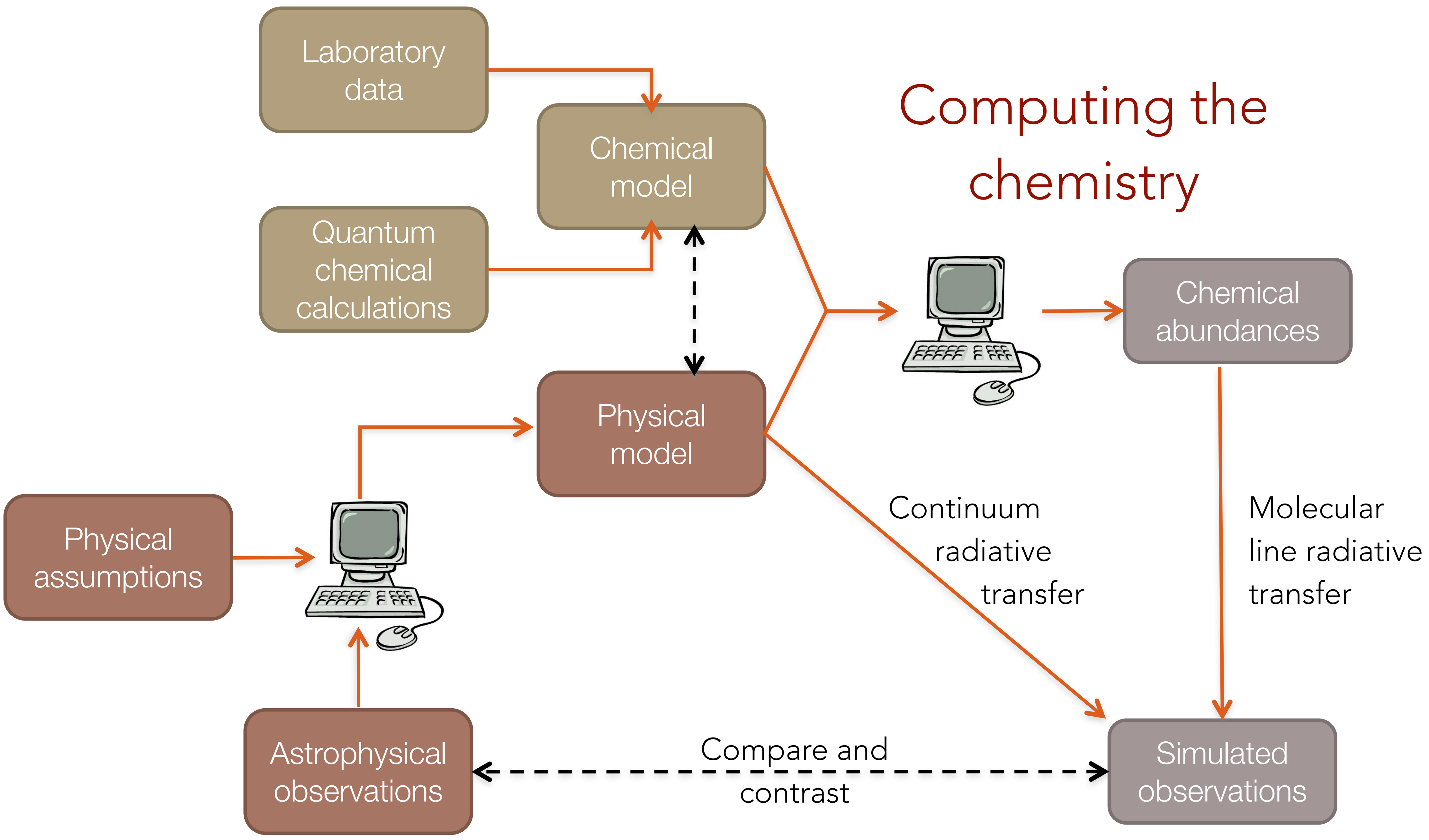
Molecular/atomic emission lines

^{12}CO J =3-2



Dullemond, C. P., et al. 2006, PPV, 555; Thi, W.-F., et al. 2004, A&A, 425, 955; Guilloteau, S., et al. 2006, A&A, 448, L5

General outline of a physico-chemical model



Outline

Disk physical structure:

✳ dust

✳ gas

Disk chemical structure:

✳ gas-phase (vapour)

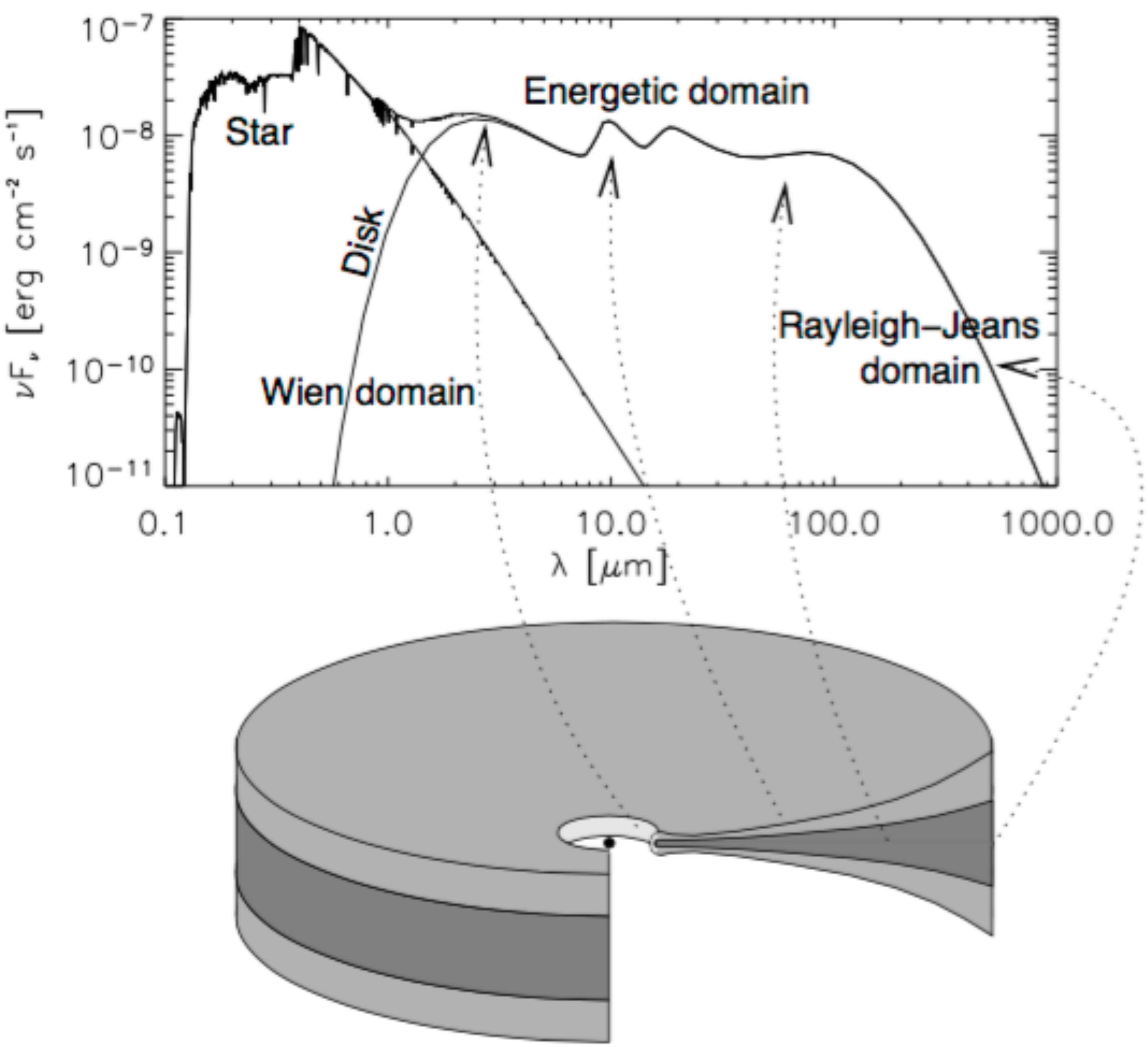
✳ solid-phase (ice)

Building physico-chemical models

Observations of dust in protoplanetary disks

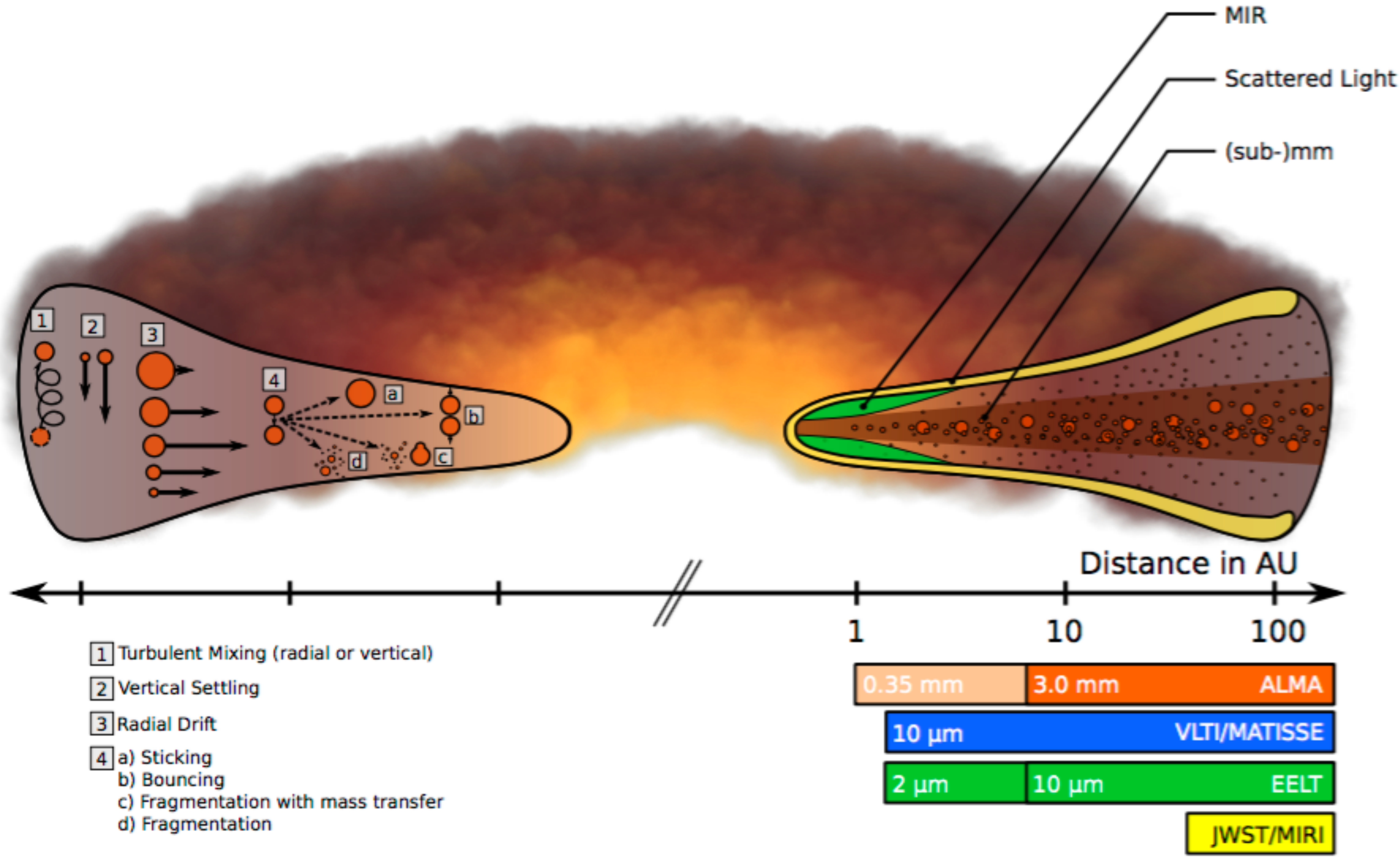
Early modelling efforts concerning the dust focussed primarily on reproducing the spectral energy distribution (SED)

Dust spectral energy distribution



- Optical wavelengths: scattered light; hence no temperature/density information
- Near-infrared wavelengths: originates mainly from "hot" inner rim
- Mid-infrared wavelengths: originates from "warm" dust close to the star (< 10 AU) and is typically optically thick; hence, no density information but probes temperature of dust photosphere
- Sub-mm/mm wavelengths: originates from "cold" dust in outer disk (> 10 AU) and is typically optically thin; hence, has both temperature and density information

Observations of dust in protoplanetary disks

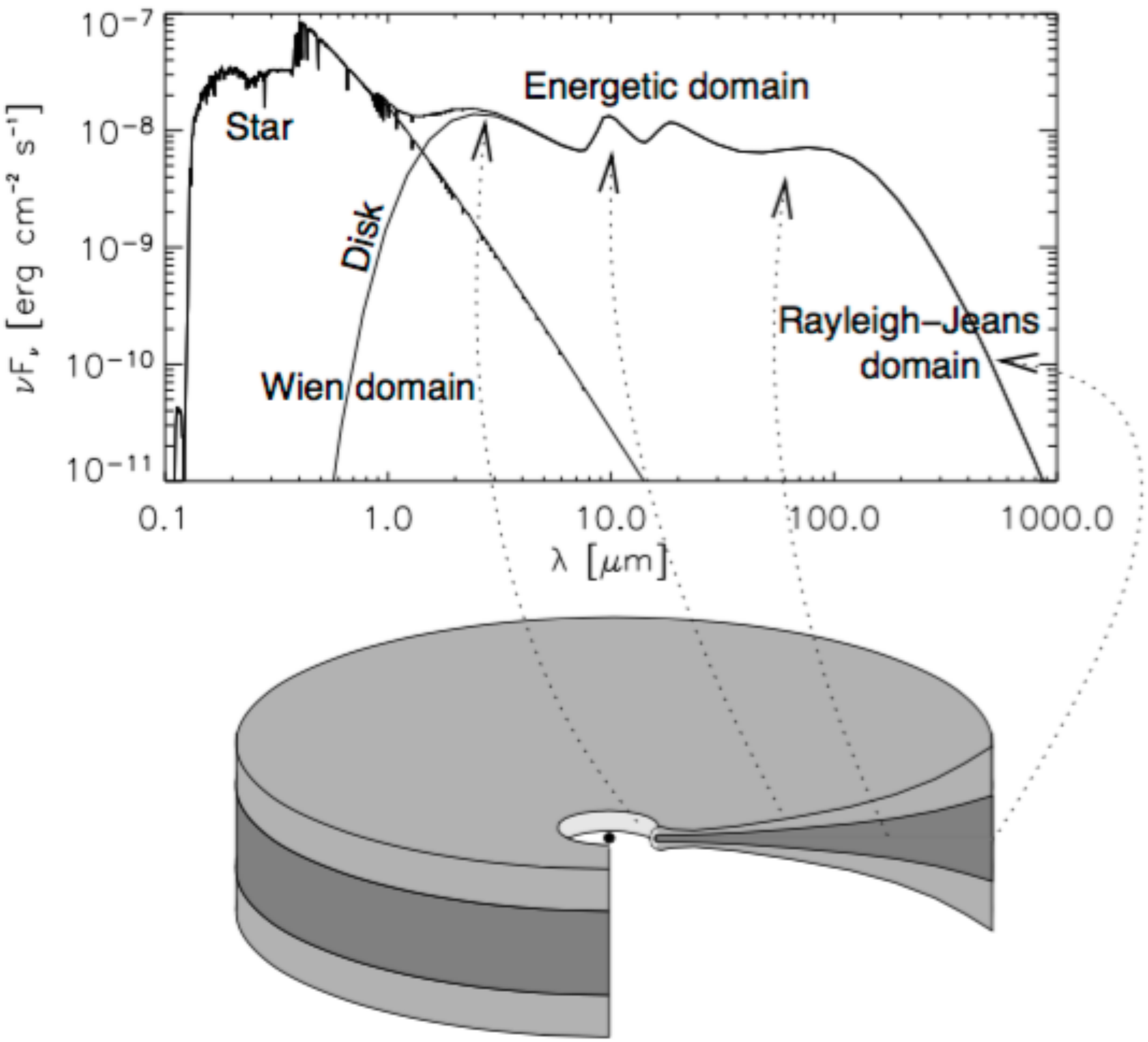


Testi, L., et al. 2014, PPVI, 339

Observations of dust in protoplanetary disks

Some simple assumptions about the (sub)mm opacity and dust temperature can yield an estimation of the disk mass

Dust spectral energy distribution



Optical depth

$$\tau_\nu = \int \rho \kappa_\nu ds = \kappa_\nu \Sigma,$$

Dust mass opacity

$$\kappa_\nu = 0.1 \left(\frac{\nu}{10^{12}\,\mathrm{Hz}}\right)^\beta \mathrm{cm}^2\,\mathrm{g}^{-1}.$$

Disk mass

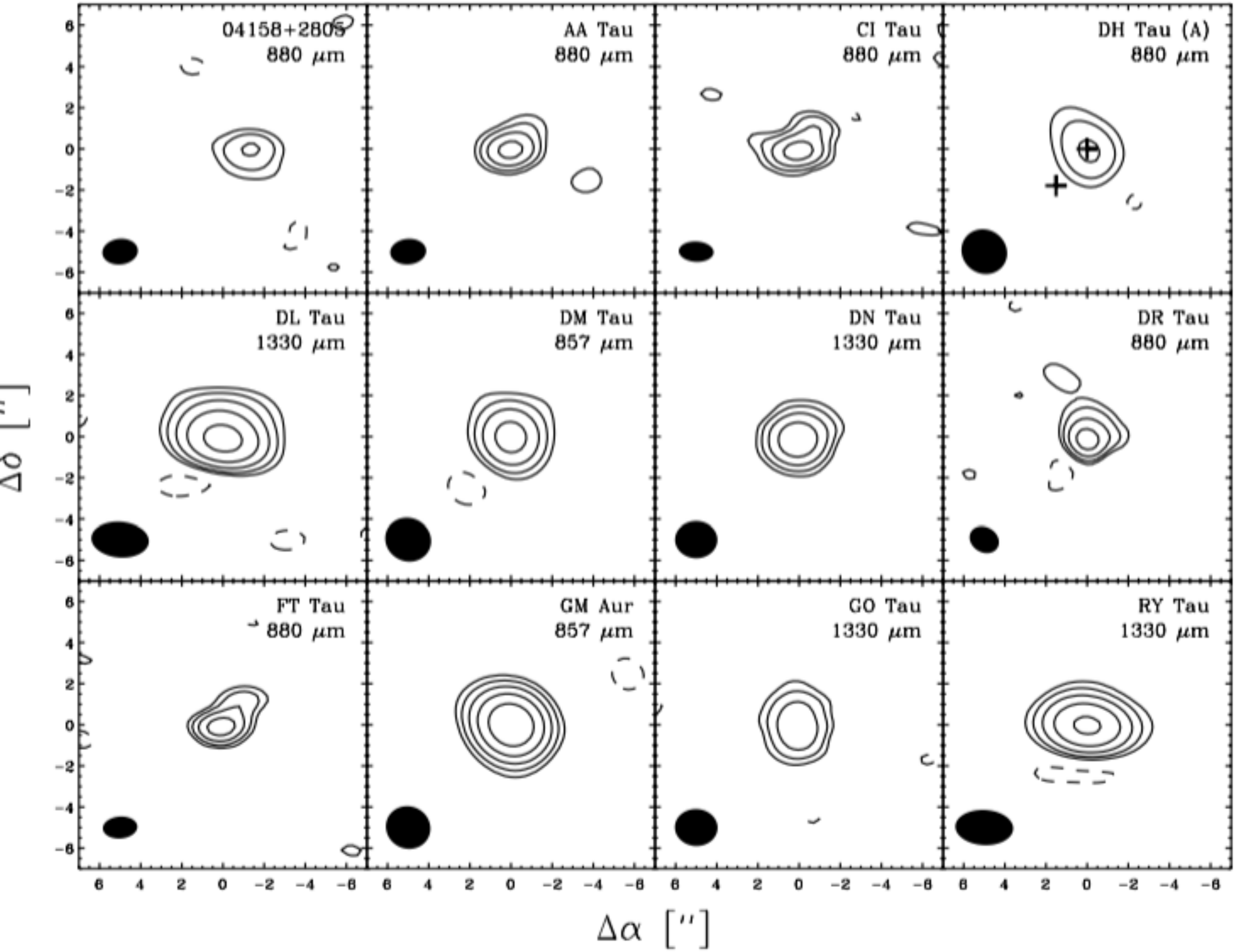
$$M(\mathrm{gas} + \mathrm{dust}) = \frac{F_\nu d^2}{\kappa_\nu B_\nu(T)},$$

Gas-to-dust mass ratio ~ 100

Beckwith et al. 1990, AJ, 99, 924; Andrews & Williams 2005, ApJ, 631, 1134; Williams & Cieza 2011, ARA&A, 49, 67

Observations of dust in protoplanetary disks

The advent of (sub)mm interferometry required more sophisticated models to describe the radial disk structure



Disk surface density, temperature, and dust mass opacity were "well-fit" using power laws

$$T_r = T_1 \left(\frac{r}{1\ \mathrm{AU}}\right)^{-q},$$

$$\Sigma_r = \Sigma_5 \left(\frac{r}{5\ \mathrm{AU}}\right)^{-p},$$

$$\kappa_\nu = \kappa_0 \left(\frac{\nu}{\nu_0}\right)^{\beta},$$

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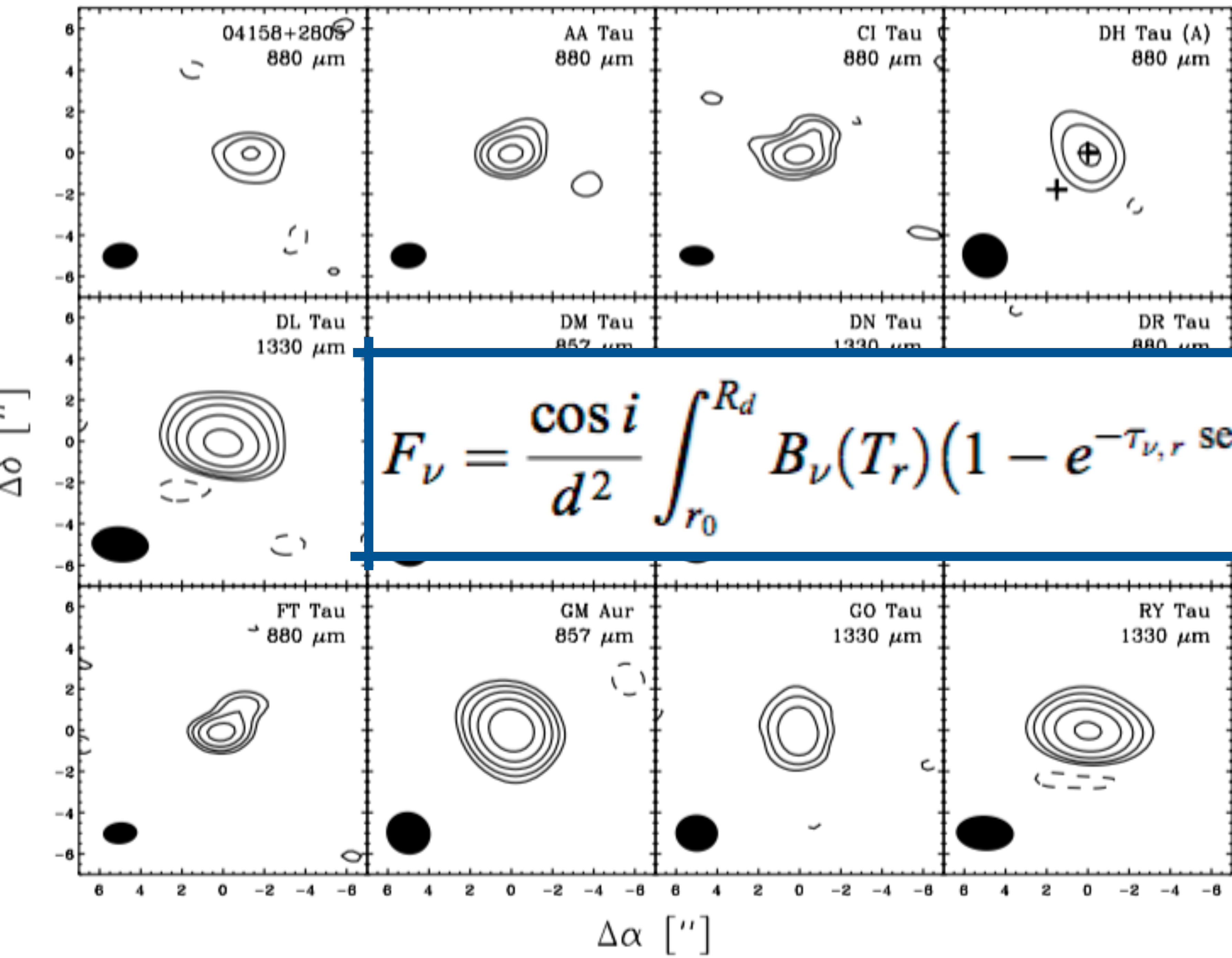

$$F_\nu = \frac{\cos i}{d^2} \int_{r_0}^{R_d} B_\nu(T_r)\left(1 - e^{-\tau_{\nu,r} \sec i}\right) 2\pi r \, dr,$$

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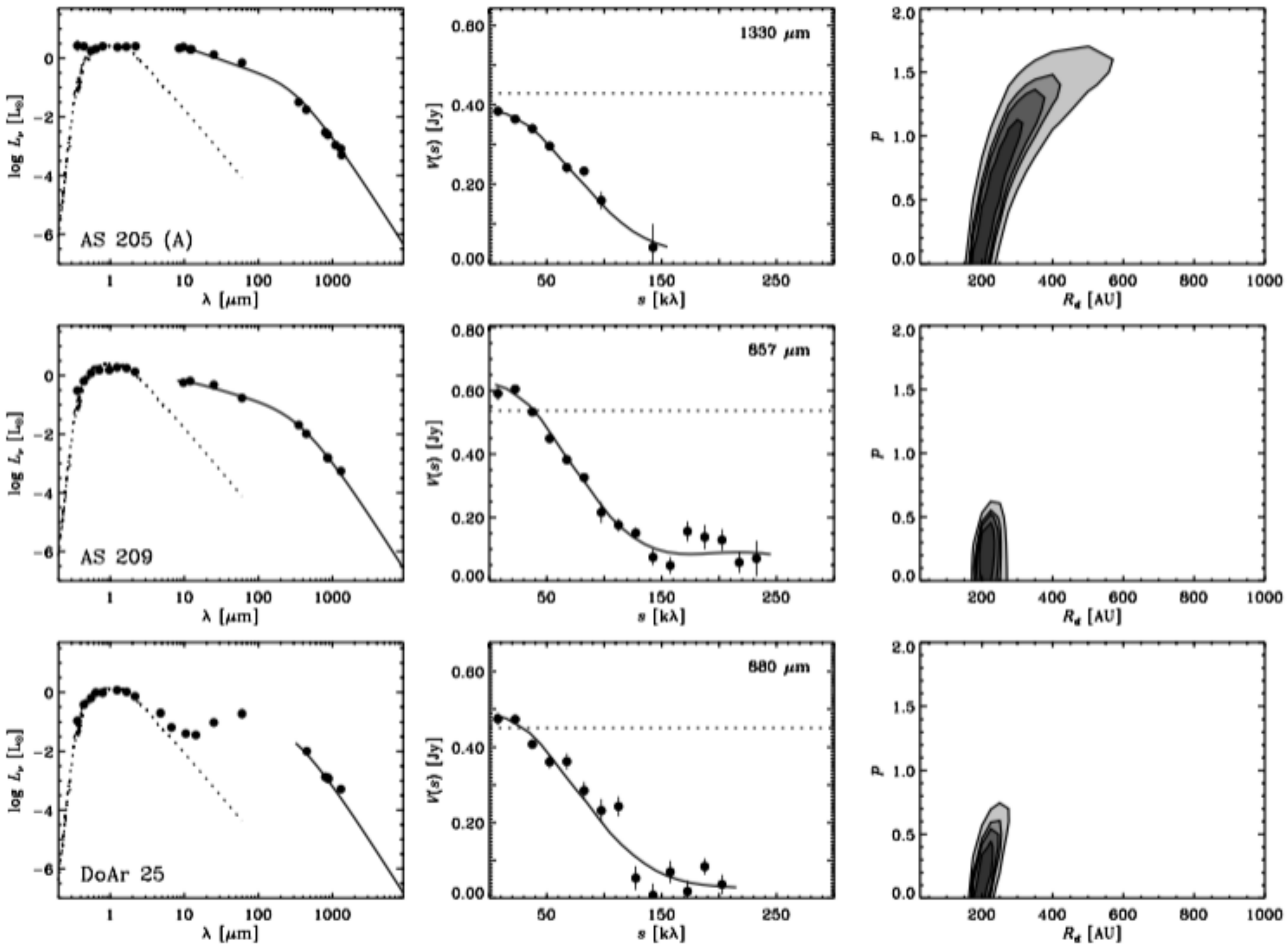
Observations of dust in protoplanetary disks

Fitting is done directly to the interferometric data (so-called visibilities) which are the Fourier transform of the intensity distribution

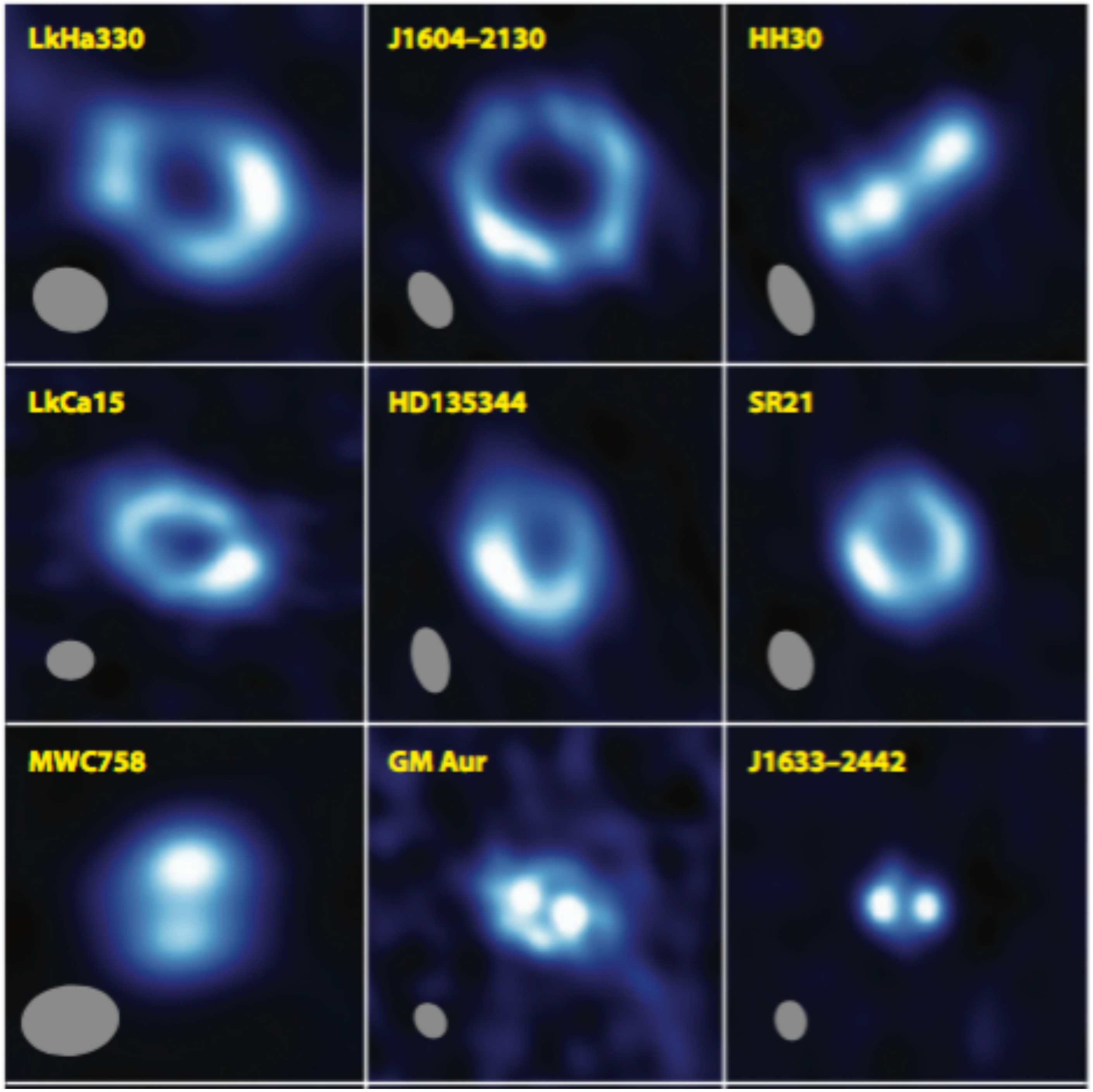


Andrews & Williams 2007, ApJ, 659, 705; Williams & Cieza 2011, ARA&A, 49, 67

Observations of dust in protoplanetary disks

Higher-resolution (sub-arcsecond) interferometric data required additional considerations for models of the dust emission: cavities and rings

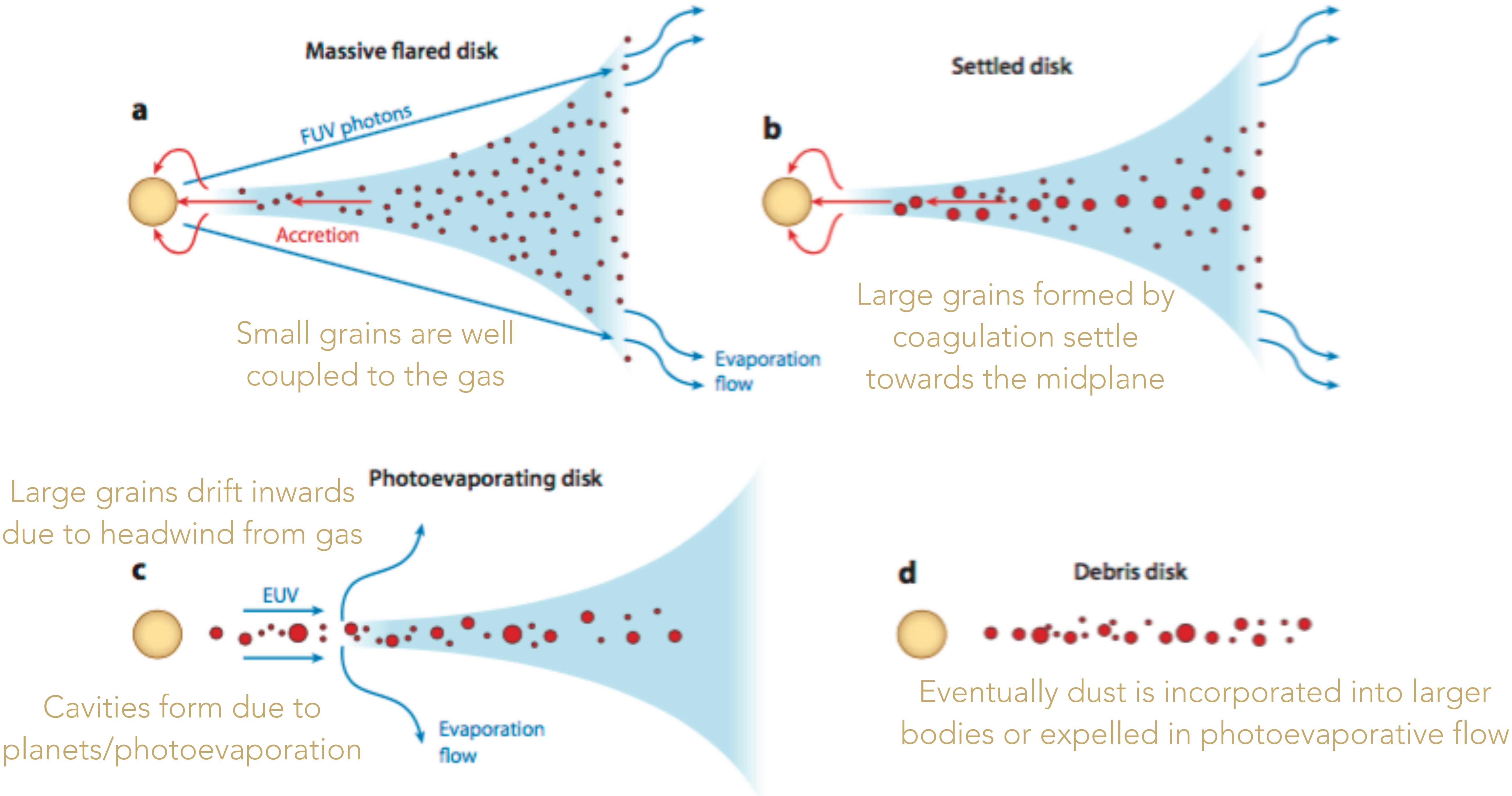
SMA observations



Williams & Cieza 2011, ARA&A, 49, 67

Evolution of dust in protoplanetary disks

Generalised picture of dust evolution in protoplanetary disks

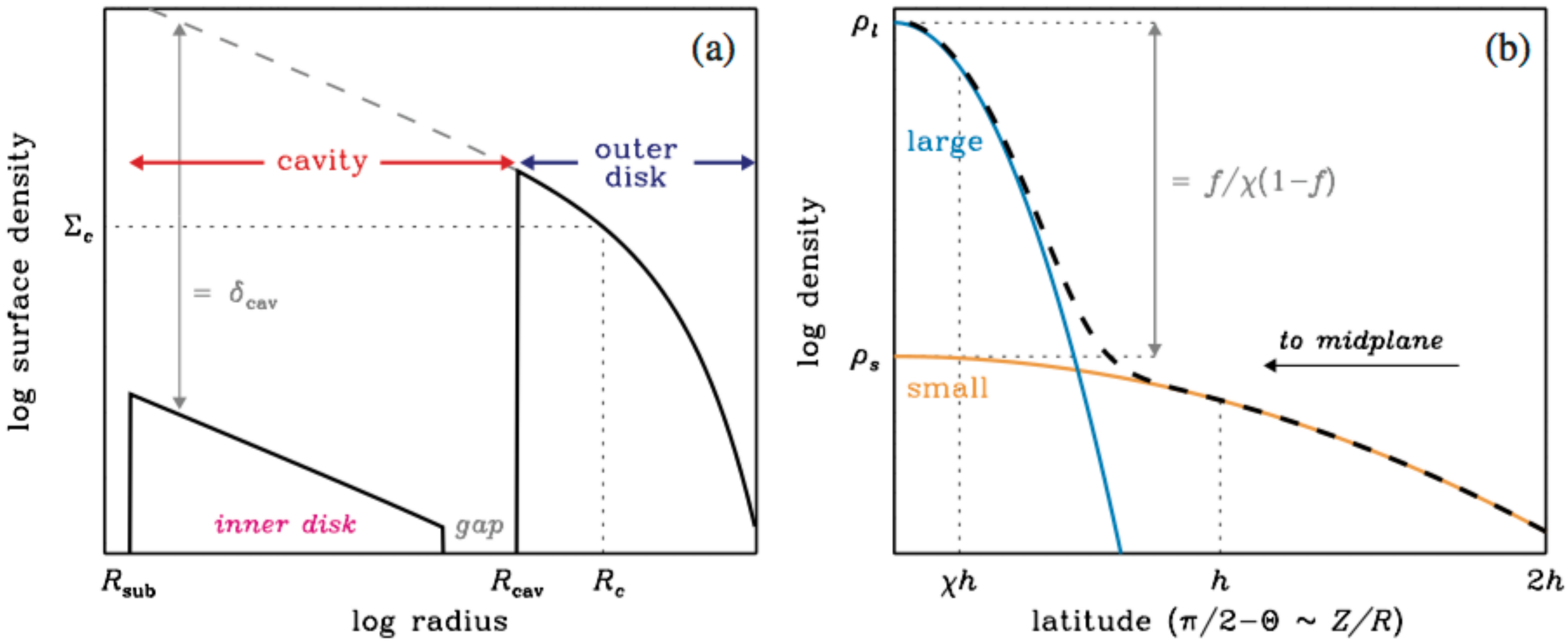


Small (~ μm-sized) and large (~ mm-sized) grains follow different paths

Williams & Cieza 2011, ARA&A, 49, 67

Modelling of dust in protoplanetary disks

Simple power-law models are still used, but with gaps and cavities, and "small" and "large" grains are decoupled to simulate settling



Despite more complex models being using to model more complex data, significant degeneracies still remain in the models

Andrews S. M., et al. 2011, ApJ, 732, 42l Bruderer, S 2013, A&A, 559, A46

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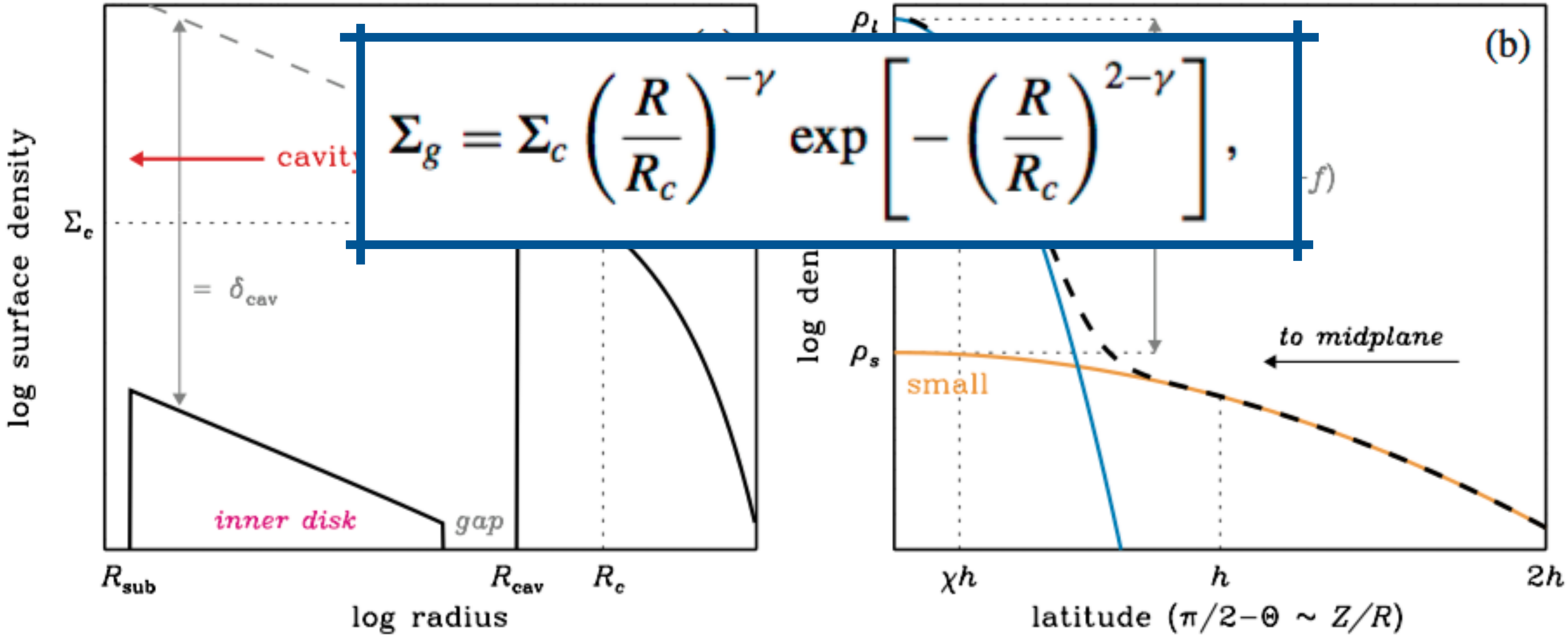

$$\Sigma_g = \Sigma_c \left(\frac{R}{R_c}\right)^{-\gamma} \exp\left[-\left(\frac{R}{R_c}\right)^{2-\gamma}\right],$$

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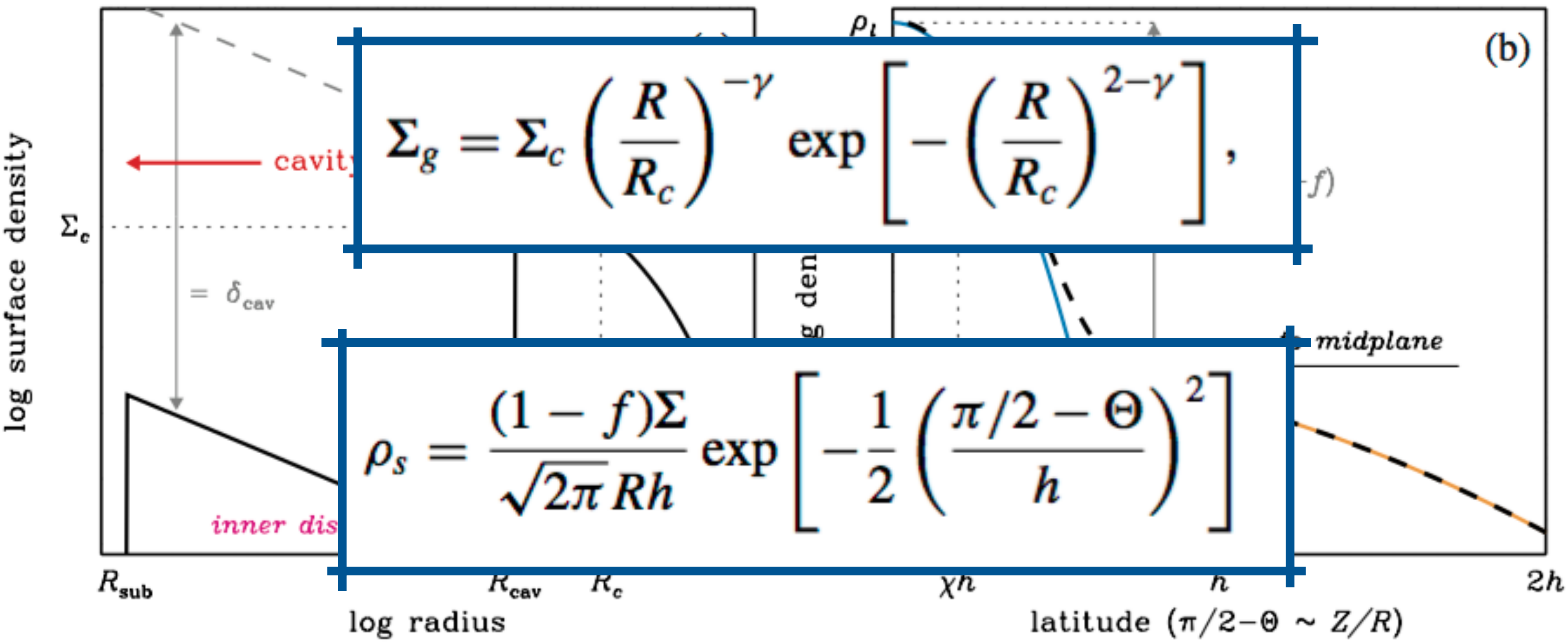


$$\Sigma_g = \Sigma_c \left(\frac{R}{R_c}\right)^{-\gamma} \exp\left[-\left(\frac{R}{R_c}\right)^{2-\gamma}\right],$$

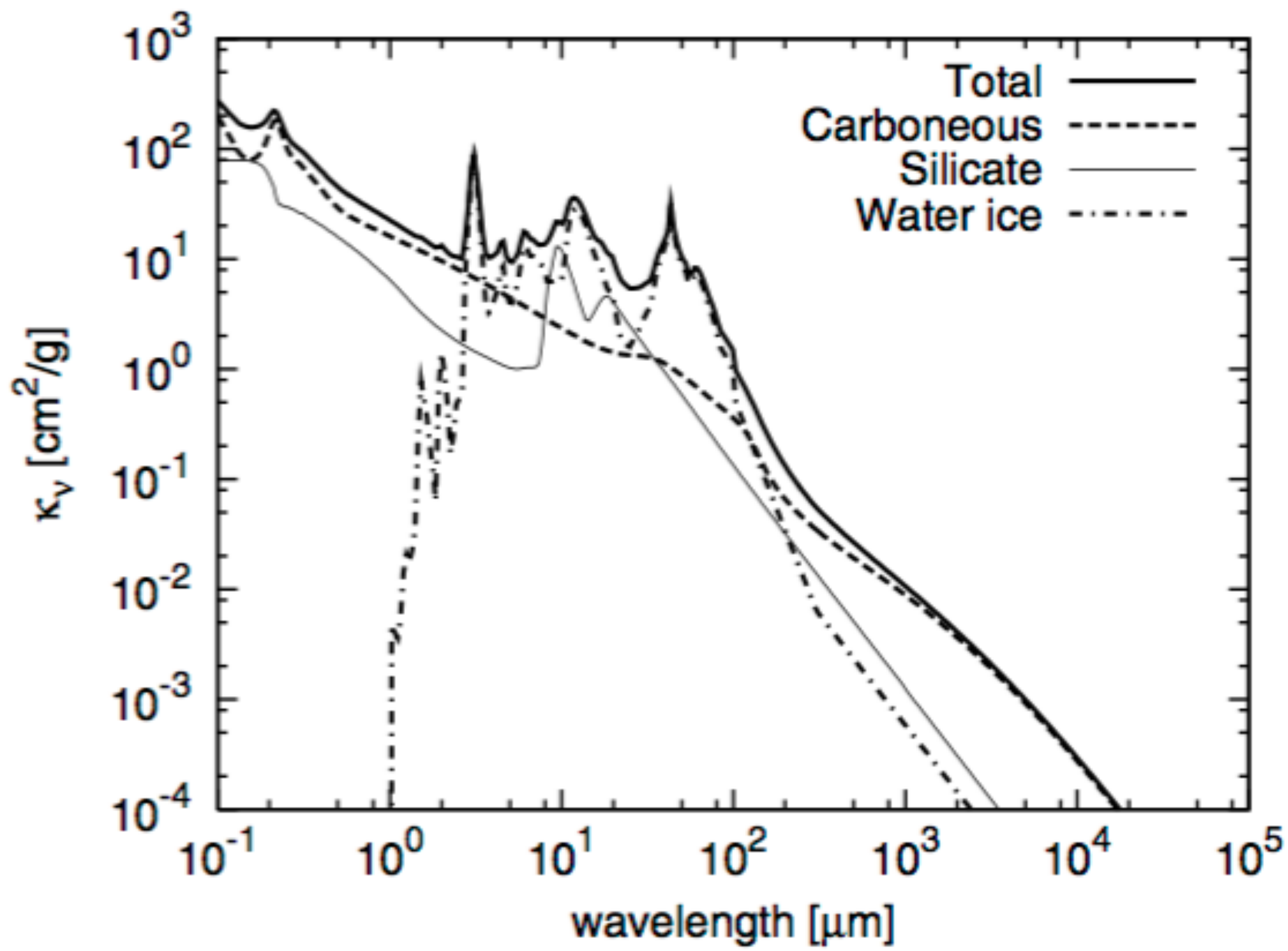
$$\rho_s = \frac{(1-f)\Sigma}{\sqrt{2\pi}\, Rh} \exp\left[-\frac{1}{2}\left(\frac{\pi/2-\Theta}{h}\right)^2\right]$$

Despite more complex models being using to model more complex data, significant degeneracies still remain in the models

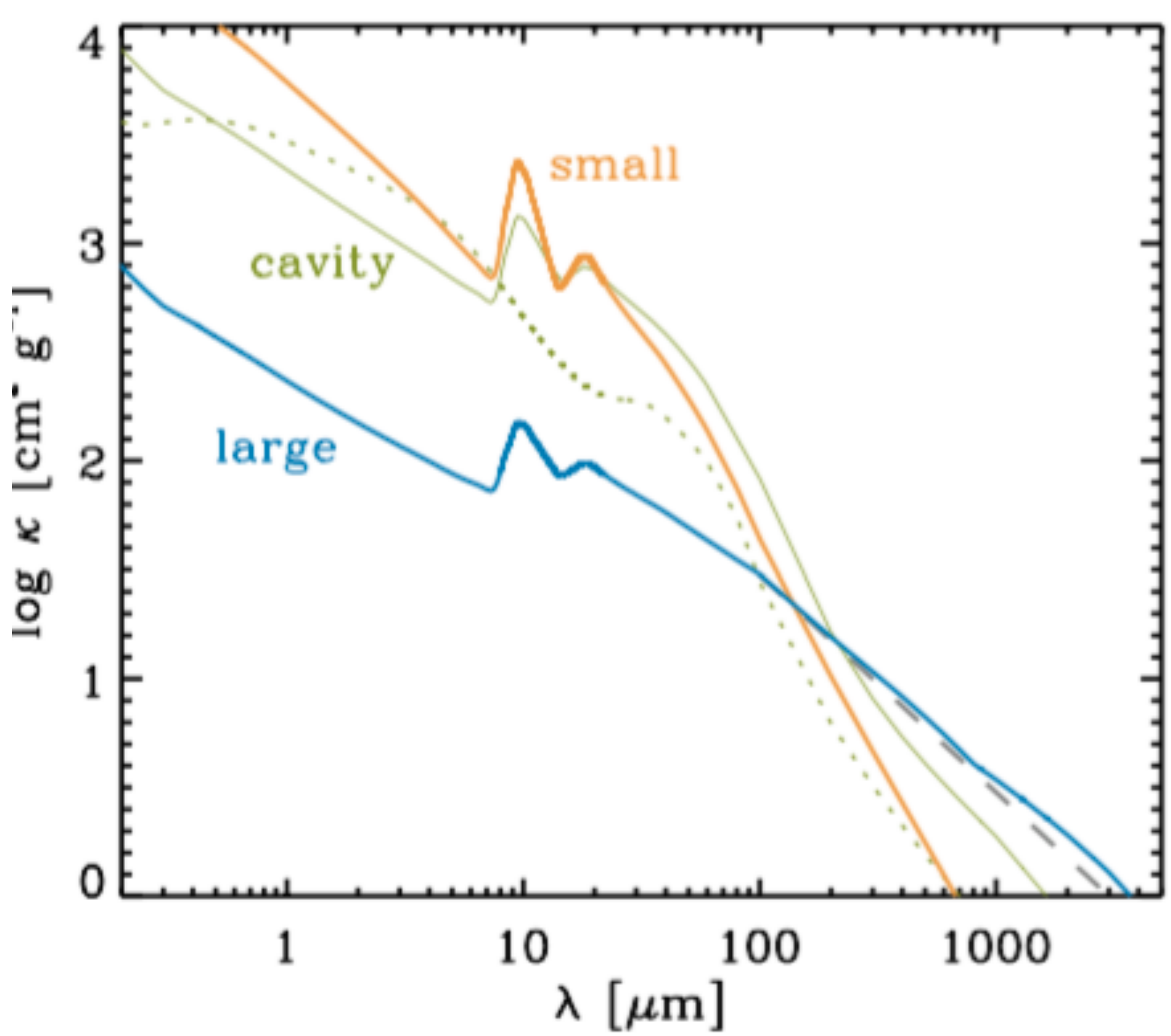
Andrews S. M., et al. 2011, ApJ, 732, 42l Bruderer, S 2013, A&A, 559, A46

Dust opacity

The dust density and size distribution sets the temperature structure of the disk: dust composition and opacity are required



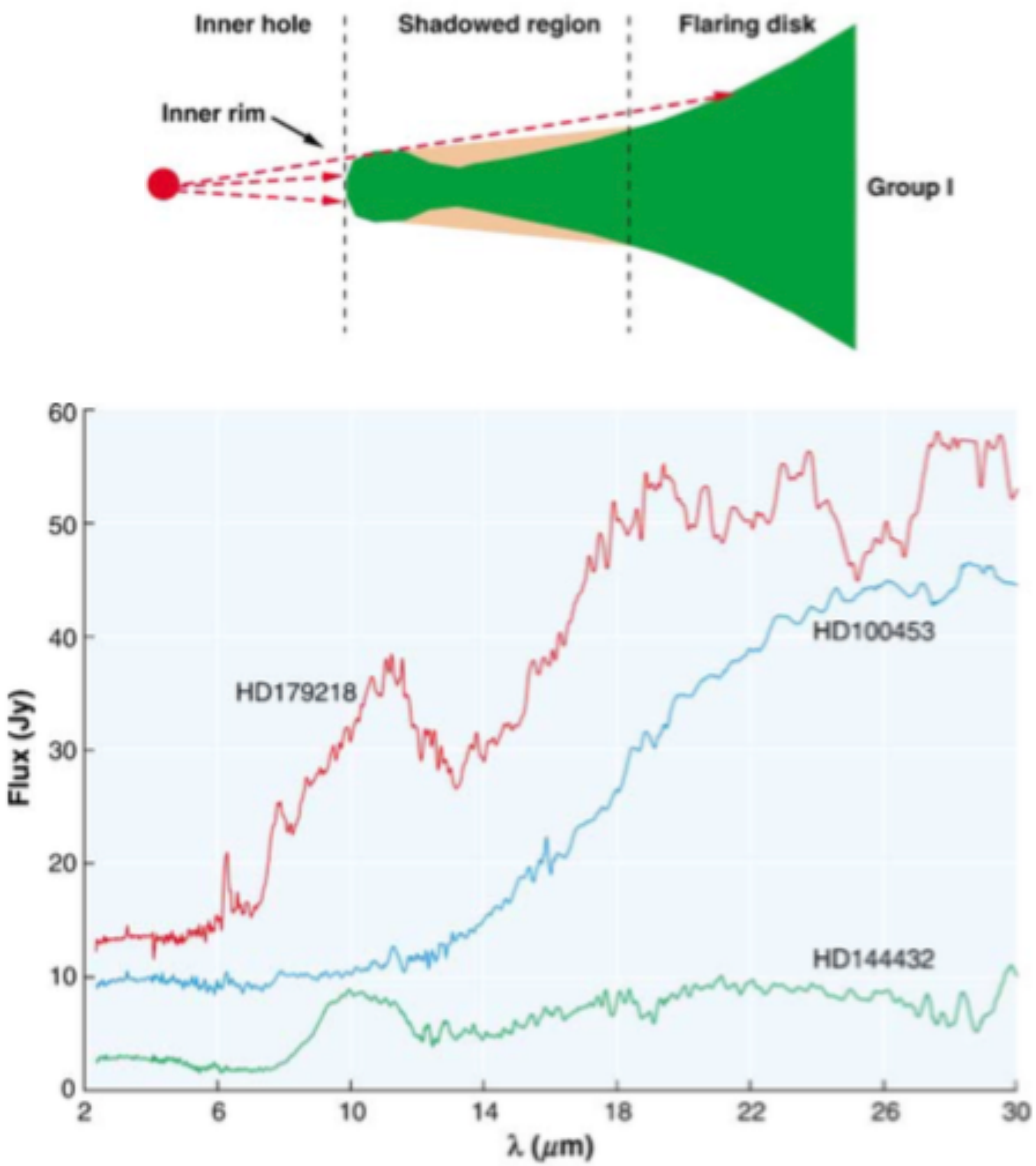
Single MRN size distribution:
$dn/da = C \times a^{-3.5}$

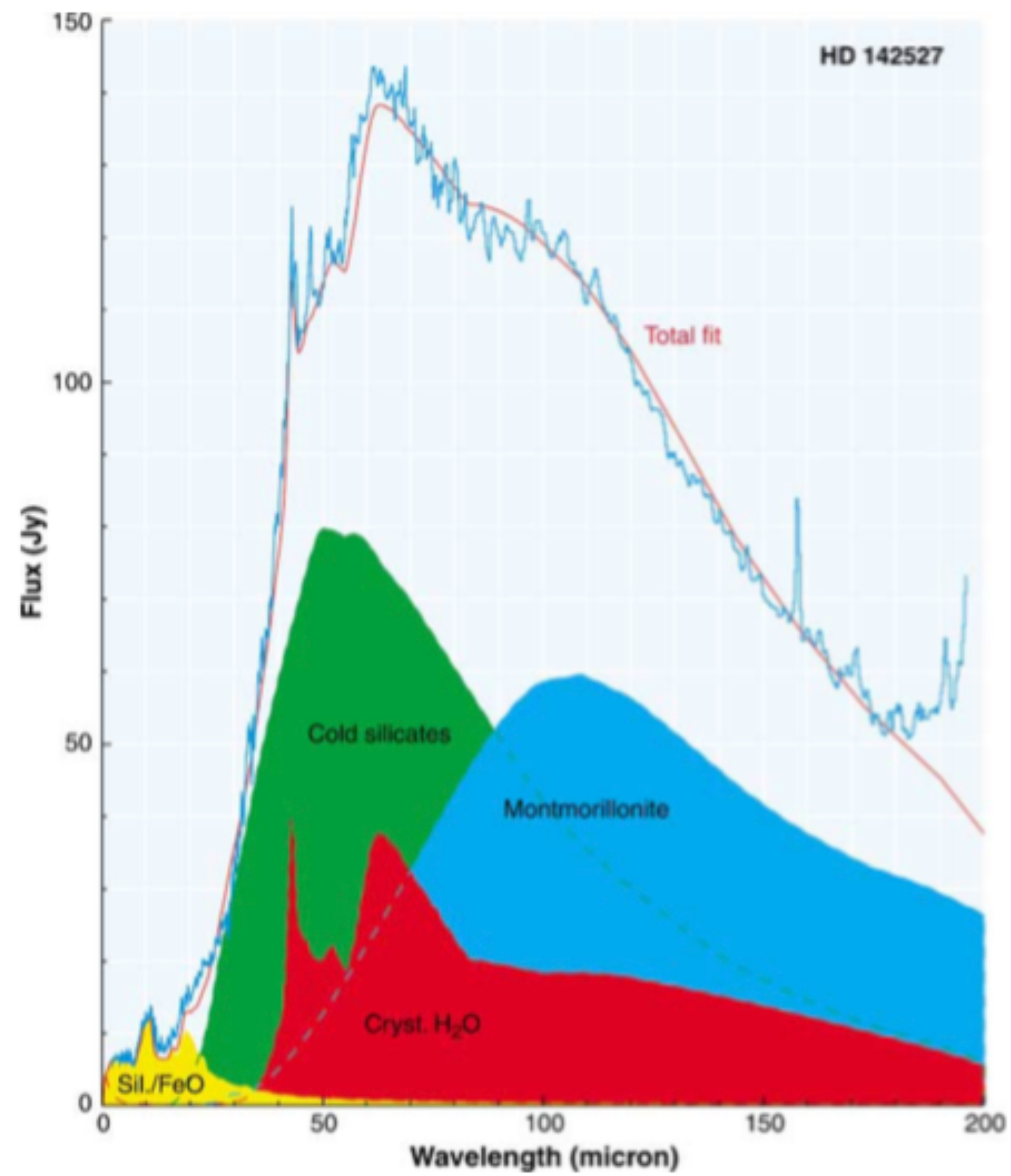


Two-populations of MRN-like grains: "small" and "large"

How do we know the composition of the dust?

The dust emission at mid- to far-IR wavelengths shows spectral features which can be attributed to different grain components

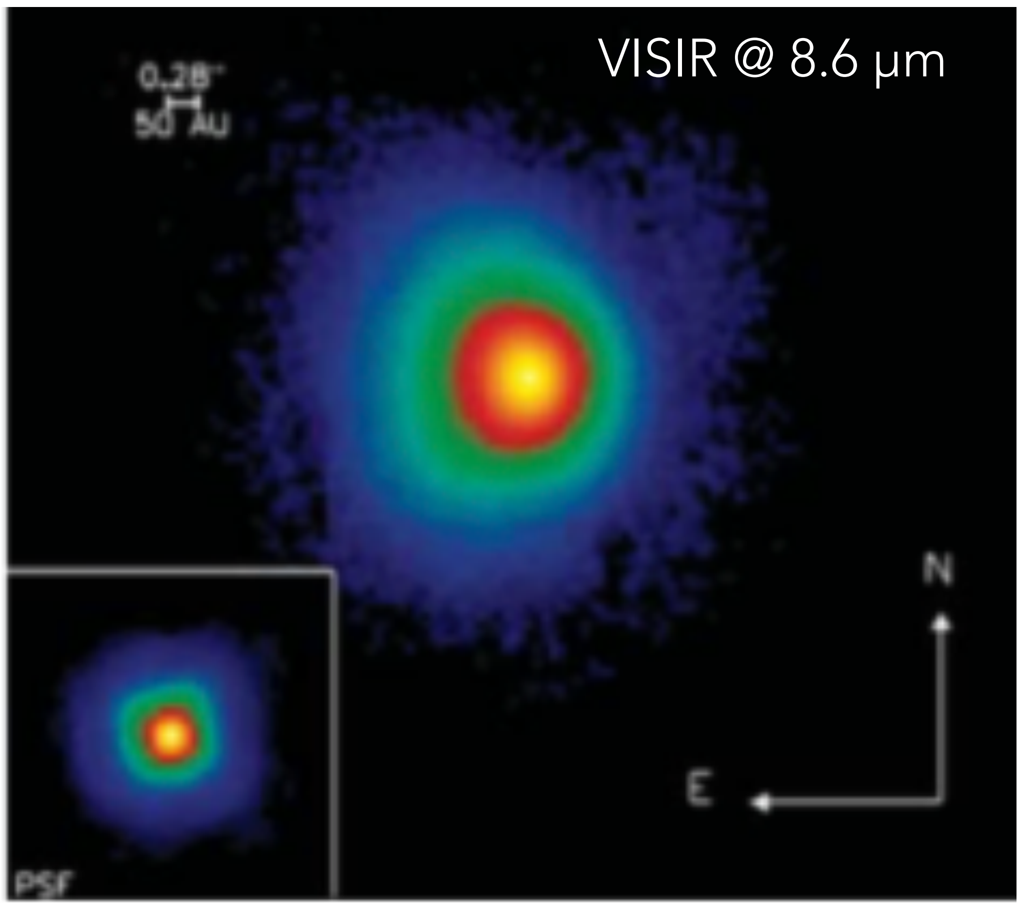


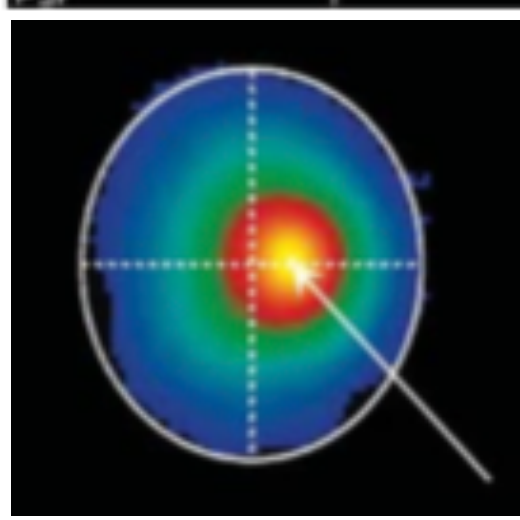


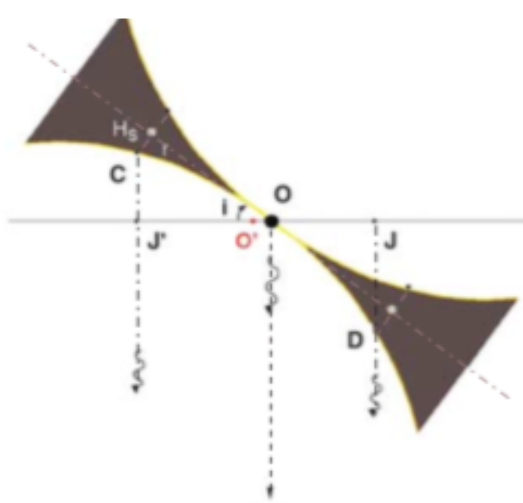
How do we know disks are flared?

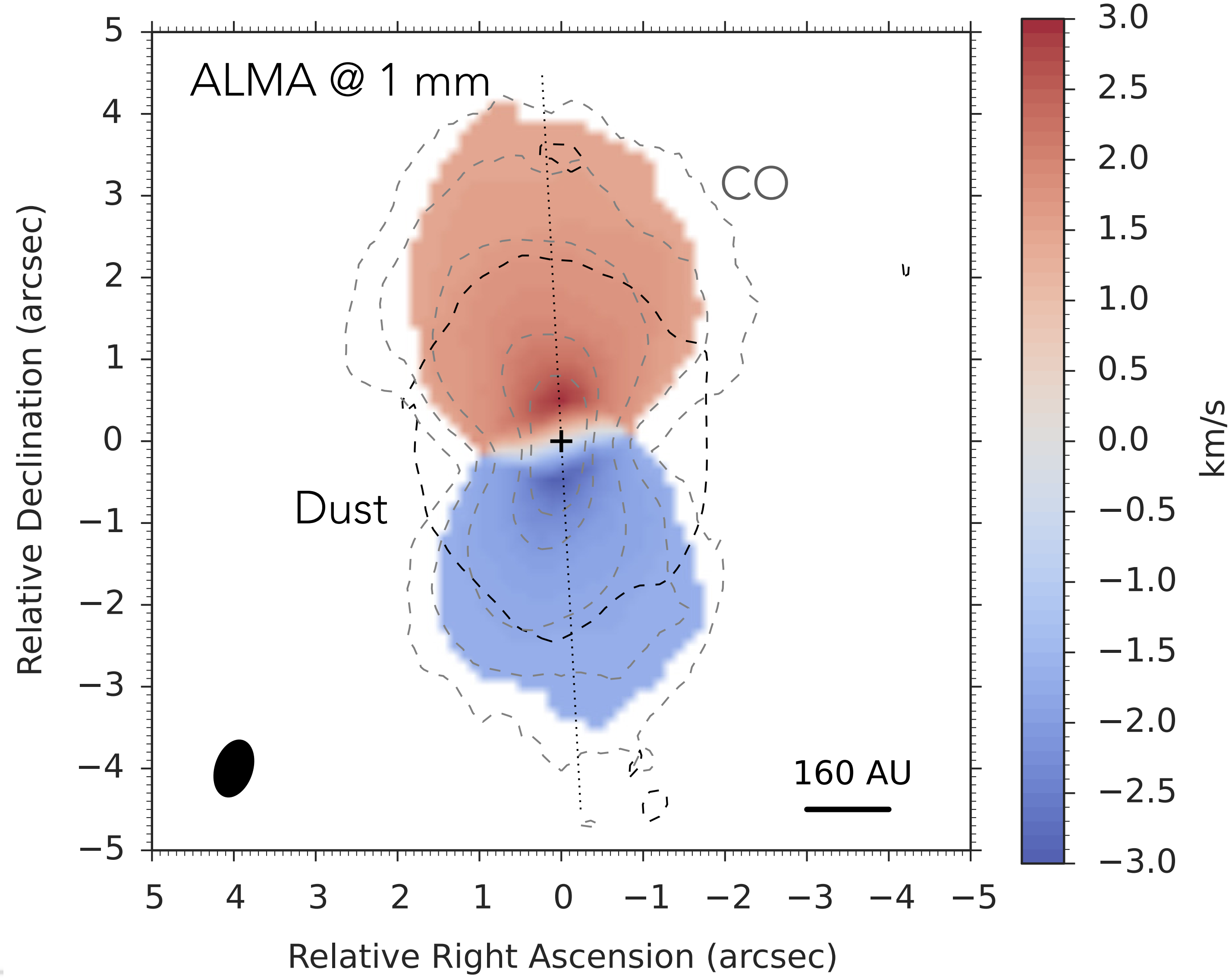
Spatially-resolved mid-IR imaging has revealed the flared morphology of emission from small grains (PAHs) in nearby protoplanetary disks

HD 97048: a group I Herbig Ae disk









Disk emission is "flat" at (sub)mm wavelengths: evidence for settling

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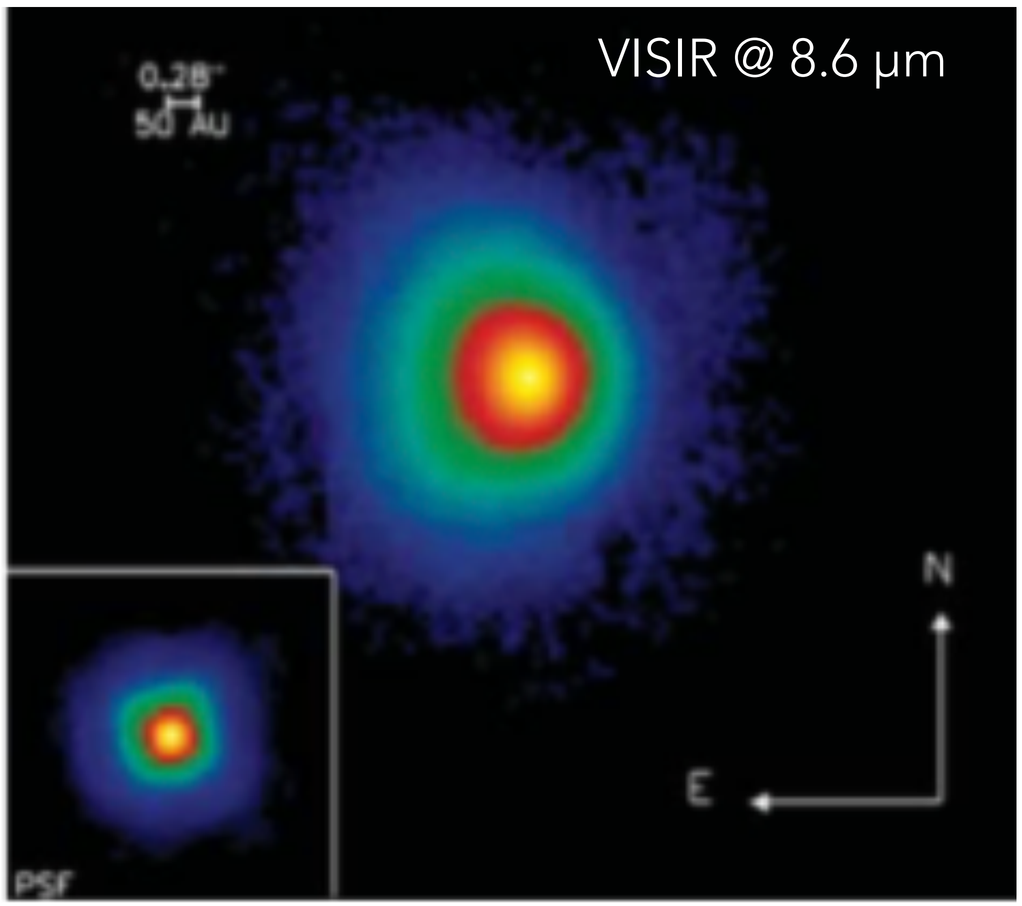
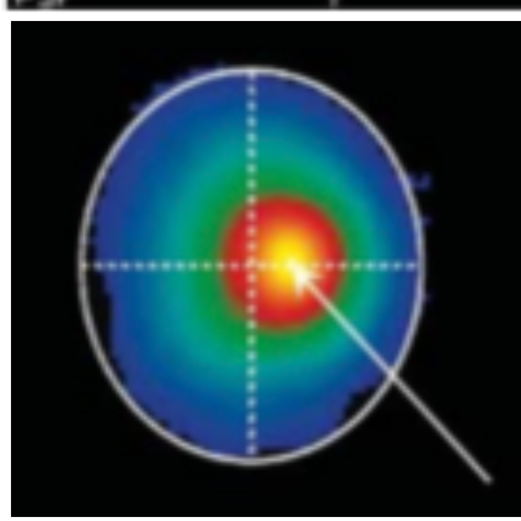
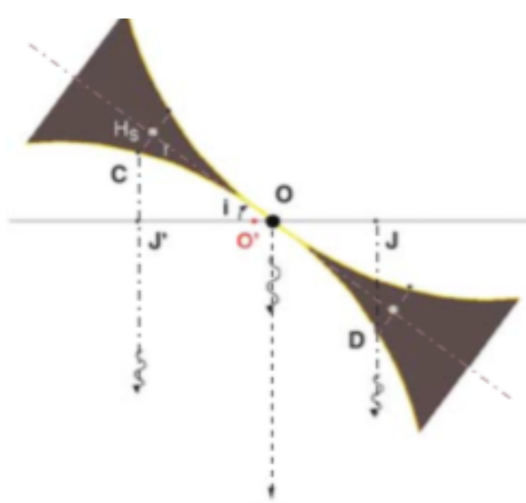
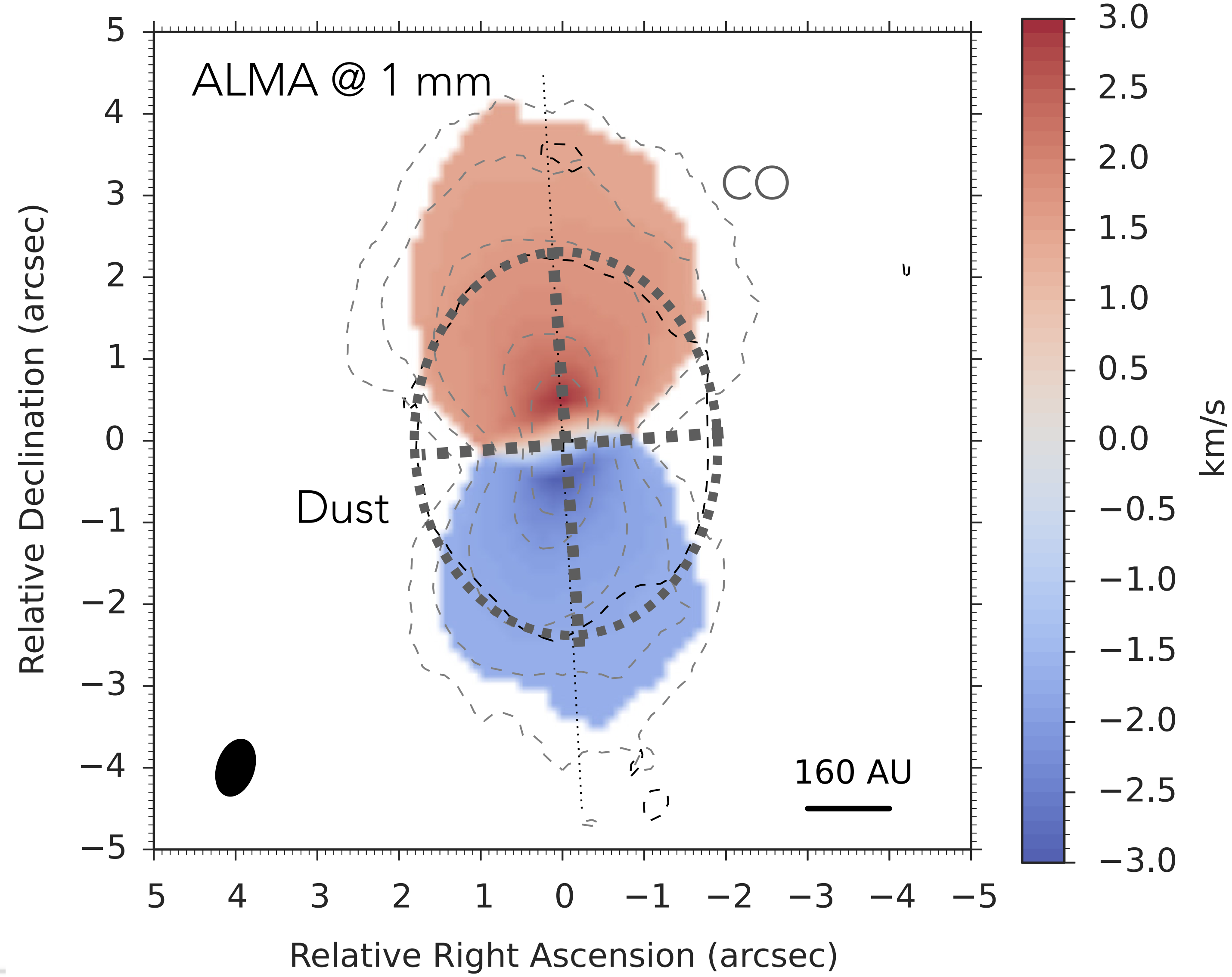








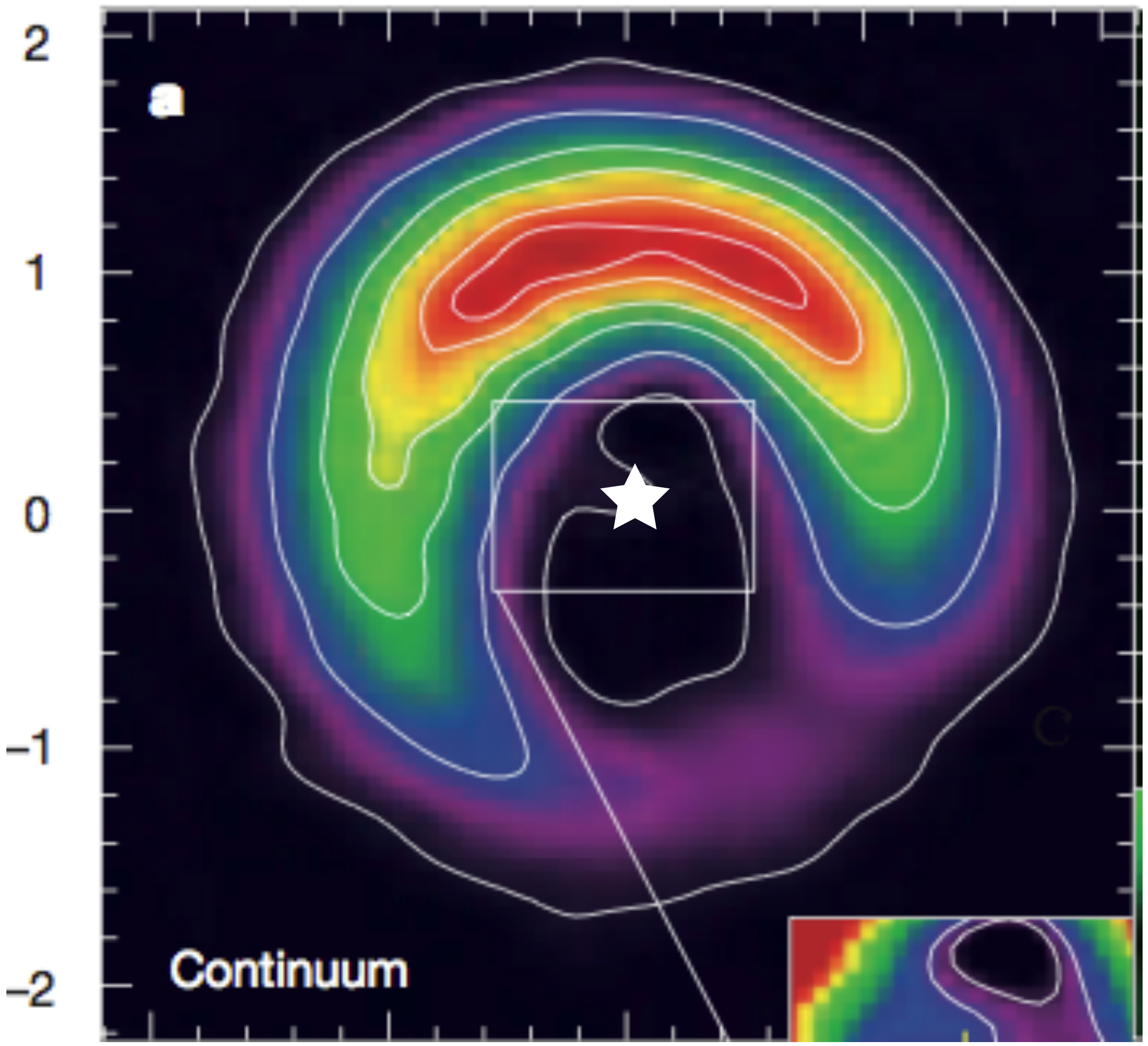
Disk emission is "flat" at (sub)mm wavelengths: evidence for settling

Lagage, P.-O., et al. 2006, Science, 314, 621; Walsh, C, et al. 2016, ApJ, under review

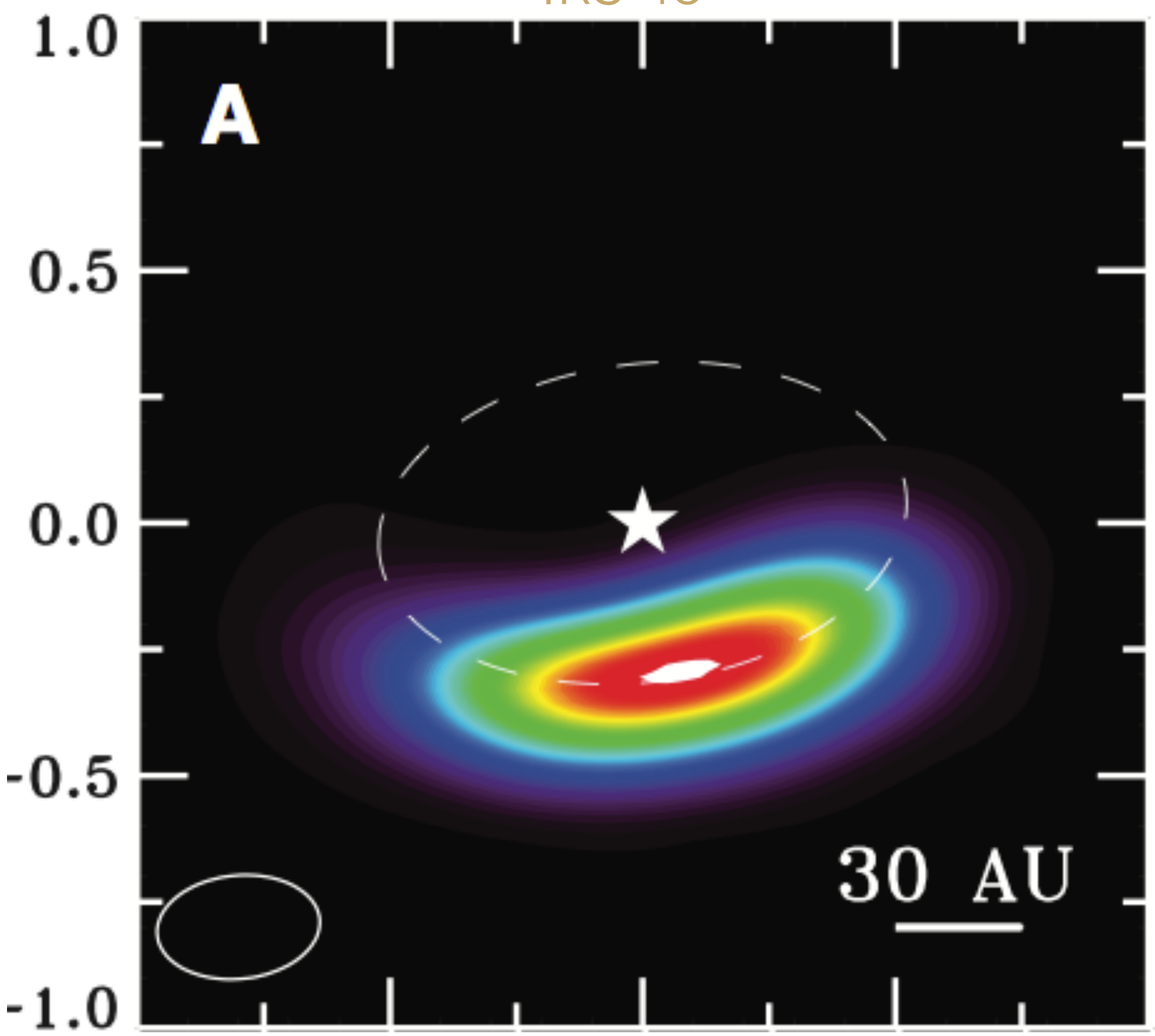
Dusty disks in the era of ALMA

Highly asymmetric (sub)mm dust emission attributed to dust trapping in vortices potentially created by forming planets

HD 142527



IRS 48

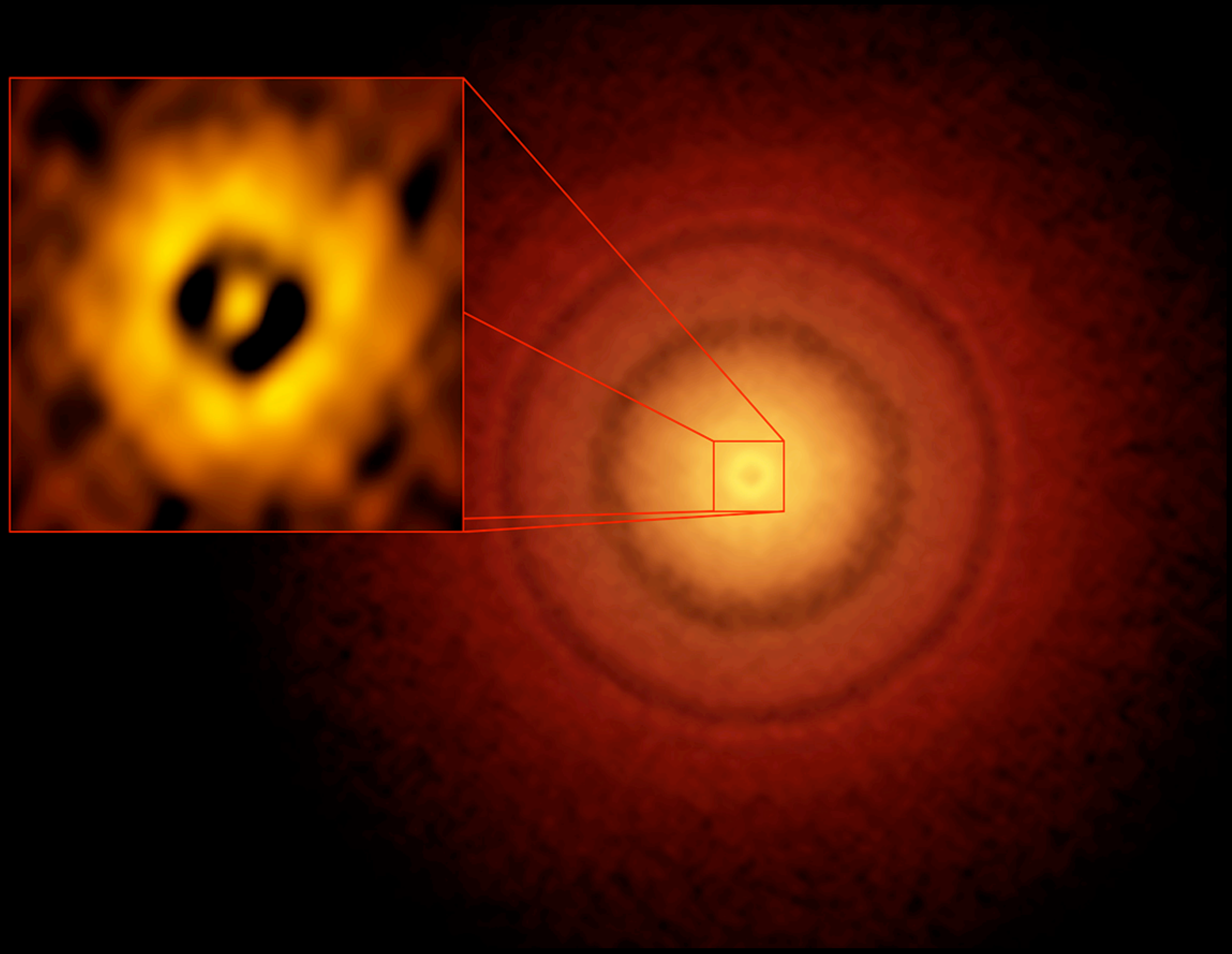


Are these the exception rather than the norm? Both are A-type stars

Casassus, S., et al. 2013, Nature, 493, 191; van der Marel, N., et al. 2013, Science, 340, 1199

Dusty disks in the era of ALMA

Highly symmetric and concentric rings attributed to various mechanisms, including dust traps, sintering, condensation fronts, …



HL Tau

TW Hya

ALMA Partnership 2015, ApJL, 808, L3; Andrews, S. M., et al, 2016, ApJ, 820, L40

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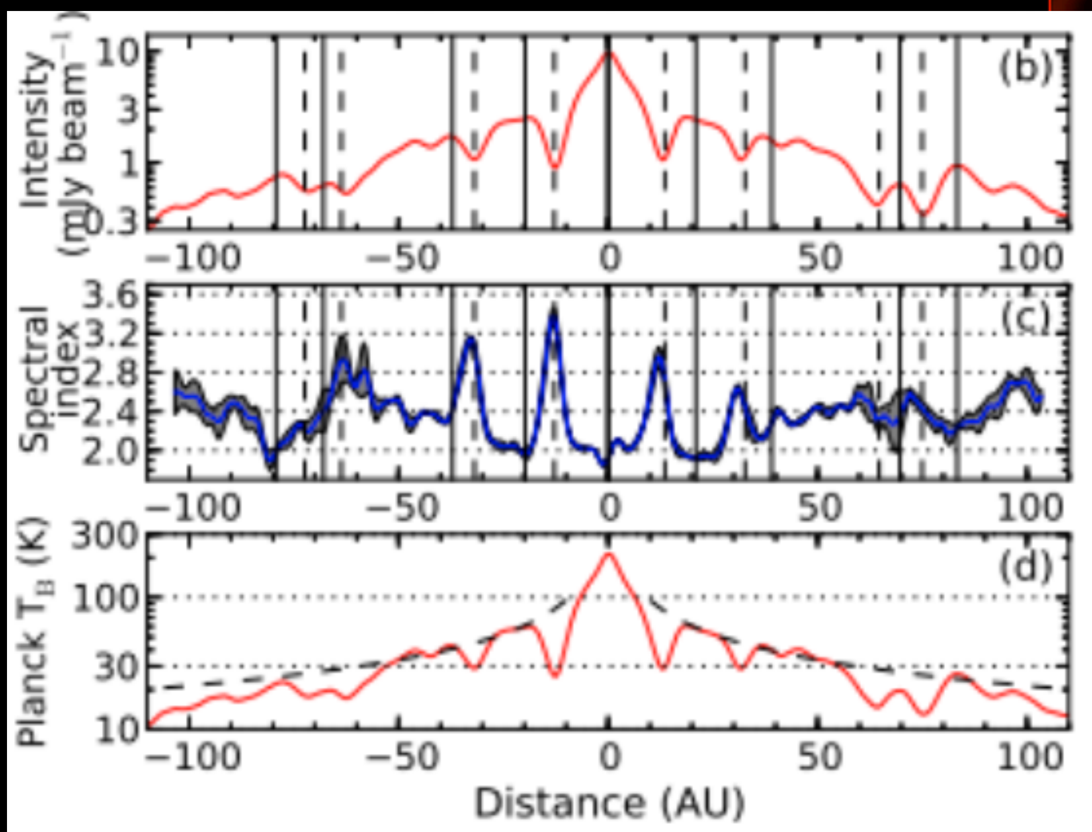

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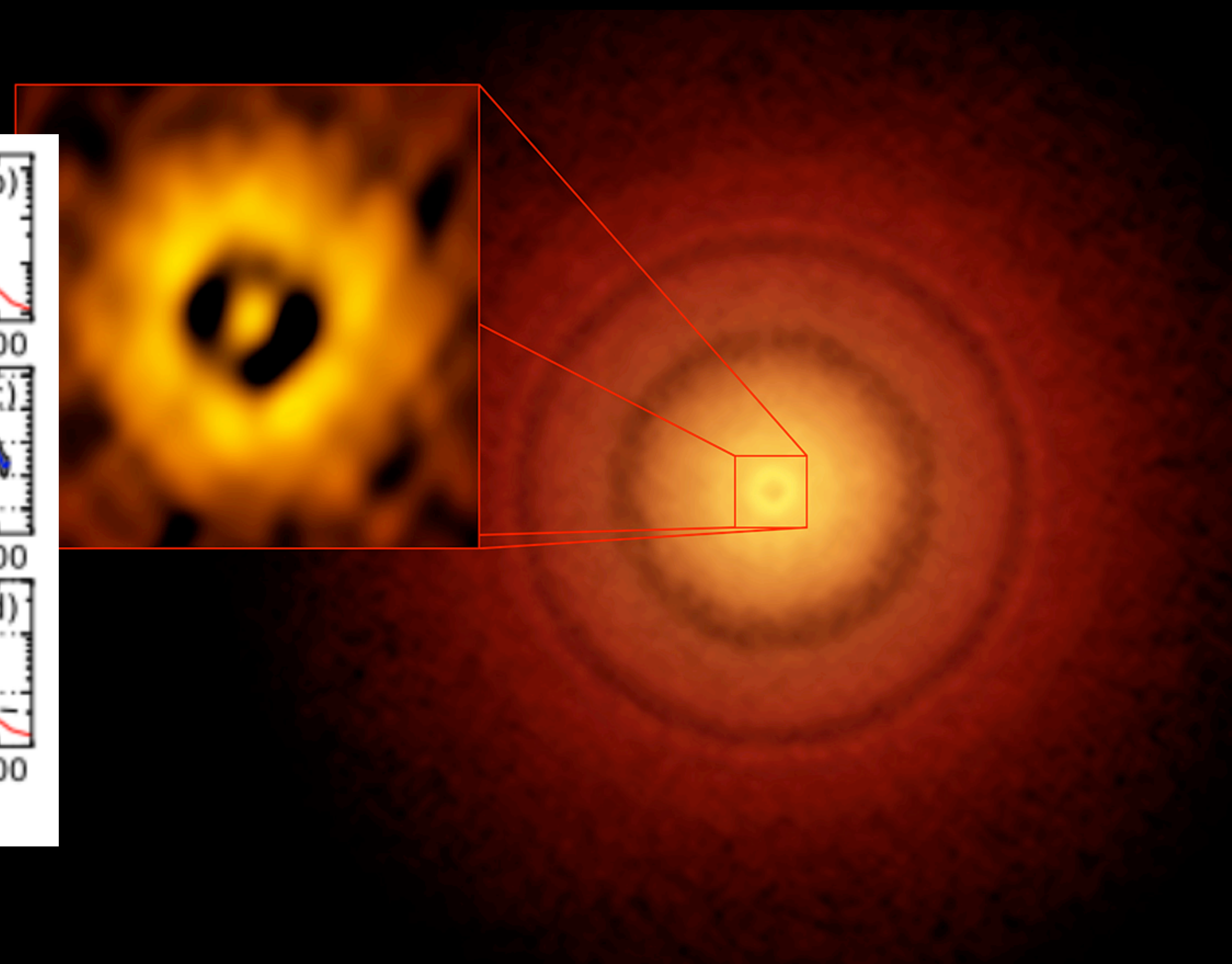

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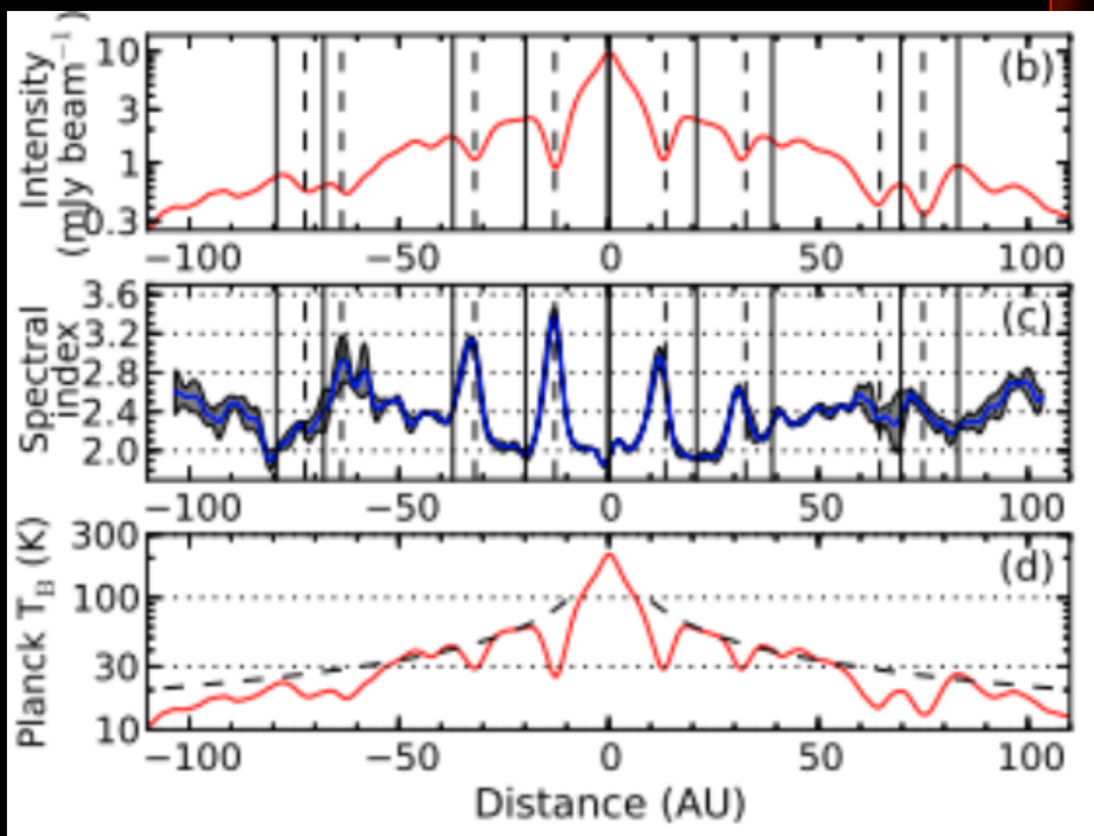

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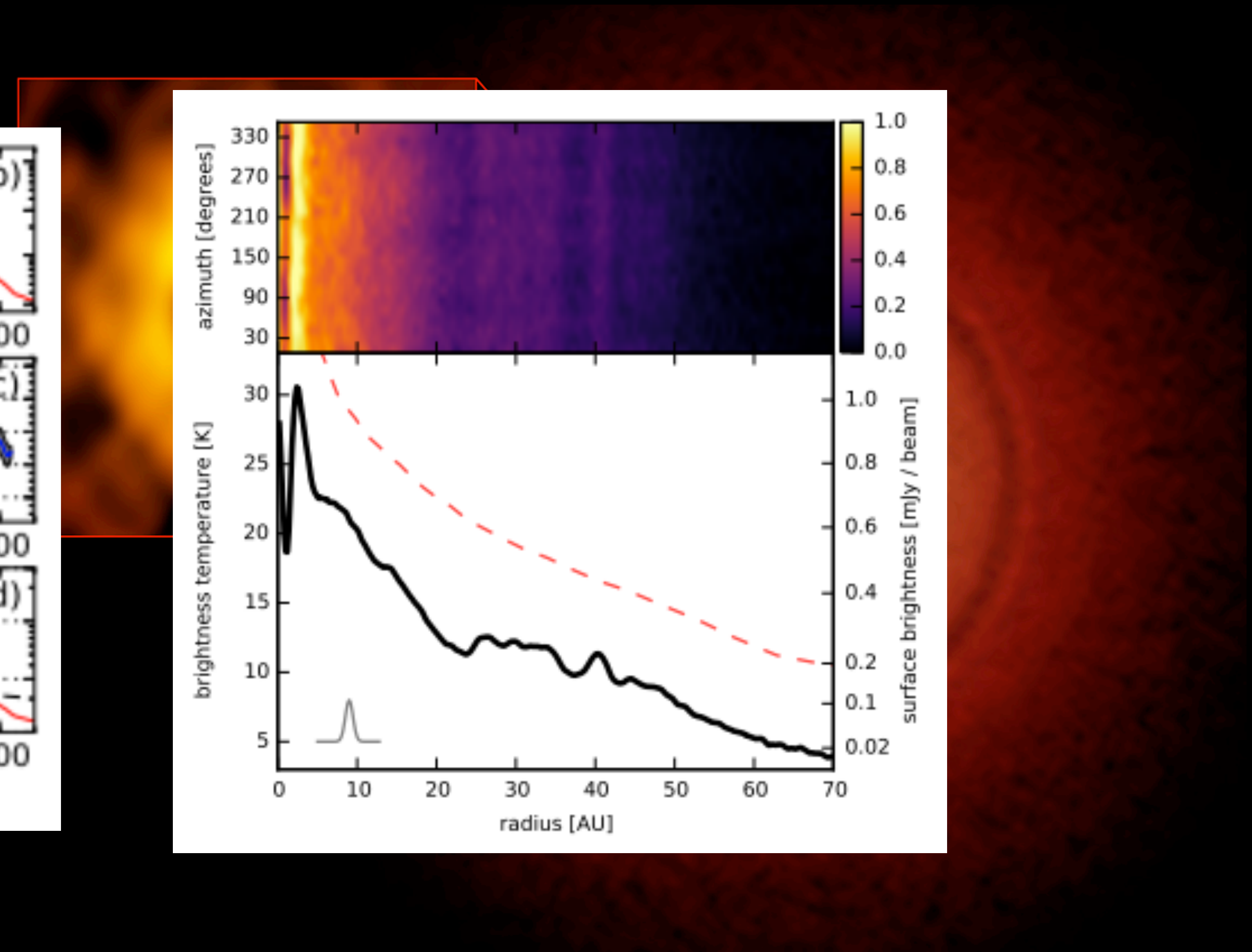
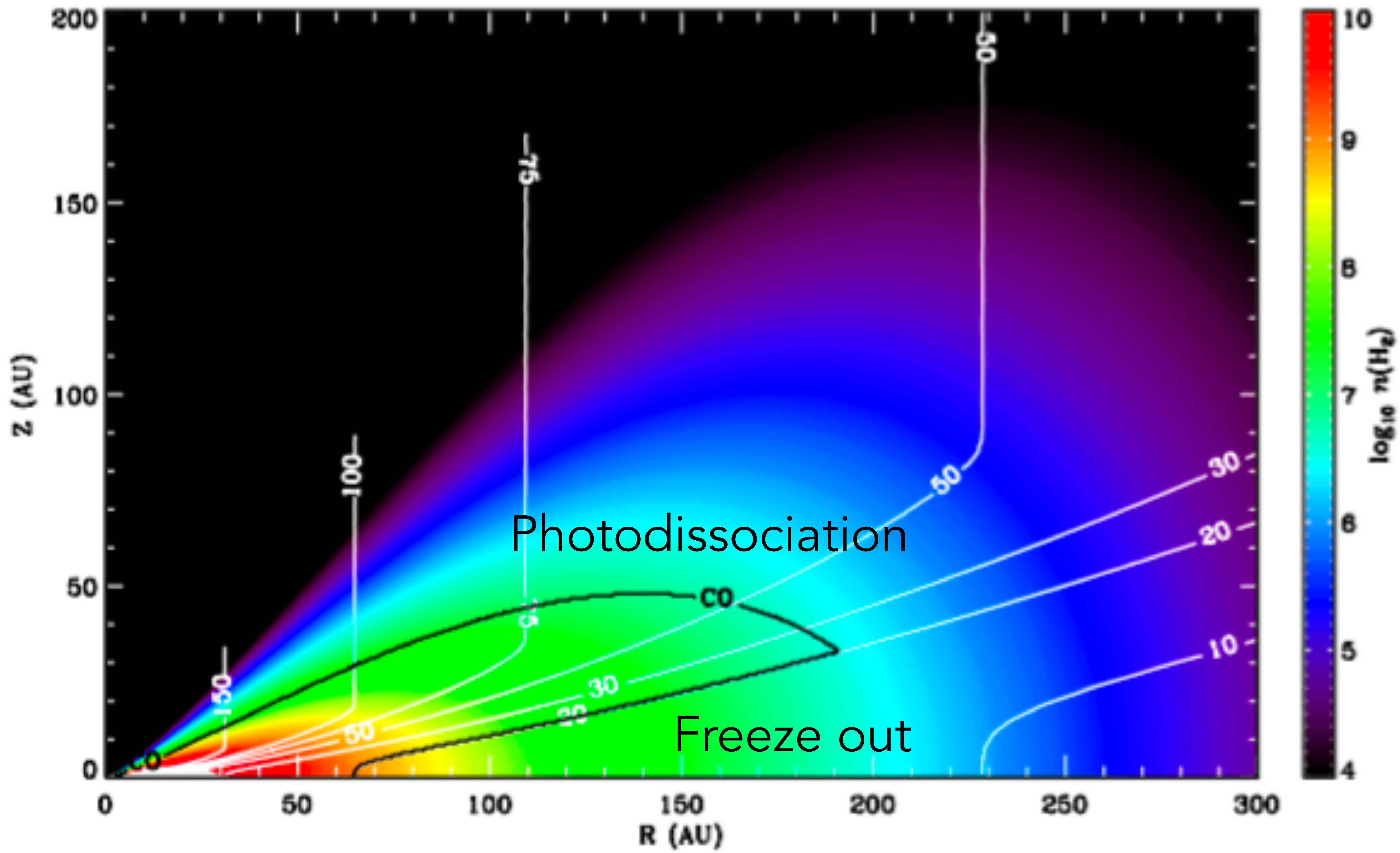


TW Hya

What about the gas?

Gas is mainly H_2 (90%) and He (10%) which are difficult to observe: CO (~0.01%) is used as a proxy as the second-most abundant molecule



Warning! CO gas can have a complex distribution due to the disk structure

Williams, J. P & Best, W. M. J. 2014, ApJ, 788, 59

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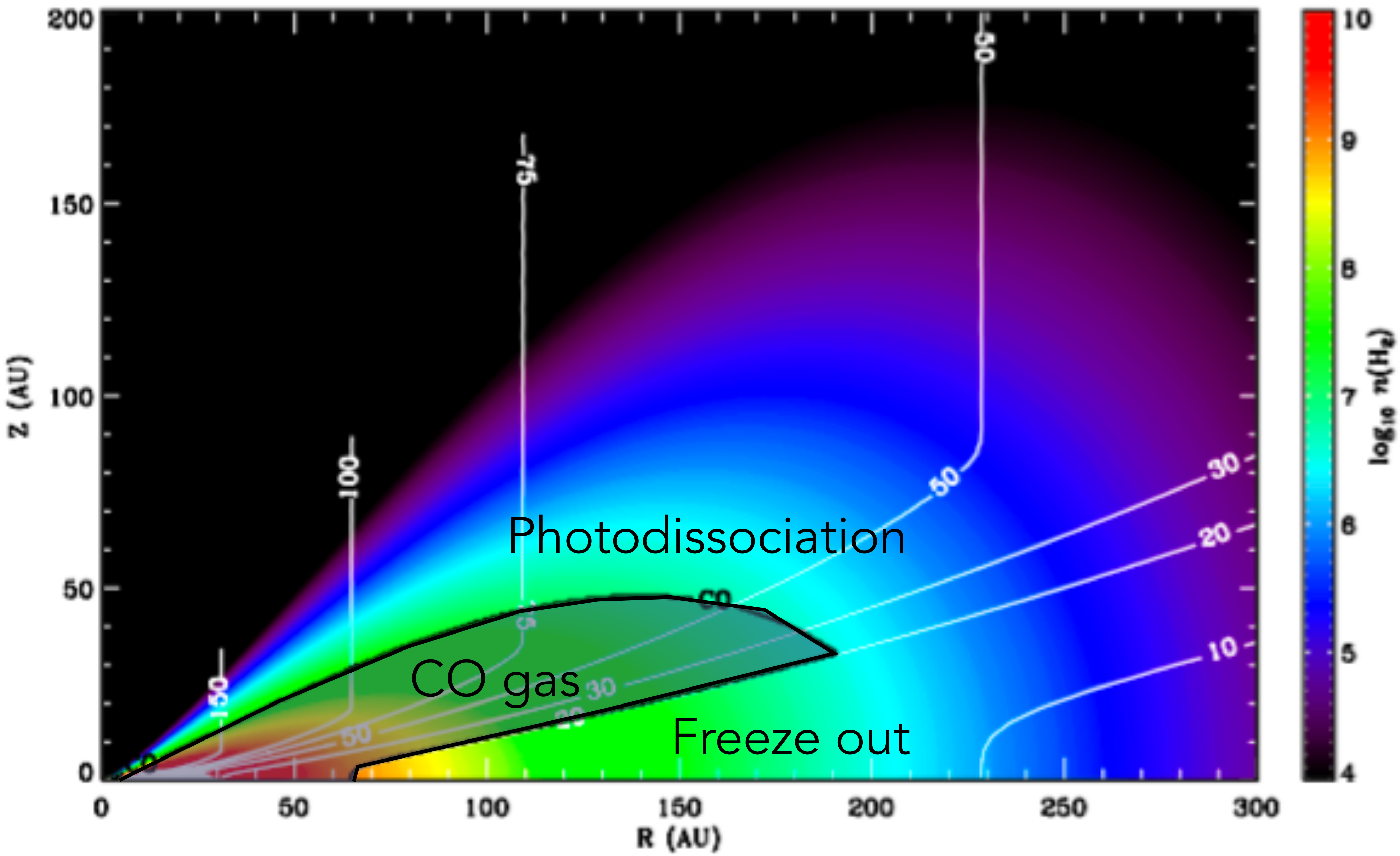

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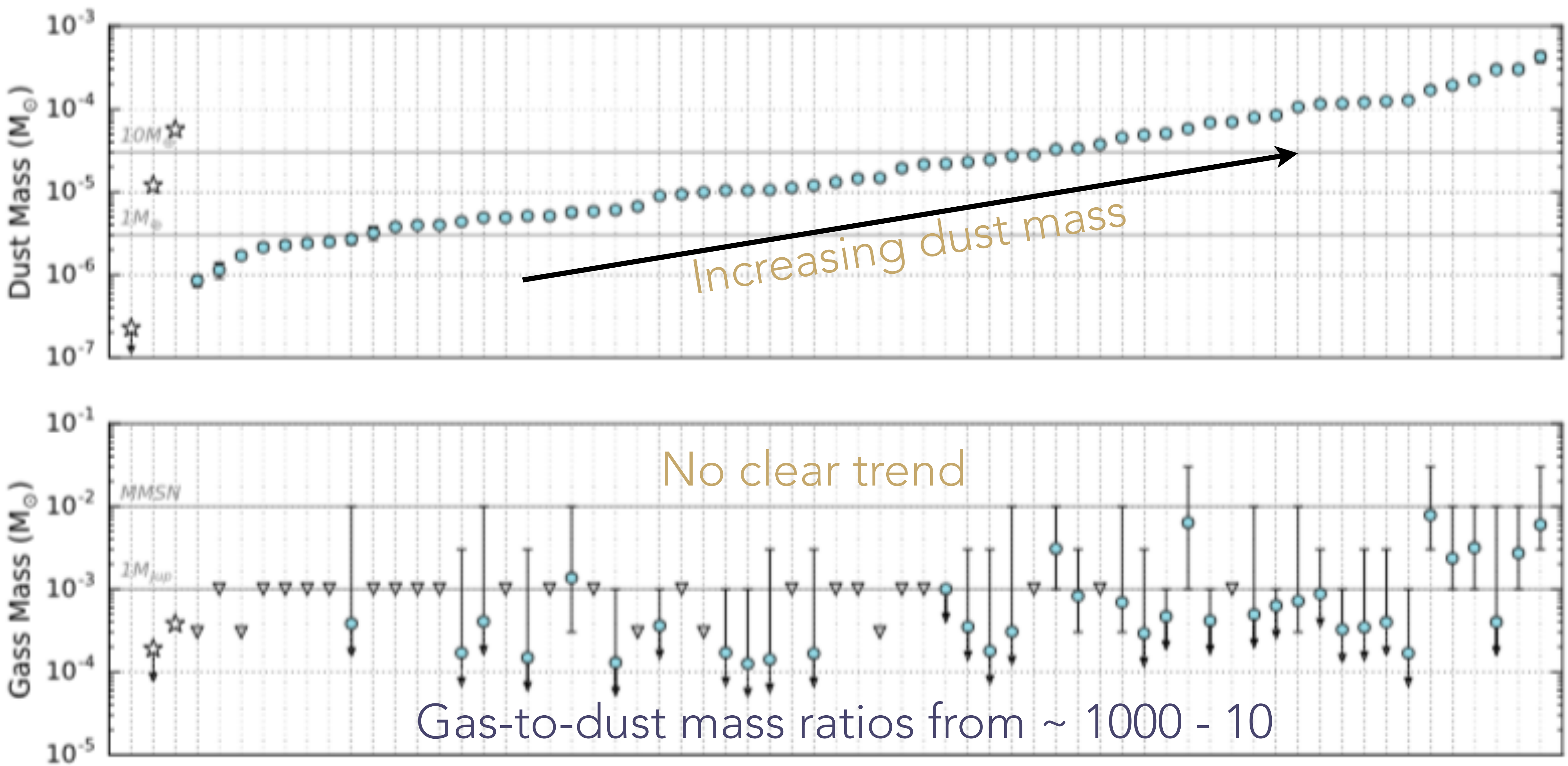
What about the gas?

Emission from the main CO isotopologues (^{12}CO and ^{13}CO) are optically thick, hence less abundant isotopologues are used ($C^{18}O$ and $C^{17}O$)



Dust and gas masses from the ALMA Survey of Lupus

Ansdell, M., et al. 2016, ApJ, in press

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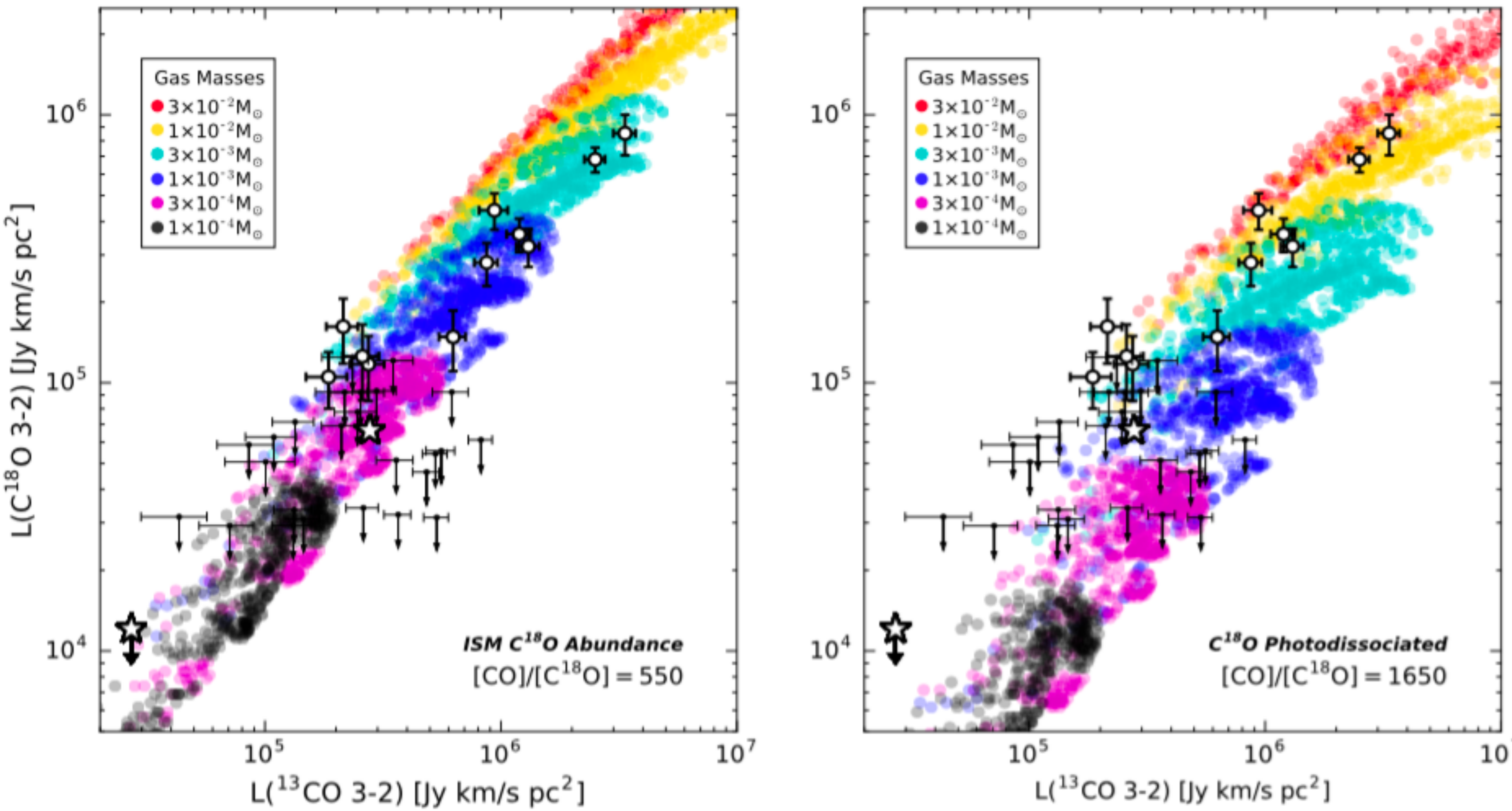
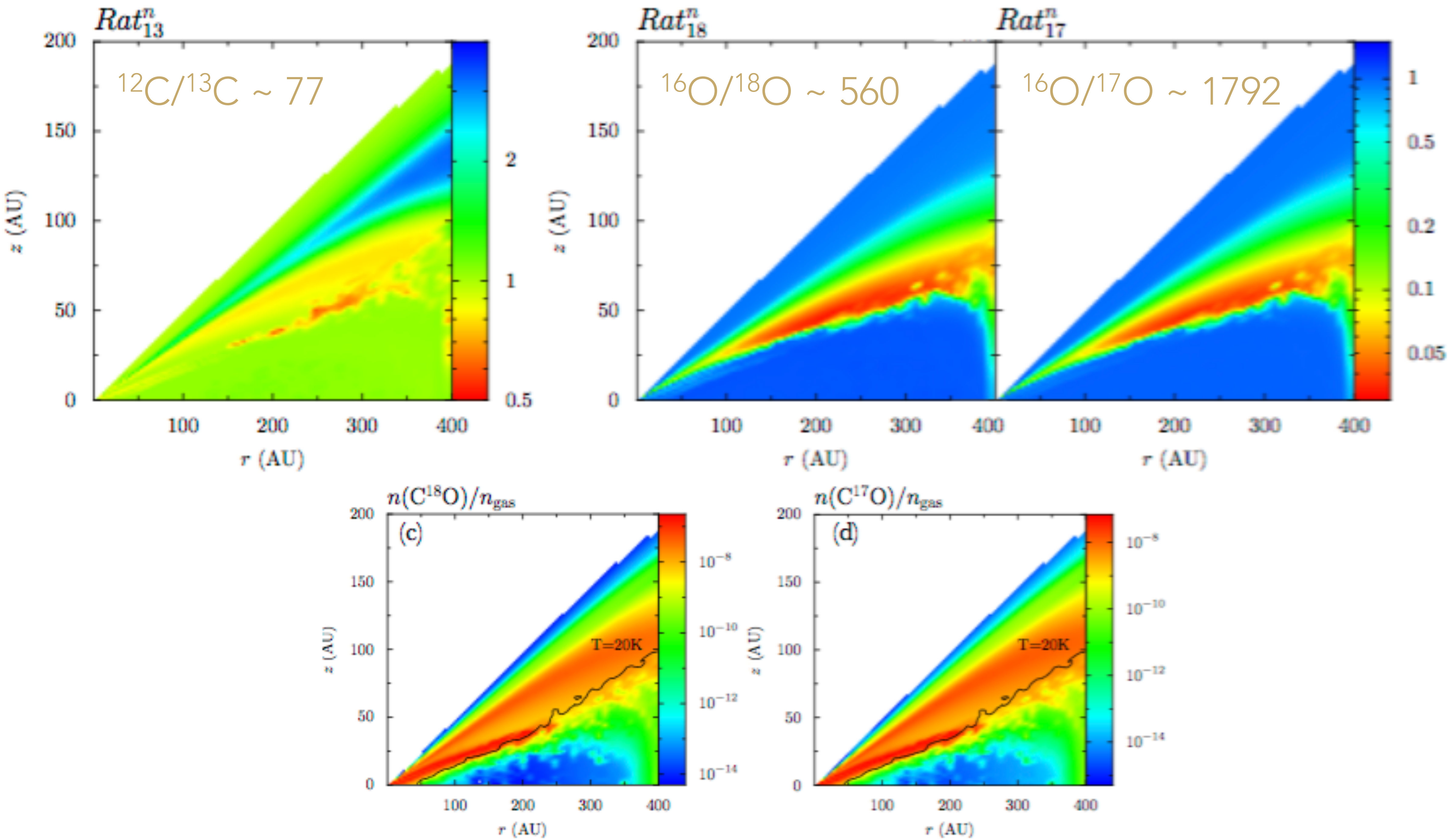


Dust and gas masses from the ALMA Survey of Lupus

What about the gas?

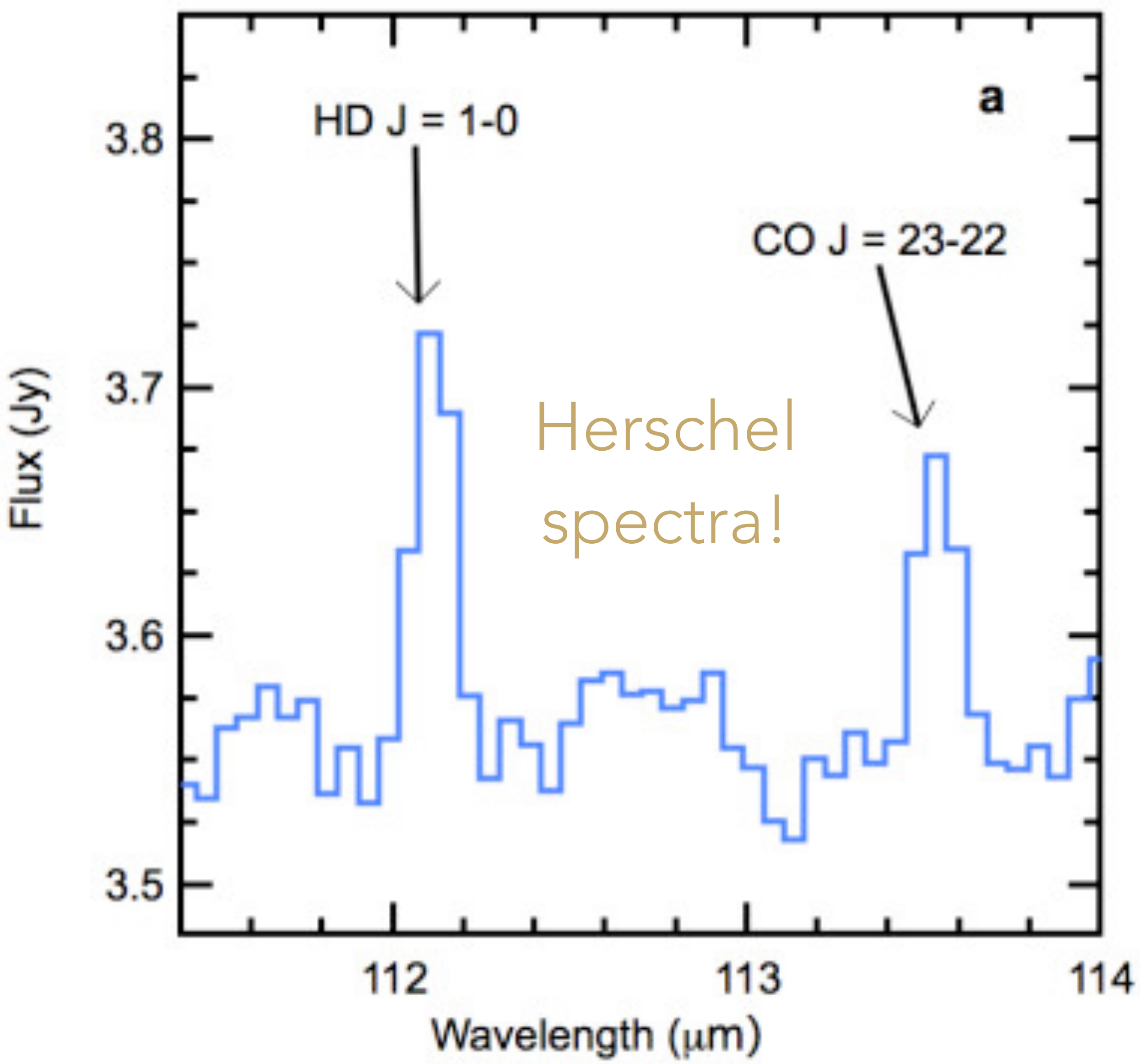
Picture is further complicated by chemical effects, namely, isotope-selective photodissociation

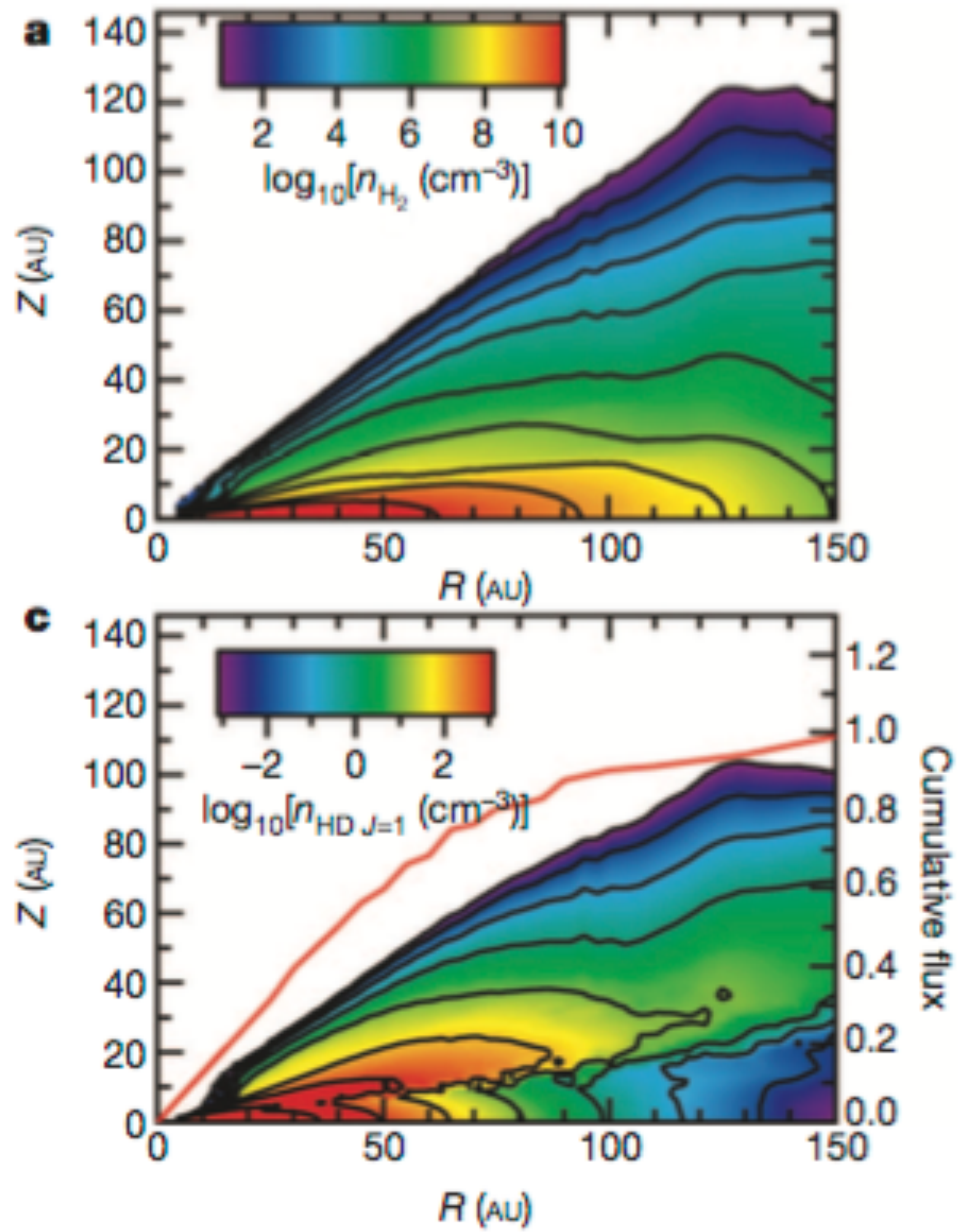


Miotello, A., et al. 2015, A&A, 572, A96

What about the gas?

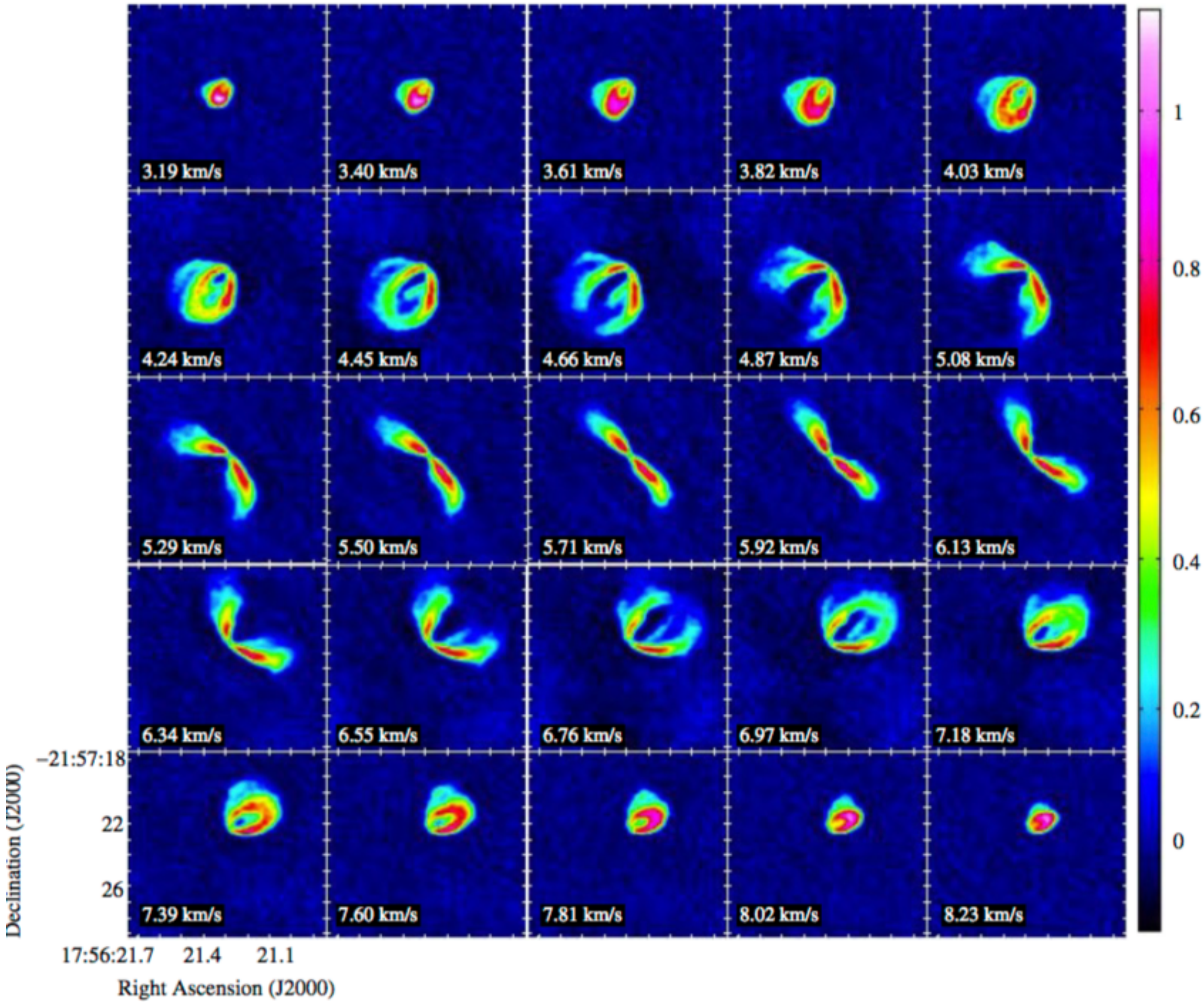
Given the relative complexity of interpreting CO observations, HD ($\sim$0.001% of H_2) is proposed as an alternative tracer of the gas mass



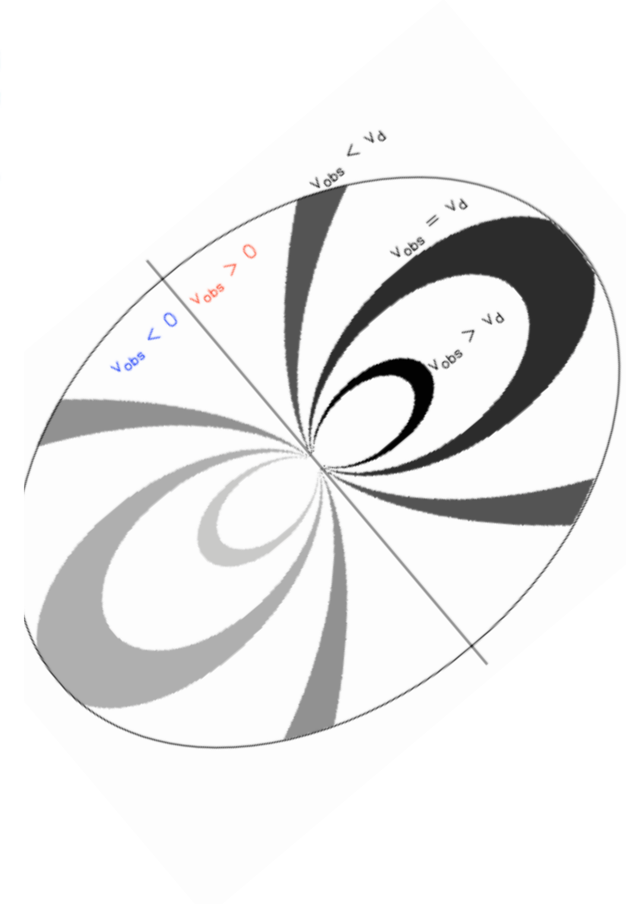


Disk mass (TW Hya) > 0.05 M_{sol}

CO line emission in the ALMA era



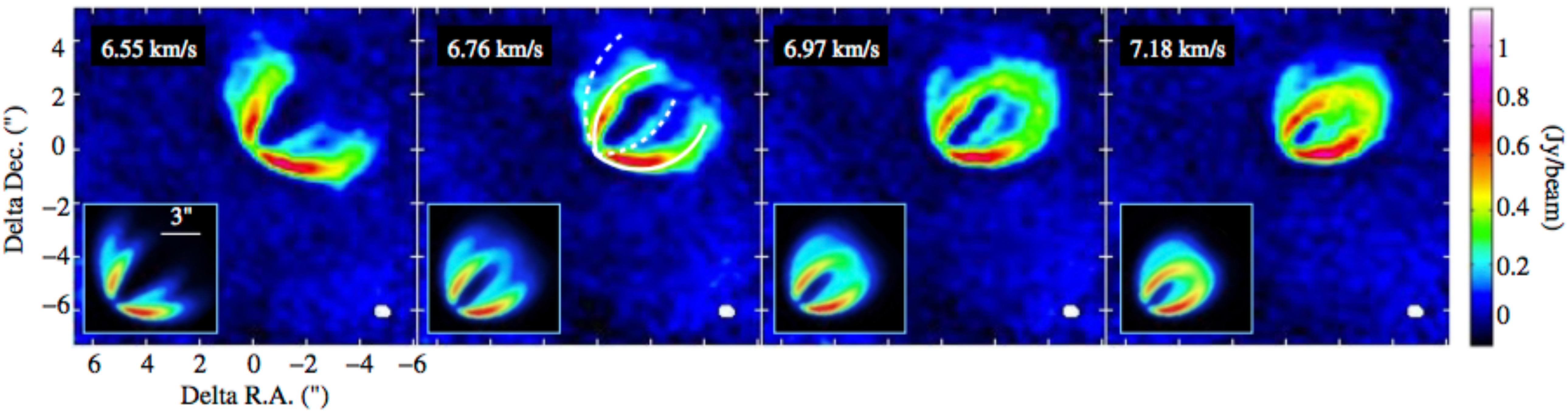
ALMA Cycle 0 observations of CO J=3-2 emission from HD 163296



de Gregorio-Monsalvo, et al. 2013, A&A, 557, 133

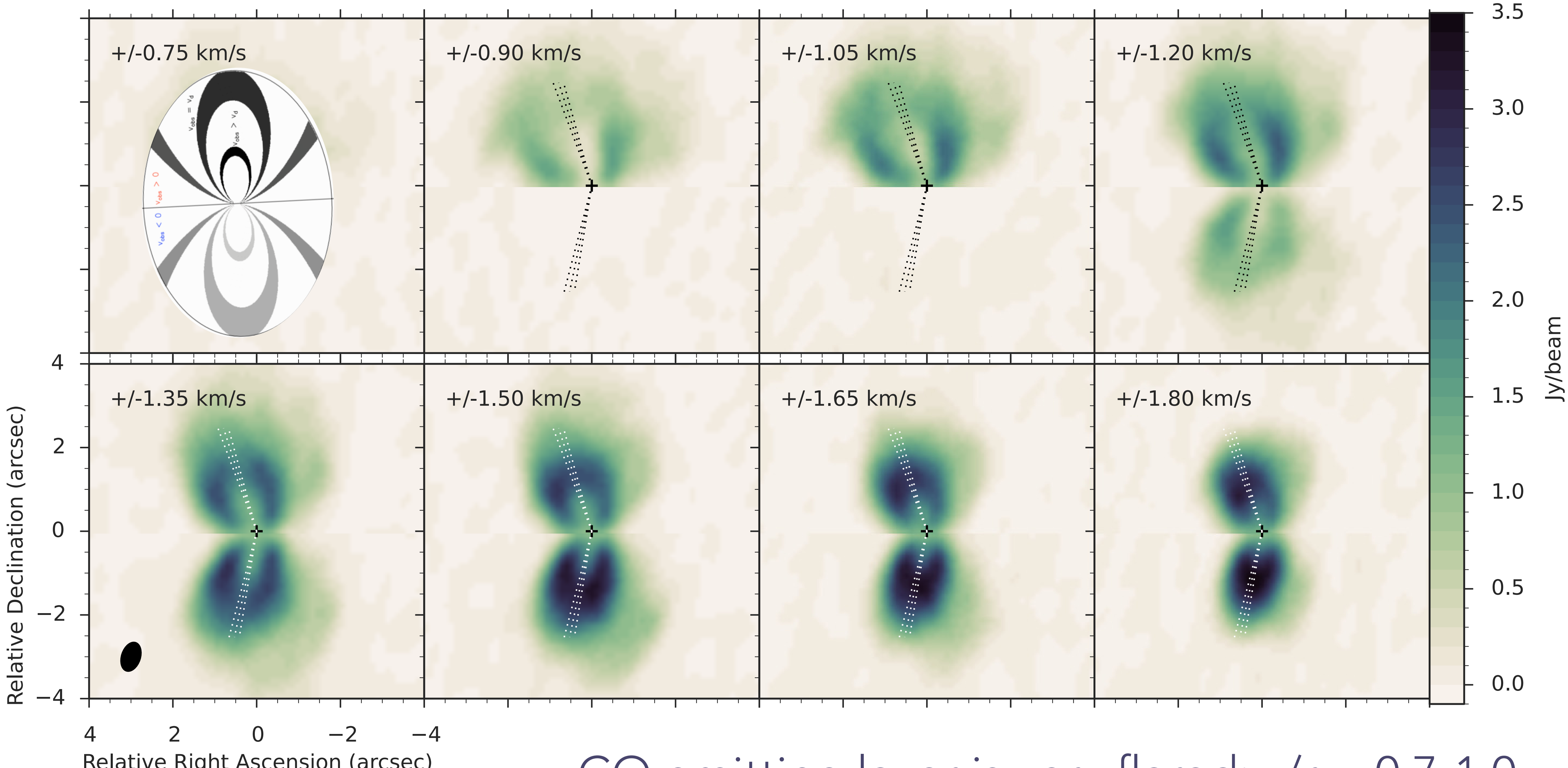
CO line emission in the ALMA era

CO J=3-2 shows emission from a moderately flared disk (z/r ~ 0.1) and reveals evidence of CO freezeout in the disk midplane



CO line emission in the ALMA era

ALMA Cycle 0 observations of CO J=3-2 emission from HD 97048

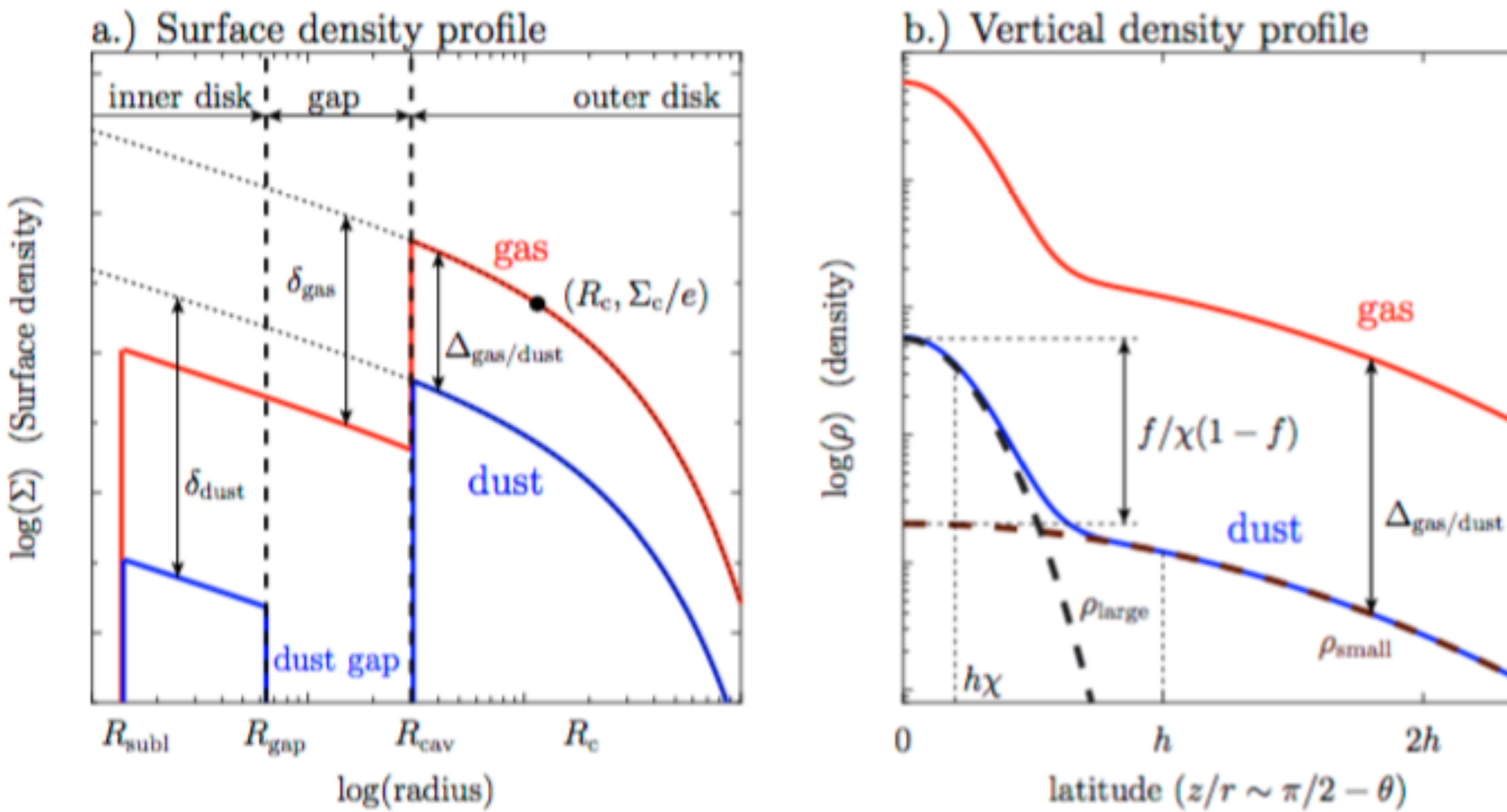


CO emitting layer is very flared: z/r ~ 0.7-1.0

Walsh, C., et al., 2016, ApJ, under review; ; Guilloteau, S., et al. 2006, A&A, 448, L5

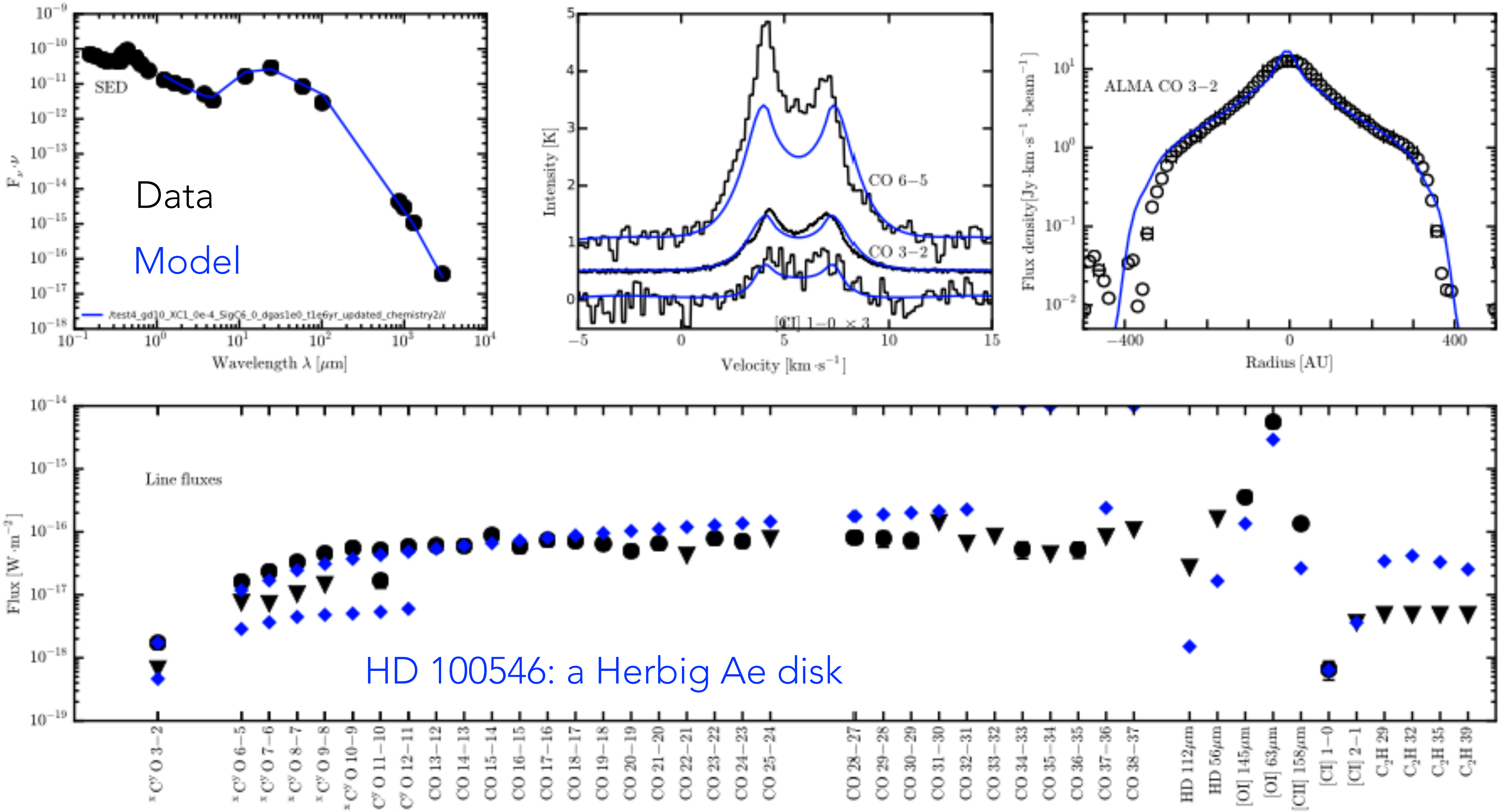
Modelling the gas and dust in tandem

Gas surface density still assumed to follow the dust: gas-to-dust mass ratio is now a "free" (yet still global) parameter



Towards a global prescription of gas and dust

Modern models now fit the dust SED and spectrally and spatially resolved molecular line observations simultaneously



Kama, M., et al. 2016, A&A, submitted

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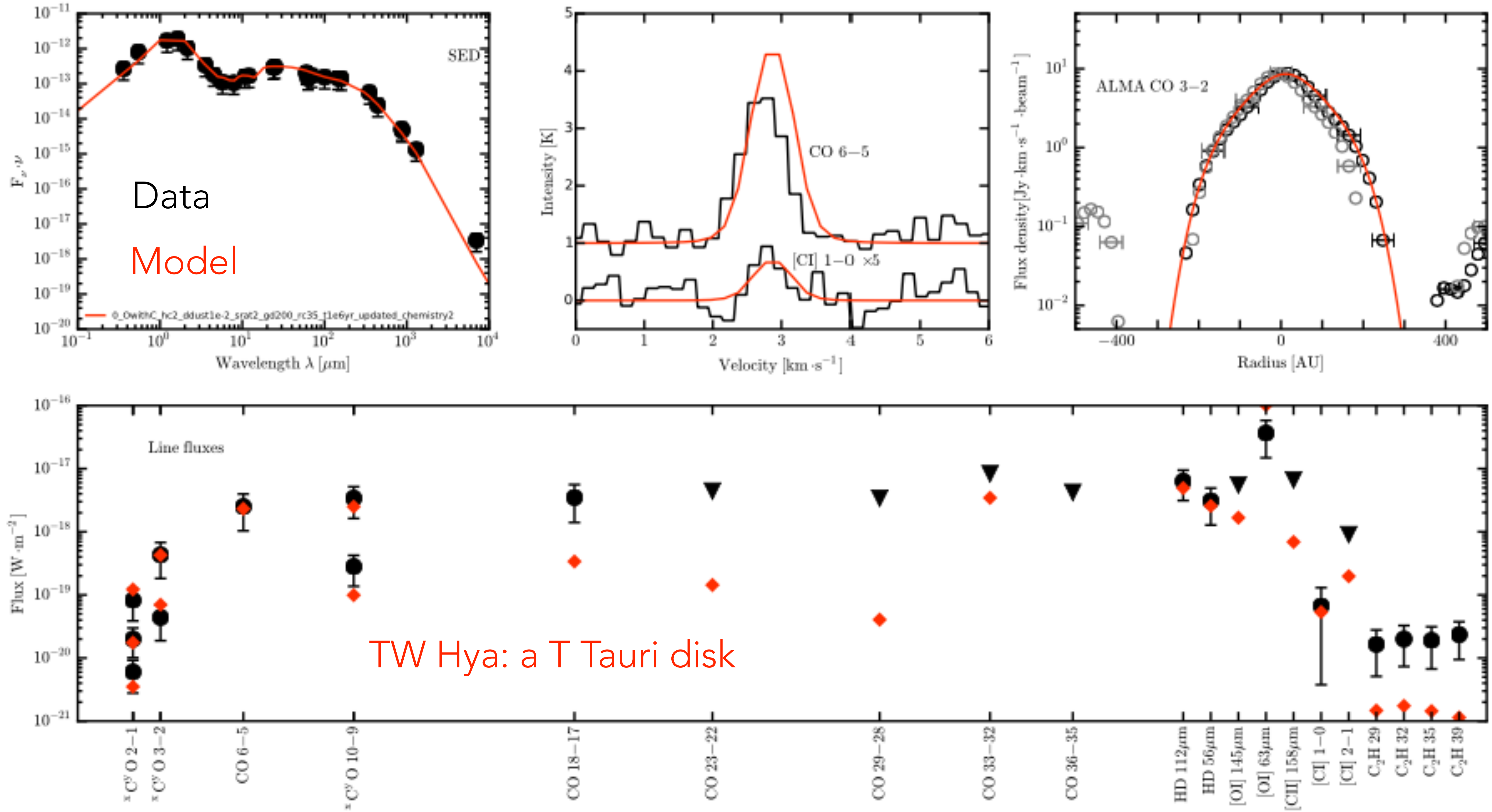
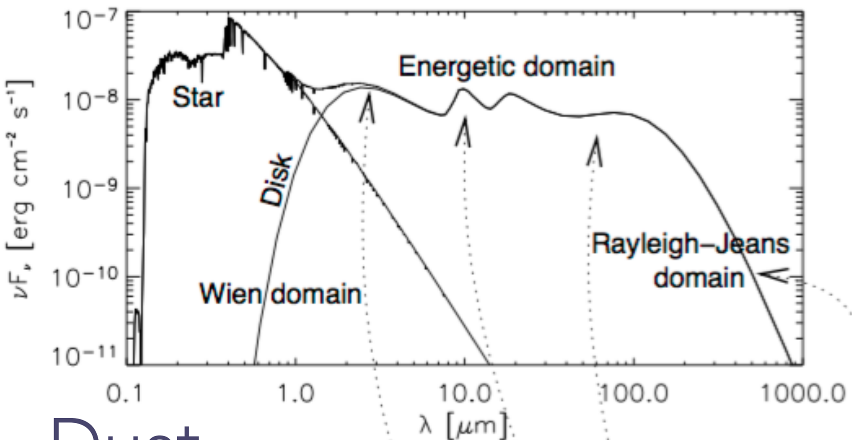
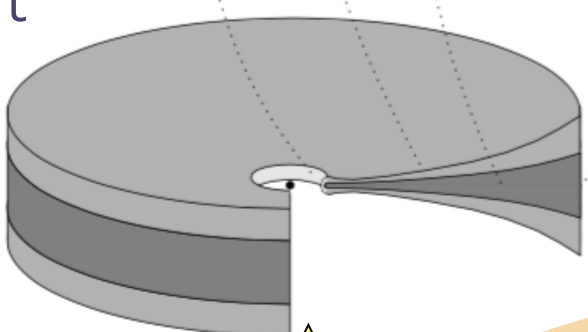


Observations of protoplanetary disks

Until recently: only spatially-unresolved observations were possible (with single-dish telescopes)

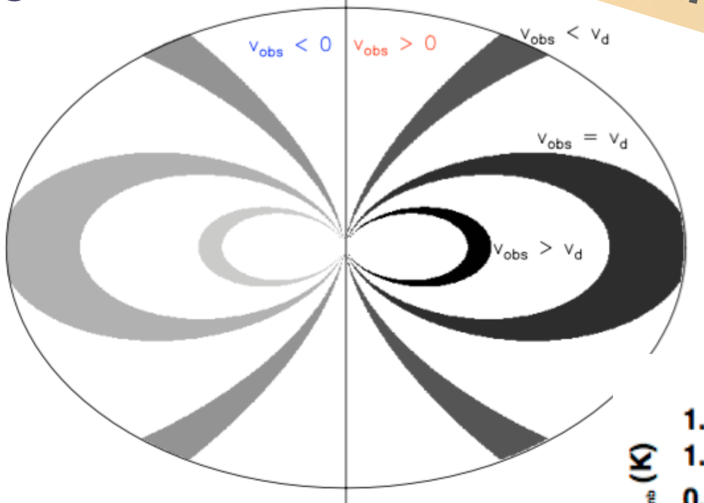
Dust





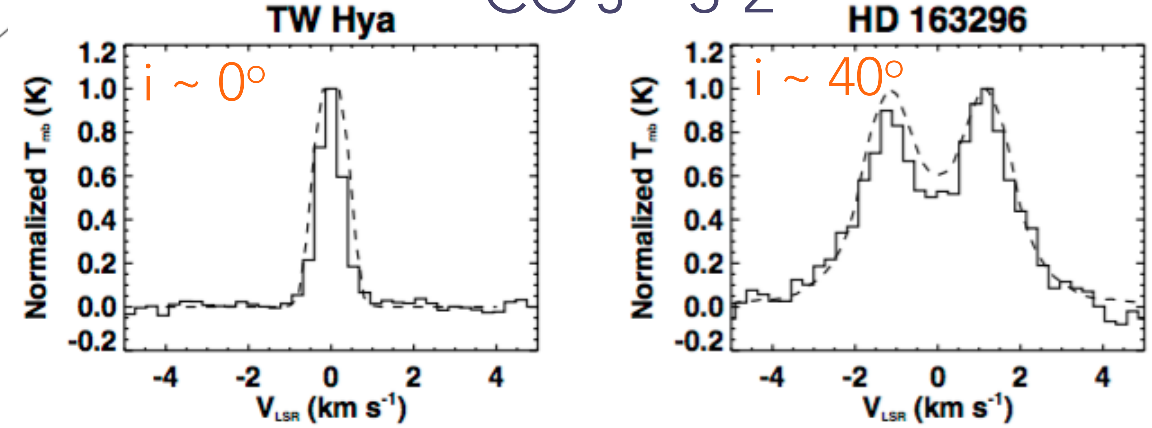
Dust spectral energy distribution

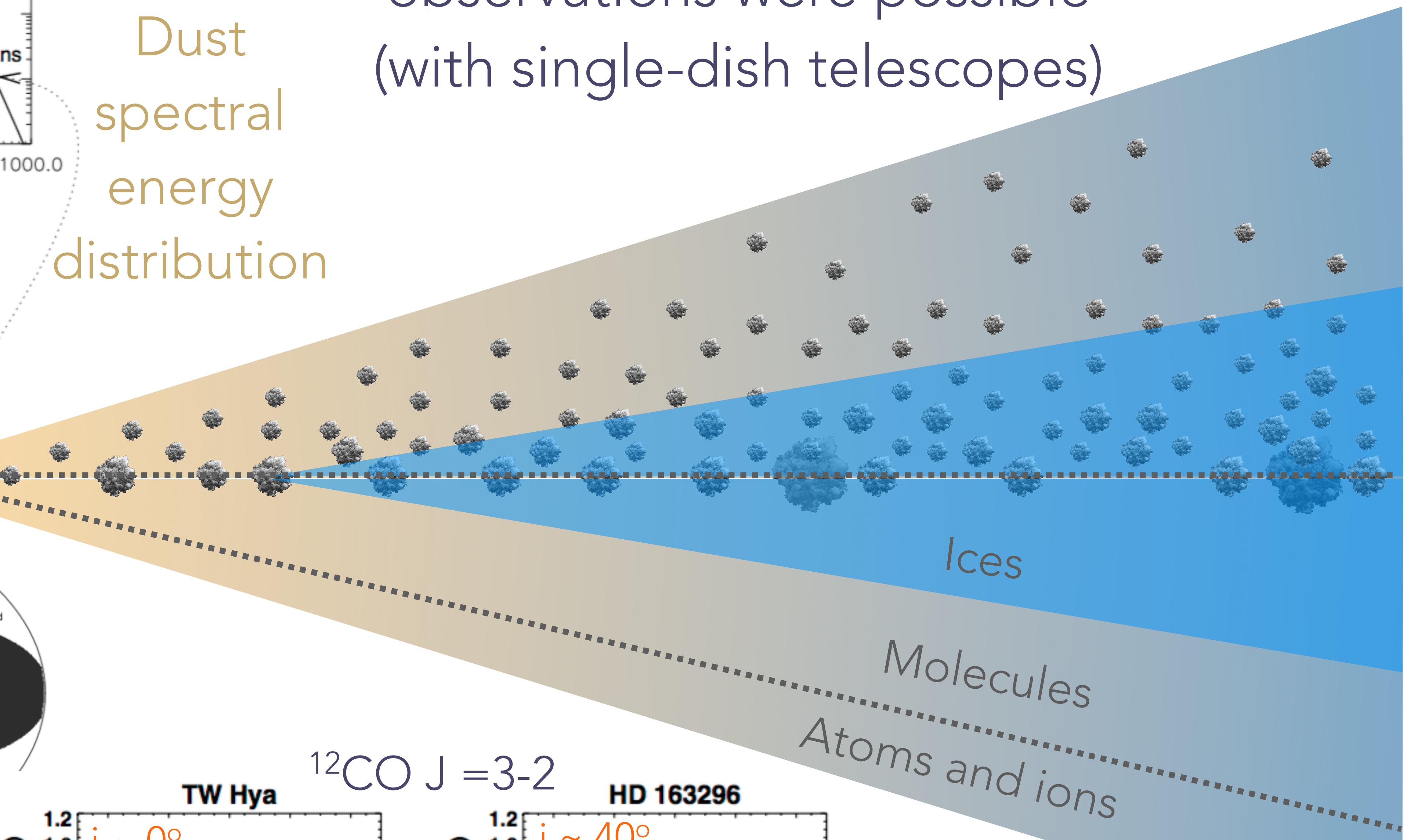
Gas



Molecular/atomic emission lines

^{12}CO J =3-2



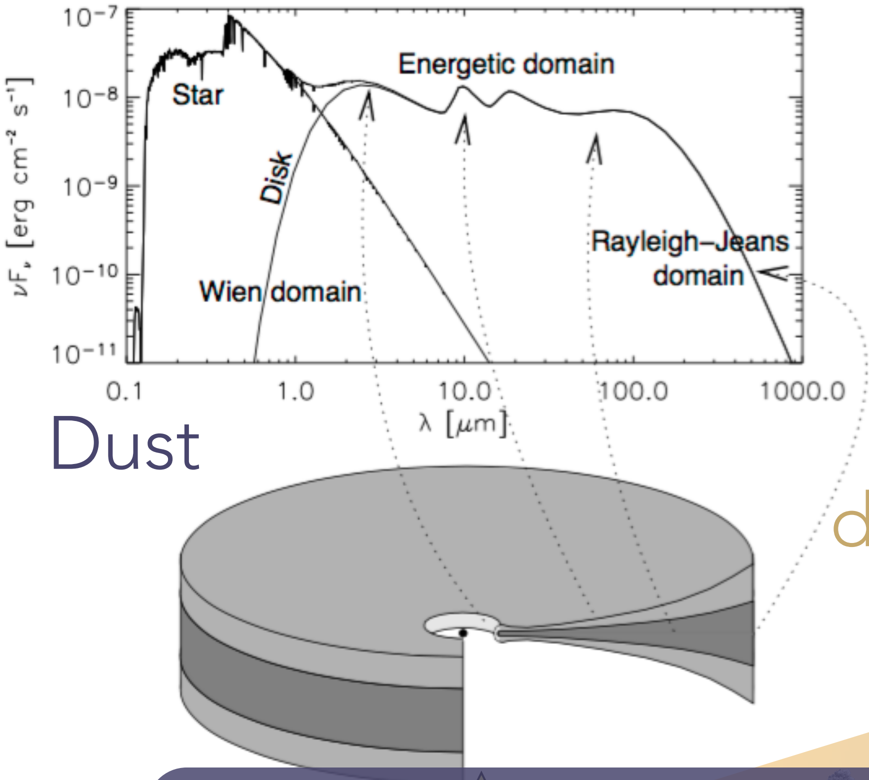


Dullemond, C. P., et al. 2006, PPV, 555; Thi, W.-F., et al. 2004, A&A, 425, 955; Guilloteau, S., et al. 2006, A&A, 448, L5

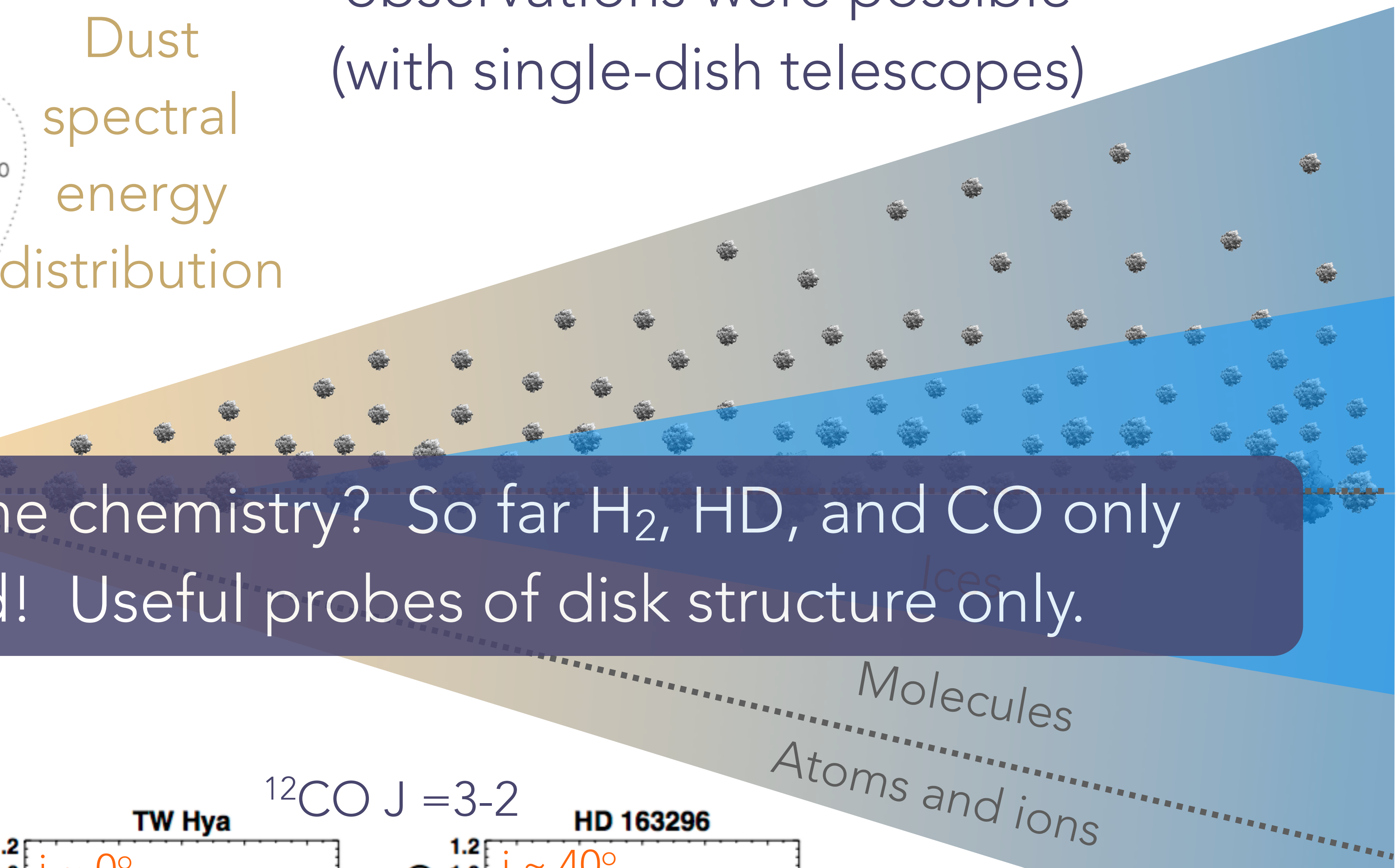
Observations of protoplanetary disks

Until recently: only spatially-unresolved observations were possible (with single-dish telescopes)

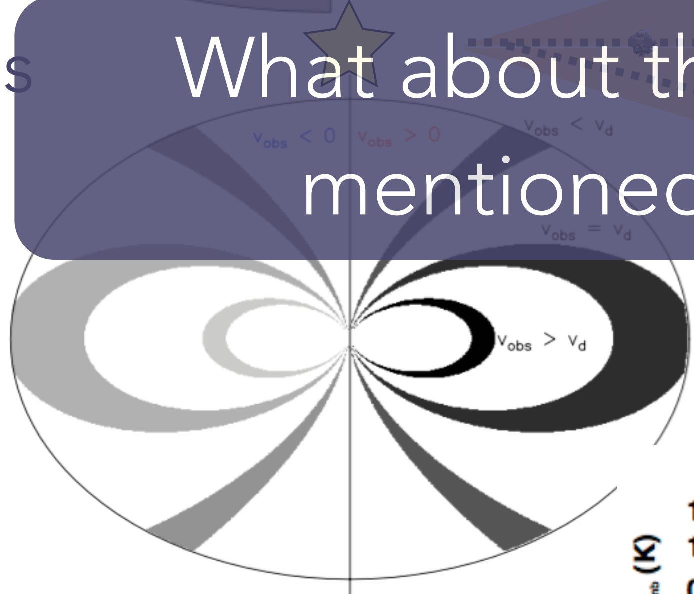
Dust



Dust spectral energy distribution

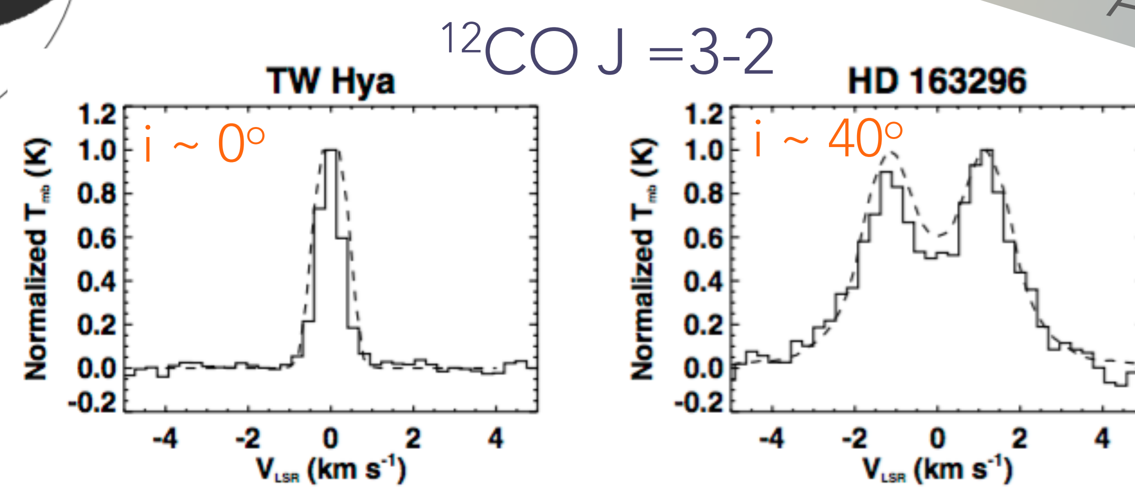


Gas



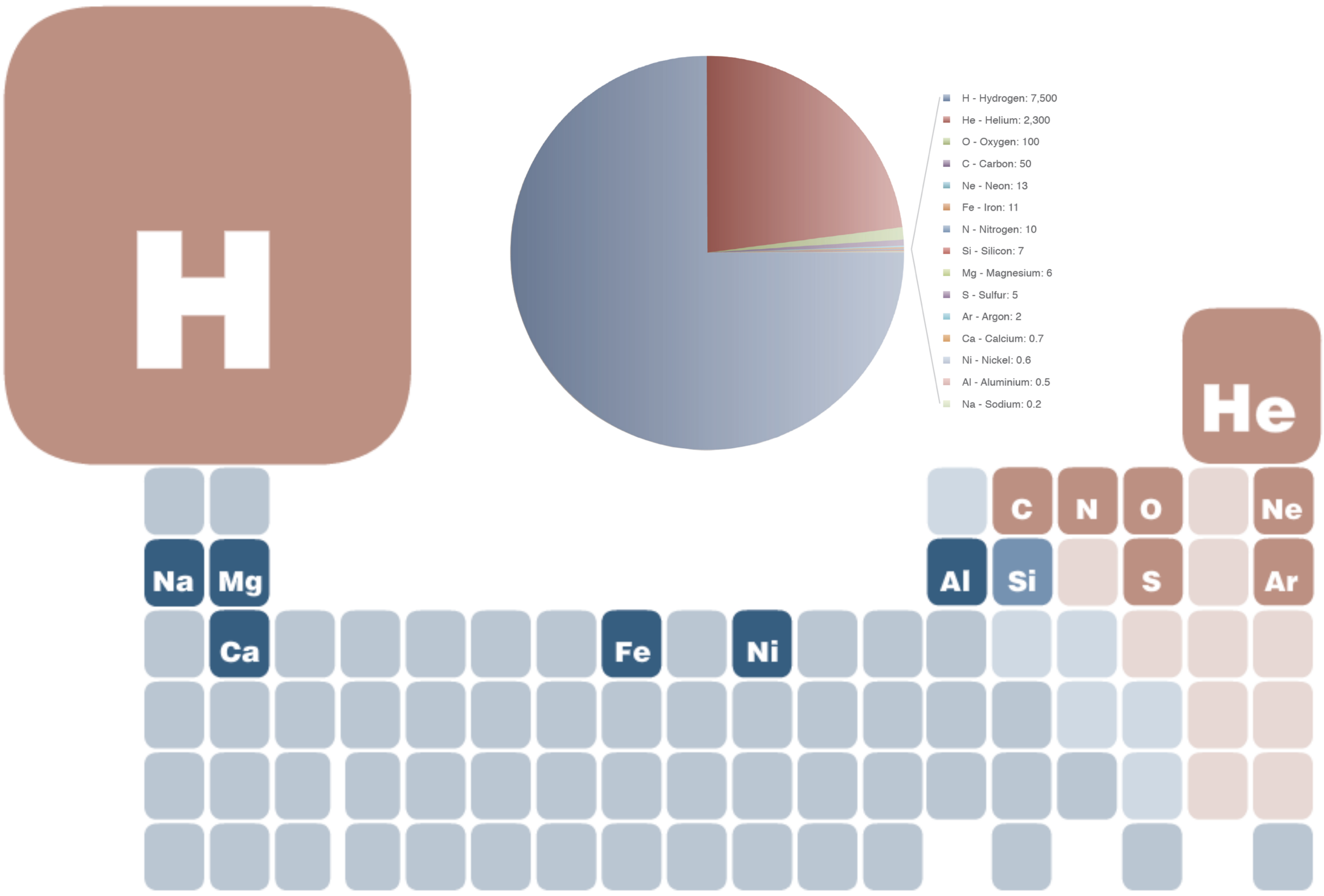
What about the chemistry? So far H_2, HD, and CO only mentioned! Useful probes of disk structure only.

Molecular/atomic emission lines



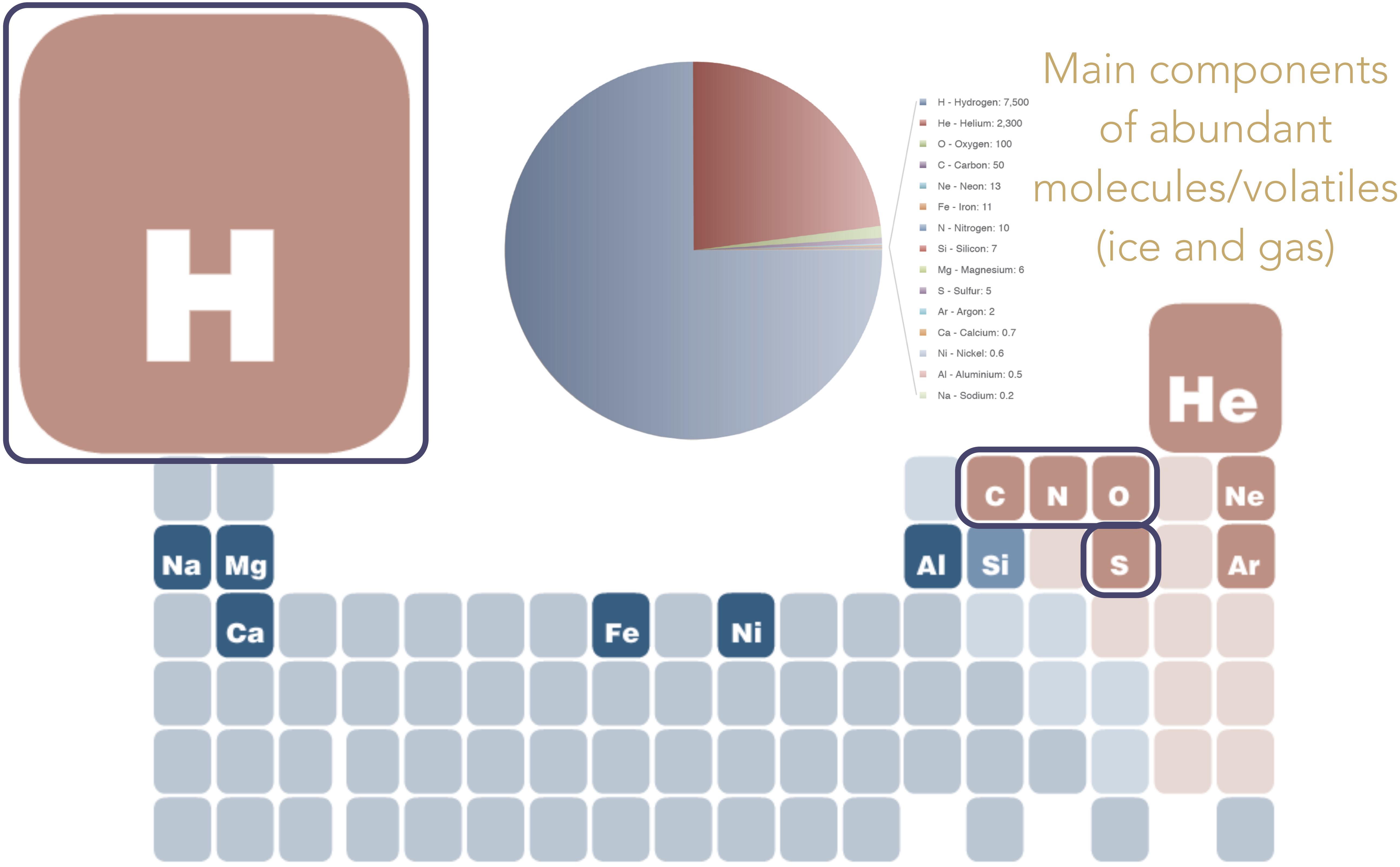
Dullemond, C. P., et al. 2006, PPV, 555; Thi, W.-F., et al. 2004, A&A, 425, 955; Guilloteau, S., et al. 2006, A&A, 448, L5

The astronomers' periodic table



http://www.chandra.harvard.edu

The astronomers' periodic table



Molecules in space

2 atoms		3 atoms		4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	≥ 10 atoms
H_2	HD	C_3	AlNC	*c*-C_3H	C5	C_5H	C_6H	CH_3C_3N	CH_3C_4H	CH_3C_5N
AlF	FeO ?	C_2H	SiNC	*l*-C_3H	C_4H	*l*-H_2C_4	CH_2CHCN	$HCOOCH_3$	CH_3CH_2CN	$(CH_3)_2CO$
AlCl	O_2	C_2O	HCP	C_3N	C_4Si	C_2H_4	CH_3C_2H	CH_3COOH	$(CH_3)_2O$	$(CH_2OH)_2$
C_2	CF^+	C_2S	CCP	C_3O	*l*-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2OH	CH_3CH_2CHO
CH	SiH ?	CH_2	AlOH	C_3S	*c*-C_3H_2	CH_3NC	CH_3CHO	C_6H_2	HC_7N	HC_9N
CH^+	PO	HCN	H_2O^+	C_2H_2	H_2CCN	CH_3OH	CH_3NH_2	CH_2OHCHO	C_8H	CH_3C_6H
CN	AlO	HCO	H_2Cl^+	NH_3	CH_4	CH_3SH	*c*-C_2H_4O	*l*-HC_6H	CH_3CONH_2	C_2H_5OCHO
CO	OH^+	HCO^+	KCN	HCCN	HC_3N	HC_3NH^+	H_2CCHOH	CH_2CHCHO ?	C_8H^-	CH_3OCOCH_3
CO^+	CN^-	HCS^+	FeCN	$HCNH^+$	HC_2NC	HC_2CHO	C_6H^-	CH_2CCHCN	C_3H_6	*c*-C_6H_6
CP	SH^+	HOC^+	O_2H	HNCO	HCOOH	NH_2CHO		H_2NCH_2CN	CH_3CH_2SH	*n*-C_3H_7CN
SiC	SH	H_2O	TiO_2	HNCS	H_2CNH	C_5N		CH_3CHNH		*i*-C_3H_7CN
HCl	HCl^+	H_2S	C_2N	$HOCO^+$	H_2C_2O	*l*-HC_4H				$HC_{11}N$
KCl	TiO	HNC	Si_2C	H_2CO	H_2NCN	*l*-HC_4N				C_{60}
NH	ArH^+	HNO		H_2CN	HNC_3	*c*-H_2C_3O				C_{70}
NO	NO^+ ?	MgCN		H_2CS	SiH_4	H_2CCNH ?				
NS		MgNC		H_3O^+	H_2COH^+	C_5N^-				
NaCl		N_2H^+		*c*-SiC_3	C_4H^-	HNCHCN				
OH		N_2O		CH_3	HCOCN					
PN		NaCN		C_3N^-	HNCNH					
SO		OCS		PH_3	CH_3O					
SO^+		SO_2		HCNO	NH_4^+					
SiN		*c*-SiC_2		HSCN	H_2NCO^+ ?					
SiO		CO_2		H_2O_2	$HCCNH^+$					
SiS		NH_2		C_3H^+						
CS		H_3^+		HMgNC						
HF		SiCN		HCCO						

- ✳ Cations (positively-charged)
- ✳ Anions (negatively-charged)
- ✳ Radicals (unpaired electrons)
- ✳ Unsaturated carbon chains
- ✳ Structural isomers
- ✳ Complex organic molecules
- ✳ Many isotopologues
- ✳ > 180 and counting ...

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

Molecules in space

2 atoms		3 atoms		4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	≥ 10 atoms
H_2	HD	C_3	AlNC	*c*-C_3H	C5	C_5H	C_6H	CH_3C_3N	CH_3C_4H	CH_3C_5N
AlF	FeO ?	C_2H	SiNC	*l*-C_3H	C_4H	*l*-H_2C_4	CH_2CHCN	$HCOOCH_3$	CH_3CH_2CN	$(CH_3)_2CO$
AlCl	O_2	C_2O	HCP	C_3N	C_4Si	C_2H_4	CH_3C_2H	CH_3COOH	$(CH_3)_2O$	$(CH_2OH)_2$
C_2	CF^+	C_2S	CCP	C_3O	*l*-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2OH	CH_3CH_2CHO
CH	SiH ?	CH_2	AlOH	C_3S	*c*-C_3H_2	CH_3NC	CH_3CHO	C_6H_2	HC_7N	HC_9N
CH^+	PO	HCN	H_2O^+	C_2H_2	H_2CCN	CH_3OH	CH_3NH_2	CH_2OHCHO	C_8H	CH_3C_6H
CN	AlO	HCO	H_2Cl^+	NH_3	CH_4	CH_3SH	*c*-C_2H_4O	*l*-HC_6H	CH_3CONH_2	C_2H_5OCHO
CO	OH^+	HCO^+	KCN	HCCN	HC_3N	HC_3NH^+	H_2CCHOH	CH_2CHCHO ?	C_8H^-	CH_3OCOCH_3
CO^+	CN^-	HCS^+	FeCN	$HCNH^+$	HC_2NC	HC_2CHO	C_6H^-	CH_2CCHCN	C_3H_6	*c*-C_6H_6
CP	SH^+	HOC^+	O_2H	HNCO	HCOOH	NH_2CHO		H_2NCH_2CN	CH_3CH_2SH	*n*-C_3H_7CN
SiC	SH	H_2O	TiO_2	HNCS	H_2CNH	C_5N		CH_3CHNH		*i*-C_3H_7CN
HCl	HCl^+	H_2S	C_2N	$HOCO^+$	H_2C_2O	*l*-HC_4H				$HC_{11}N$
KCl	TiO	HNC	Si_2C	H_2CO	H_2NCN	*l*-HC_4N				C_{60}
NH	ArH^+	HNO		H_2CN	HNC_3	*c*-H_2C_3O				C_{70}
NO	NO^+ ?	MgCN		H_2CS	SiH_4	H_2CCNH ?				
NS		MgNC		H_3O^+	H_2COH^+	C_5N^-				
NaCl		N_2H^+		*c*-SiC_3	C_4H^-	HNCHCN				
OH		N_2O		CH_3	HCOCN					
PN		NaCN		C_3N^-	HNCNH					
SO		OCS		PH_3	CH_3O					
SO^+		SO_2		HCNO	NH_4^+					
SiN		*c*-SiC_2		HSCN	H_2NCO^+ ?					
SiO		CO_2		H_2O_2	$HCCNH^+$					
SiS		NH_2		C_3H^+						
CS		H_3^+		HMgNC						
HF		SiCN		HCCO						

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AlF	FeO ?	C_2H	SiNC	l-C_3H	C_4H	l-H_2C_4	CH_2CHCN	$HCOOCH_3$	CH_3CH_2CN	$(CH_3)_2CO$
AlCl	O_2	C_2O	HCP	C_3N	C_4Si	C_2H_4	CH_3C_2H	CH_3COOH	$(CH_3)_2O$	$(CH_2OH)_2$
C_2	CF^+	C_2S	CCP	C_3O	l-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2OH	CH_3CH_2CHO
CH	SiH ?	CH_2	AlOH	C_3S	c-C_3H_2	CH_3NC	CH_3CHO	C_6H_2	HC_7N	HC_9N
CH^+	PO	HCN	H_2O^+	C_2H_2	H_2CCN	CH_3OH	CH_3NH_2	CH_2OHCHO	C_8H	CH_3C_6H
CN	AlO	HCO	H_2Cl^+	NH_3	CH_4	CH_3SH	c-C_2H_4O	l-HC_6H	CH_3CONH_2	C_2H_5OCHO
CO	OH^+	HCO^+	KCN	HCCN	HC_3N	HC_3NH^+	H_2CCHOH	CH_2CHCHO ?	C_8H^-	CH_3OCOCH_3
CO^+	CN^-	HCS^+	FeCN	$HCNH^+$	HC_2NC	HC_2CHO	C_6H^-	CH_2CCHCN	C_3H_6	c-C_6H_6
CP	SH^+	HOC^+	O_2H	HNCO	HCOOH	NH_2CHO		H_2NCH_2CN	CH_3CH_2SH	n-C_3H_7CN
SiC	SH	H_2O	TiO_2	HNCS	H_2CNH	C_5N		CH_3CHNH		i-C_3H_7CN
HCl	HCl^+	H_2S	C_2N	$HOCO^+$	H_2C_2O	l-HC_4H				$HC_{11}N$
KCl	TiO	HNC	Si_2C	H_2CO	H_2NCN	l-HC_4N				C_{60}
NH	ArH^+	HNO		H_2CN	HNC_3	c-H_2C_3O				C_{70}
NO	NO^+ ?	MgCN		H_2CS	SiH_4	H_2CCNH ?				
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NaCl		N_2H^+		c-SiC_3	C_4H^-	HNCHCN				
OH		N_2O		CH_3	HCOCN					
PN		NaCN		C_3N^-	HNCNH					
SO		OCS		PH_3	CH_3O					
SO^+		SO_2		HCNO	NH_4^+					
SiN		c-SiC_2		HSCN	H_2NCO^+ ?					
SiO		CO_2		H_2O_2	$HCCNH^+$					
SiS		NH_2		C_3H^+						
CS		H_3^+		HMgNC						
HF		SiCN		HCCO						

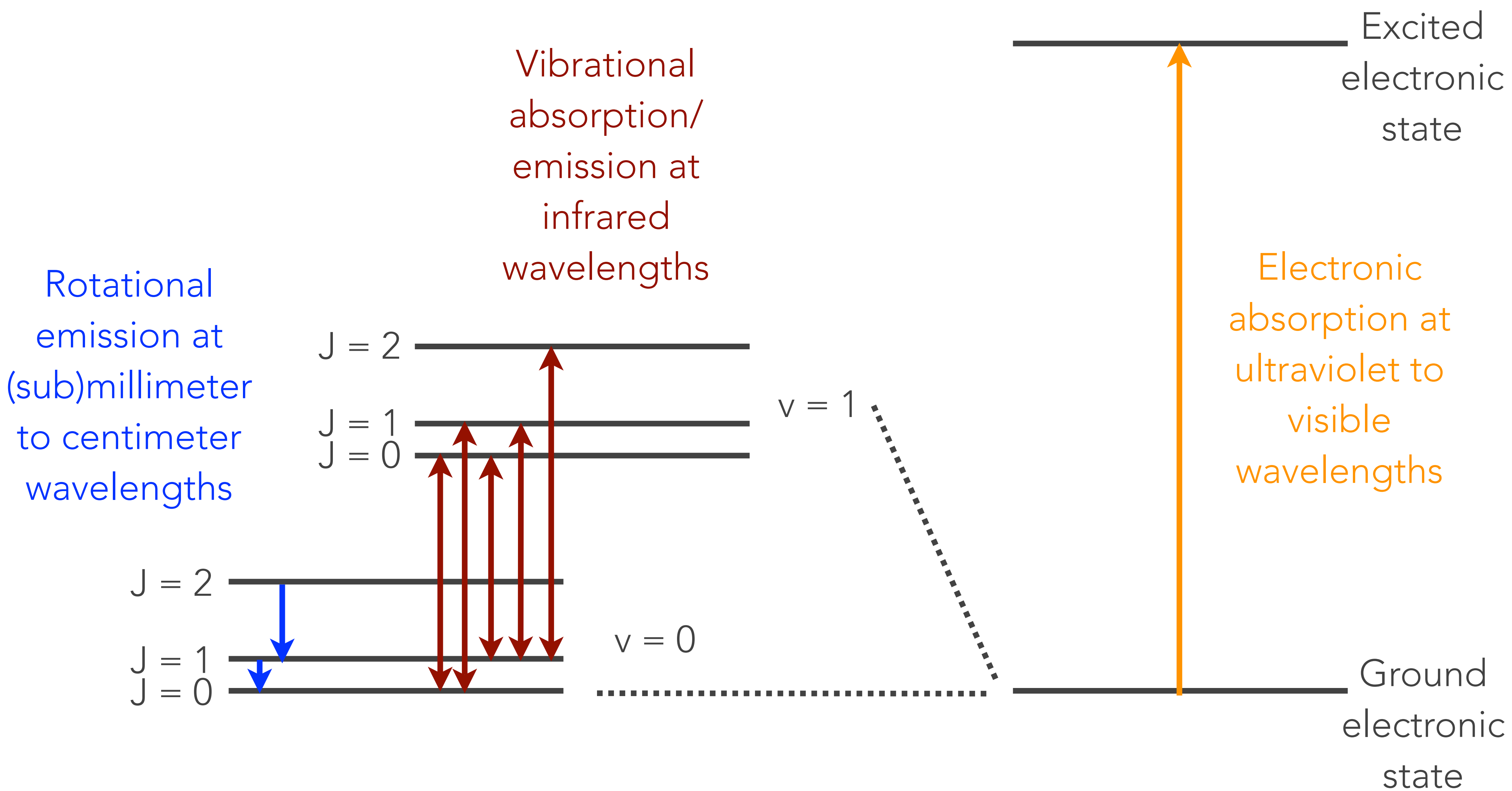
Protoplanetary disk molecules/volatiles?

21* and counting …

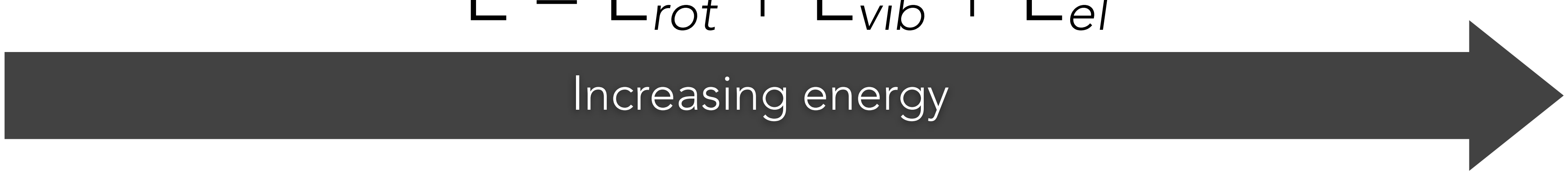
* not including isotopologues

Detection of molecules

A crash course in molecular spectroscopy

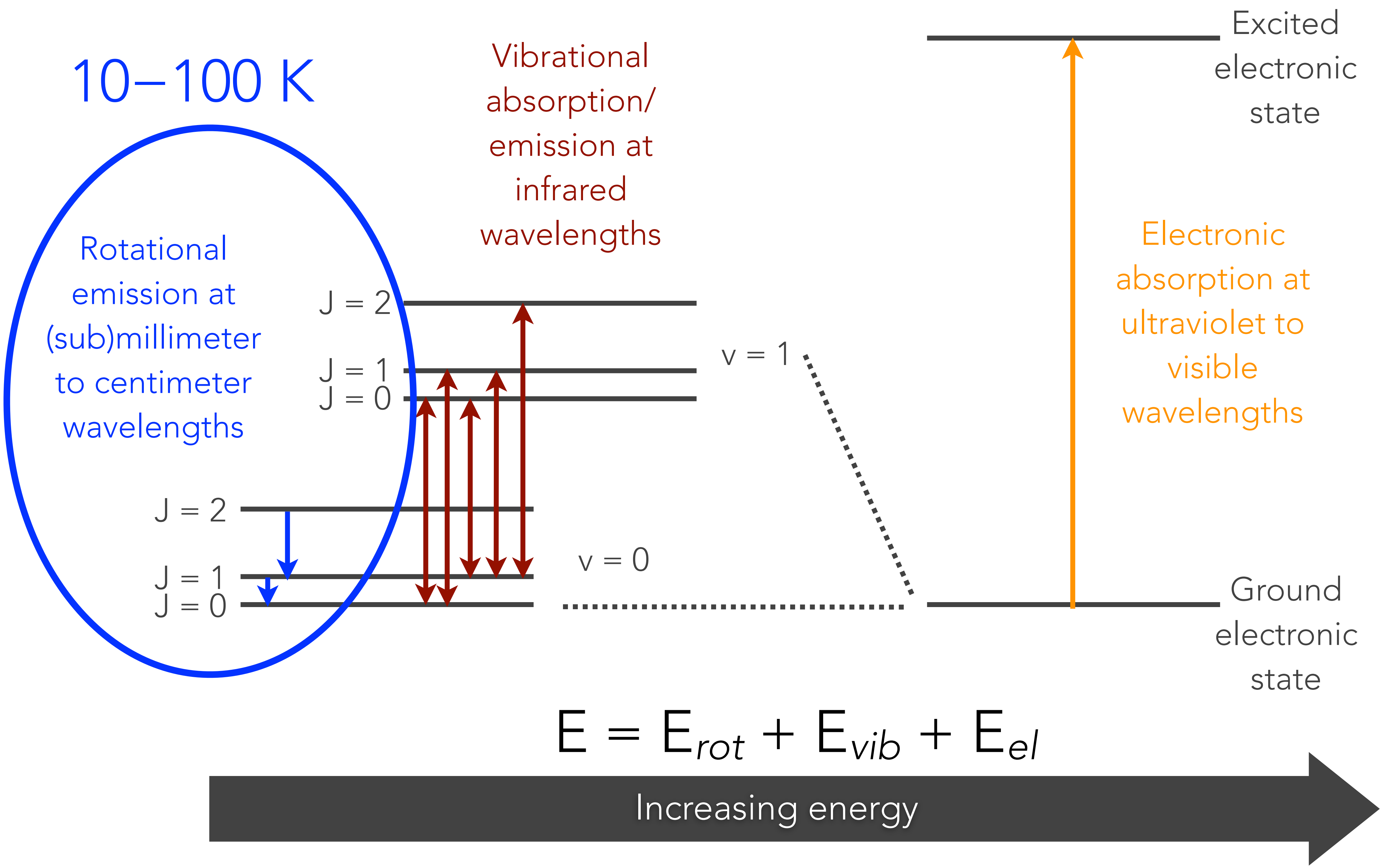


$$E = E_{rot} + E_{vib} + E_{el}$$



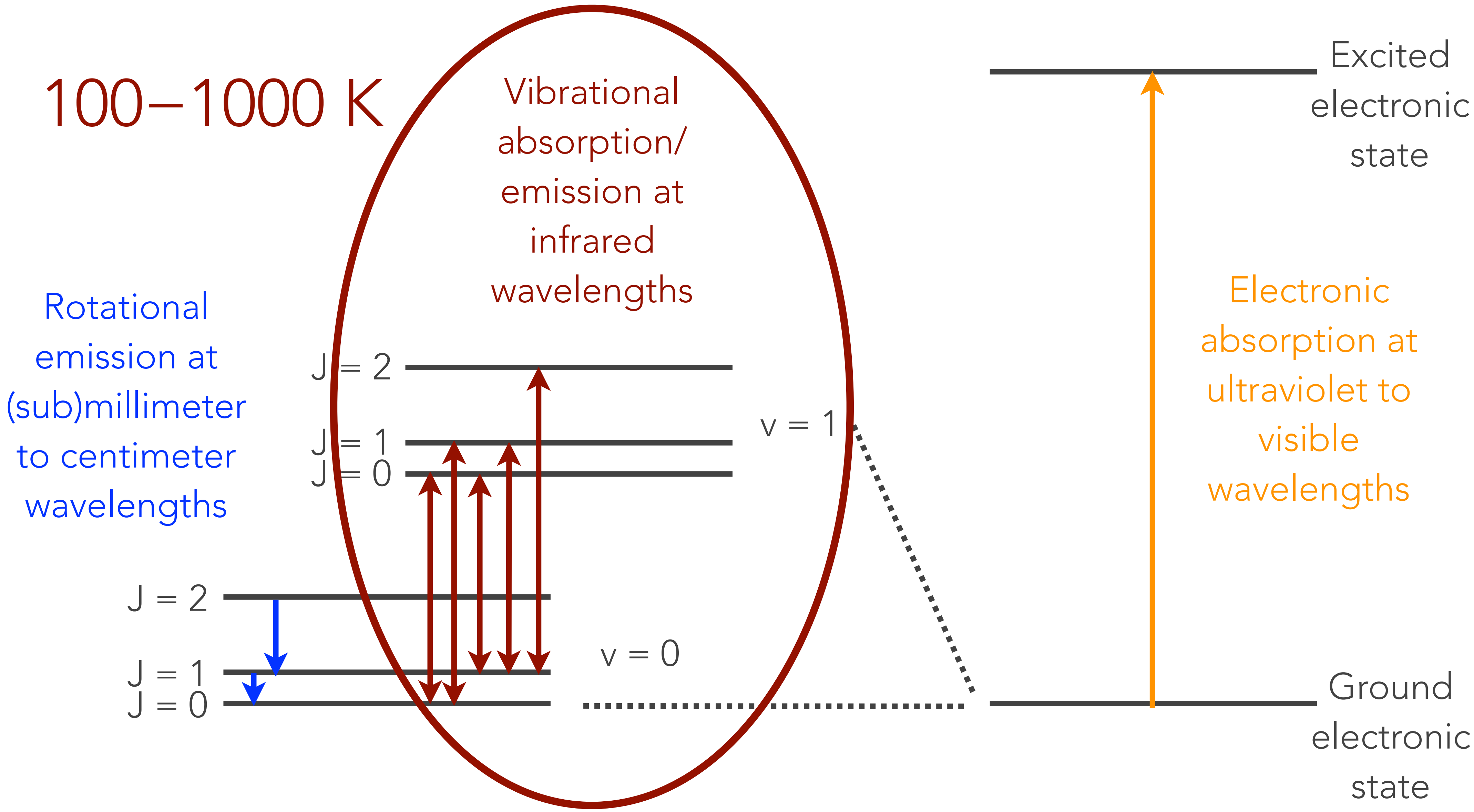
Detection of molecules

A crash course in molecular spectroscopy

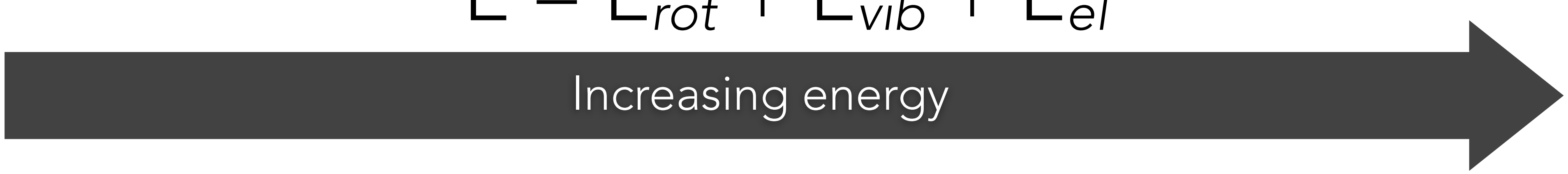


Detection of molecules

A crash course in molecular spectroscopy



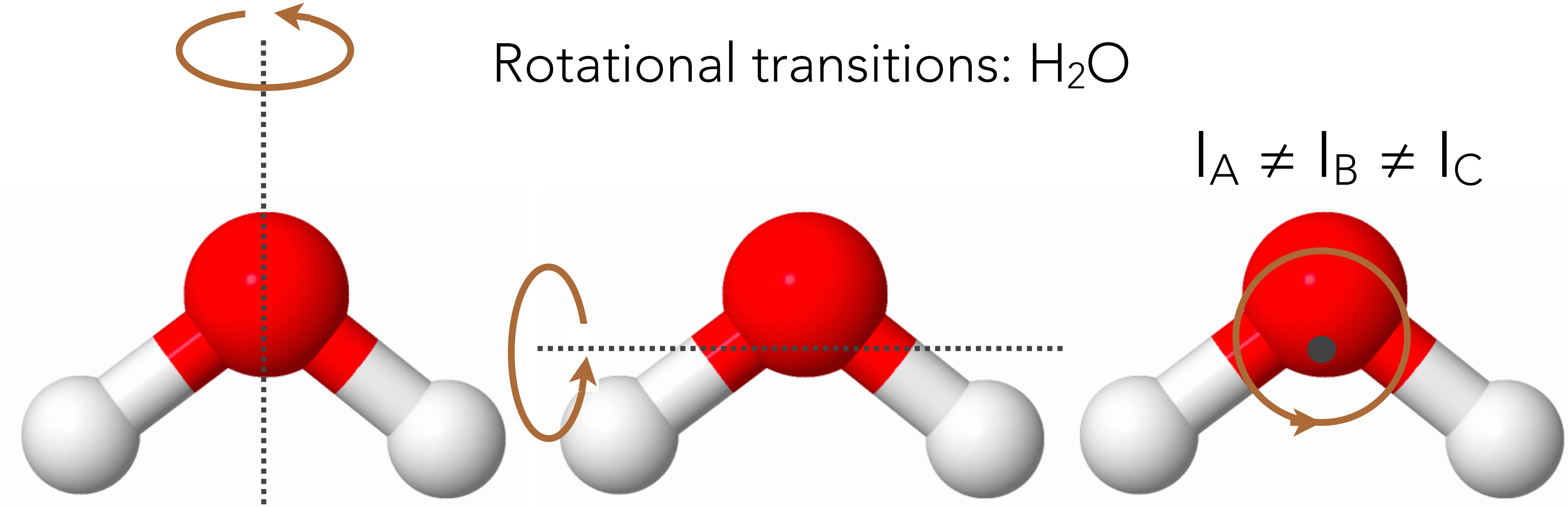
$$E = E_{rot} + E_{vib} + E_{el}$$

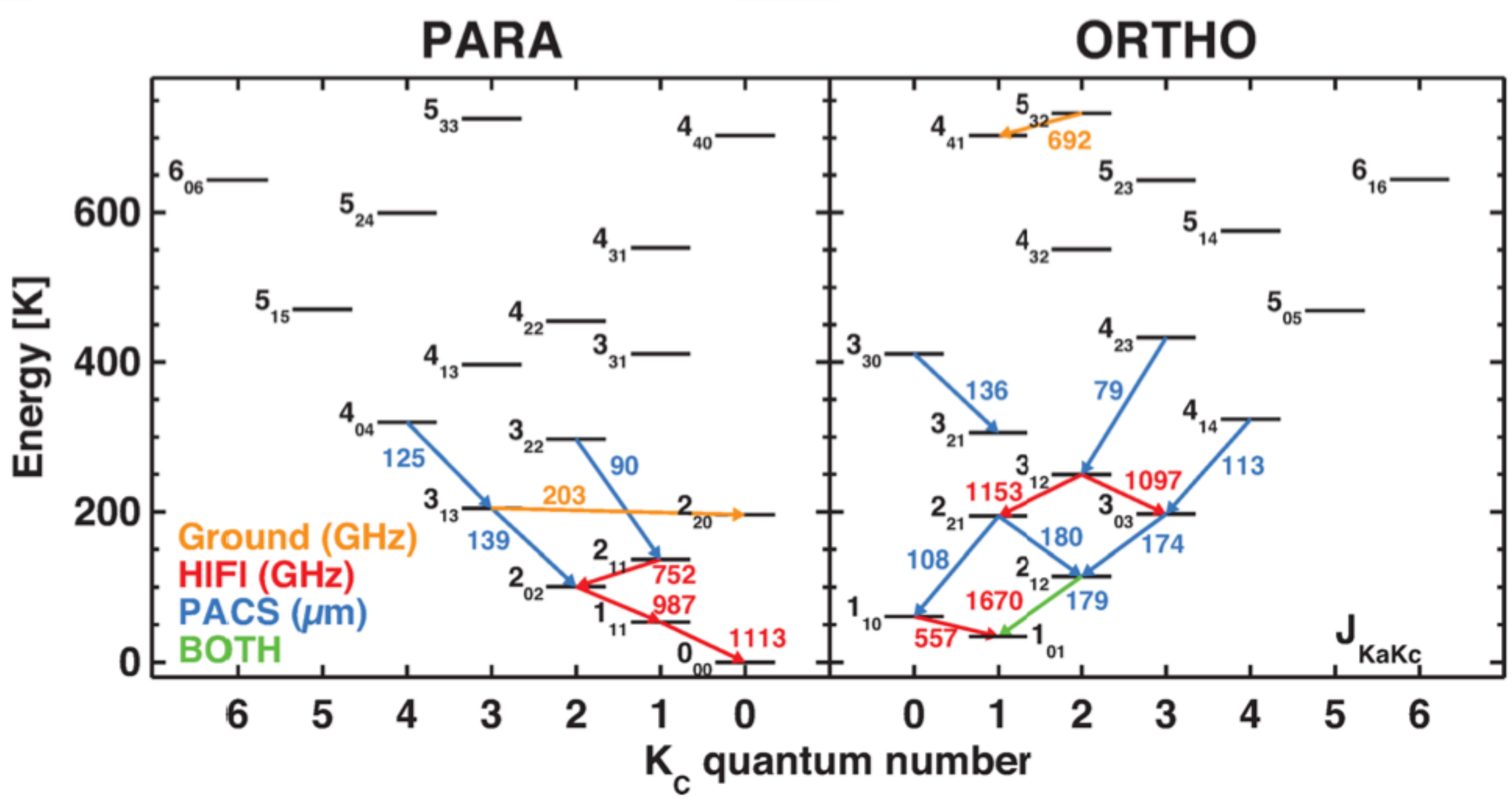


Detection of molecules

Rotational transitions: H_2O

$I_A \neq I_B \neq I_C$

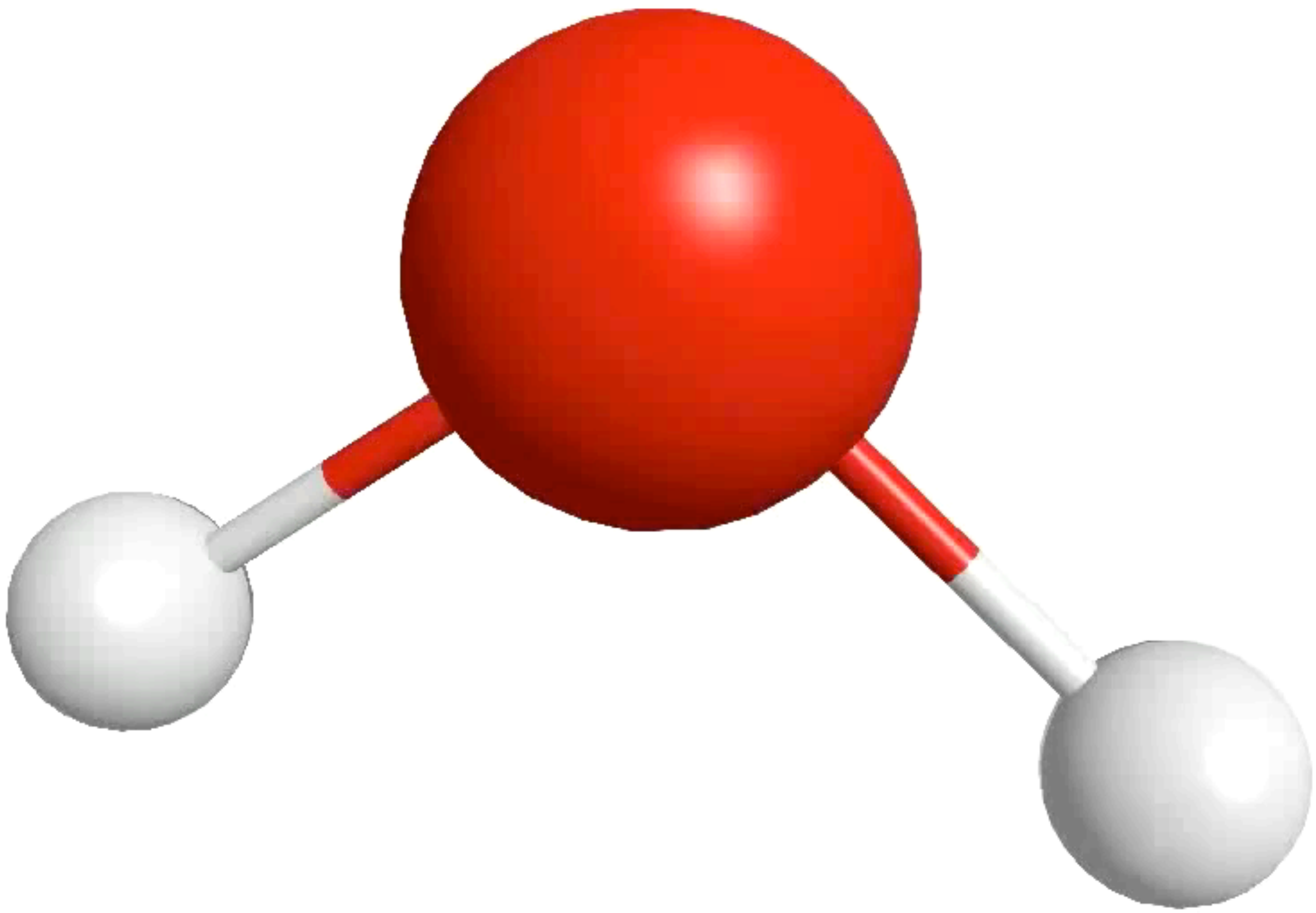




Despite only consisting of 3 atoms, H_2O has a complex rotational spectrum

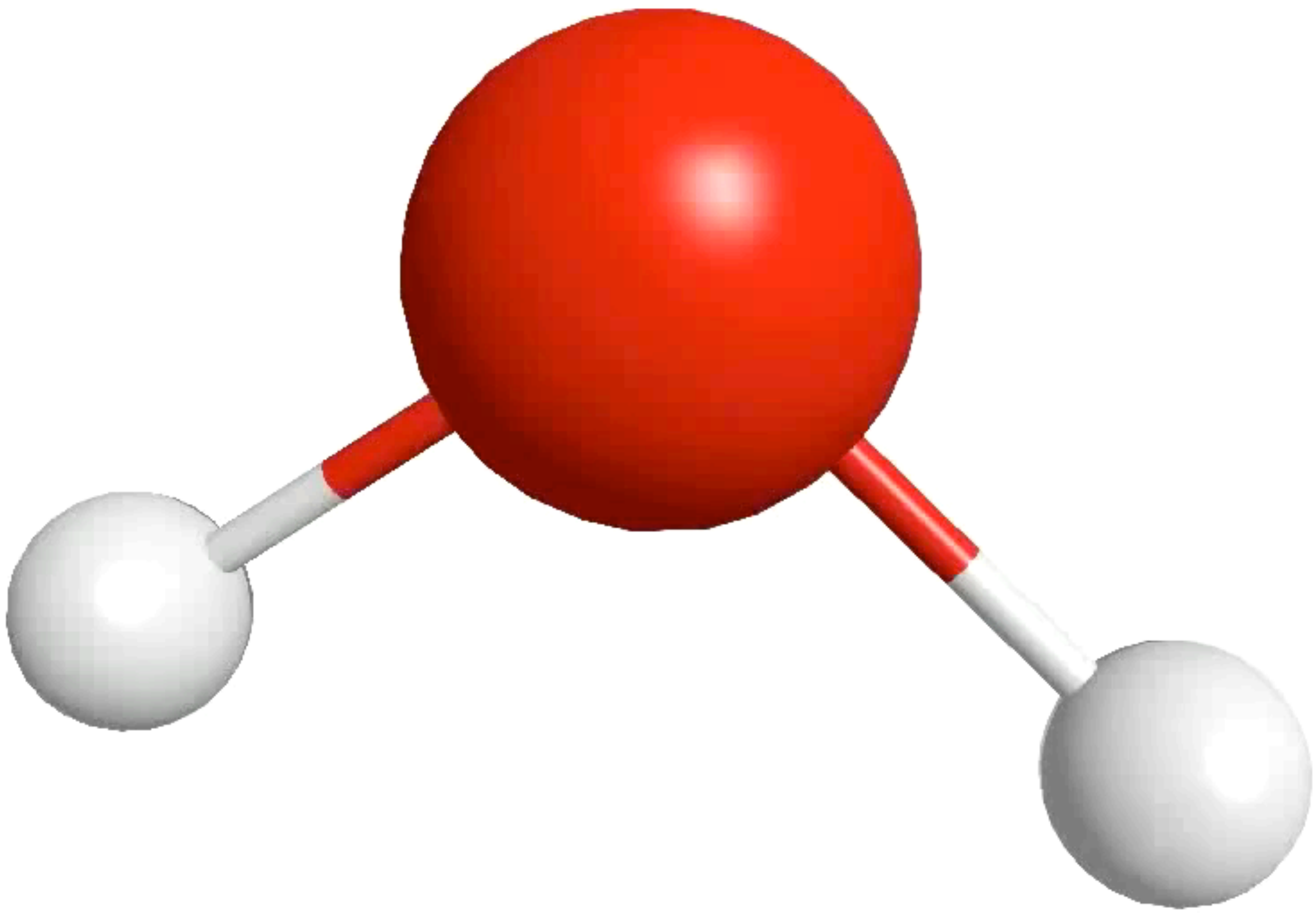
Detection of molecules

Vibrational transitions: H_2O



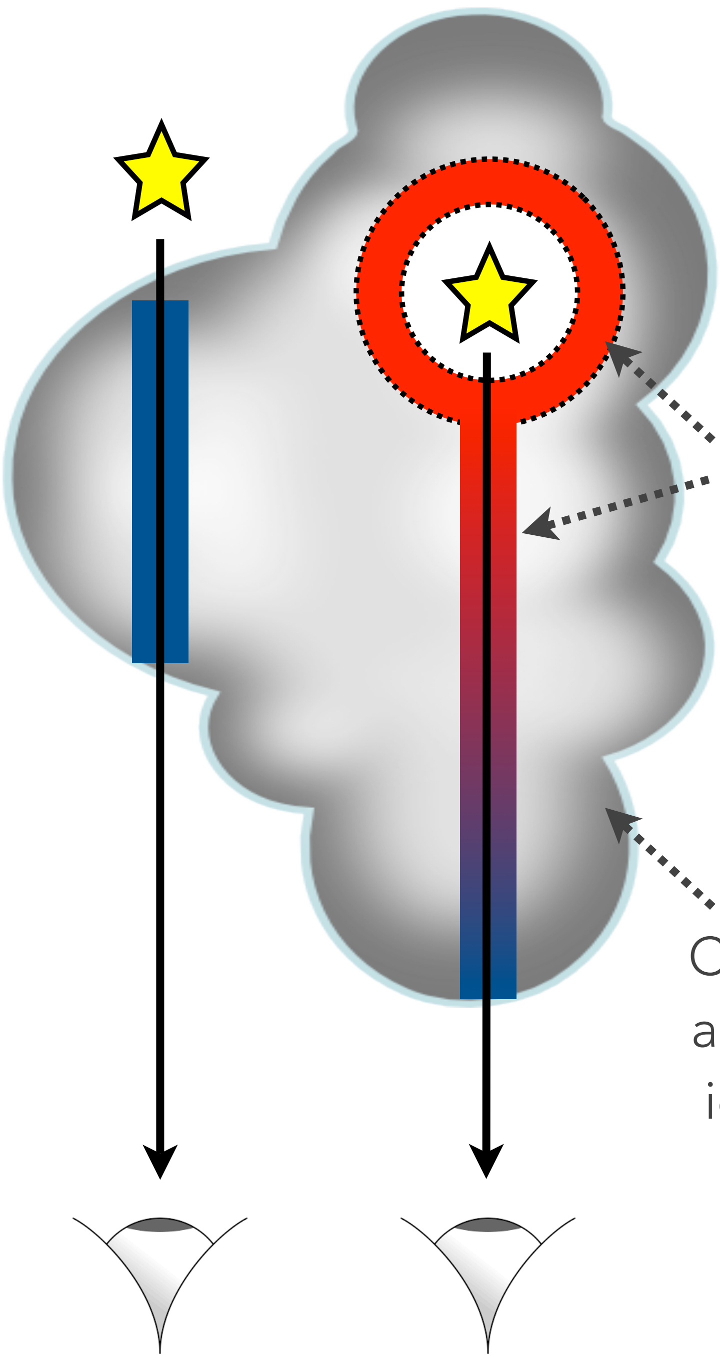
Detection of molecules

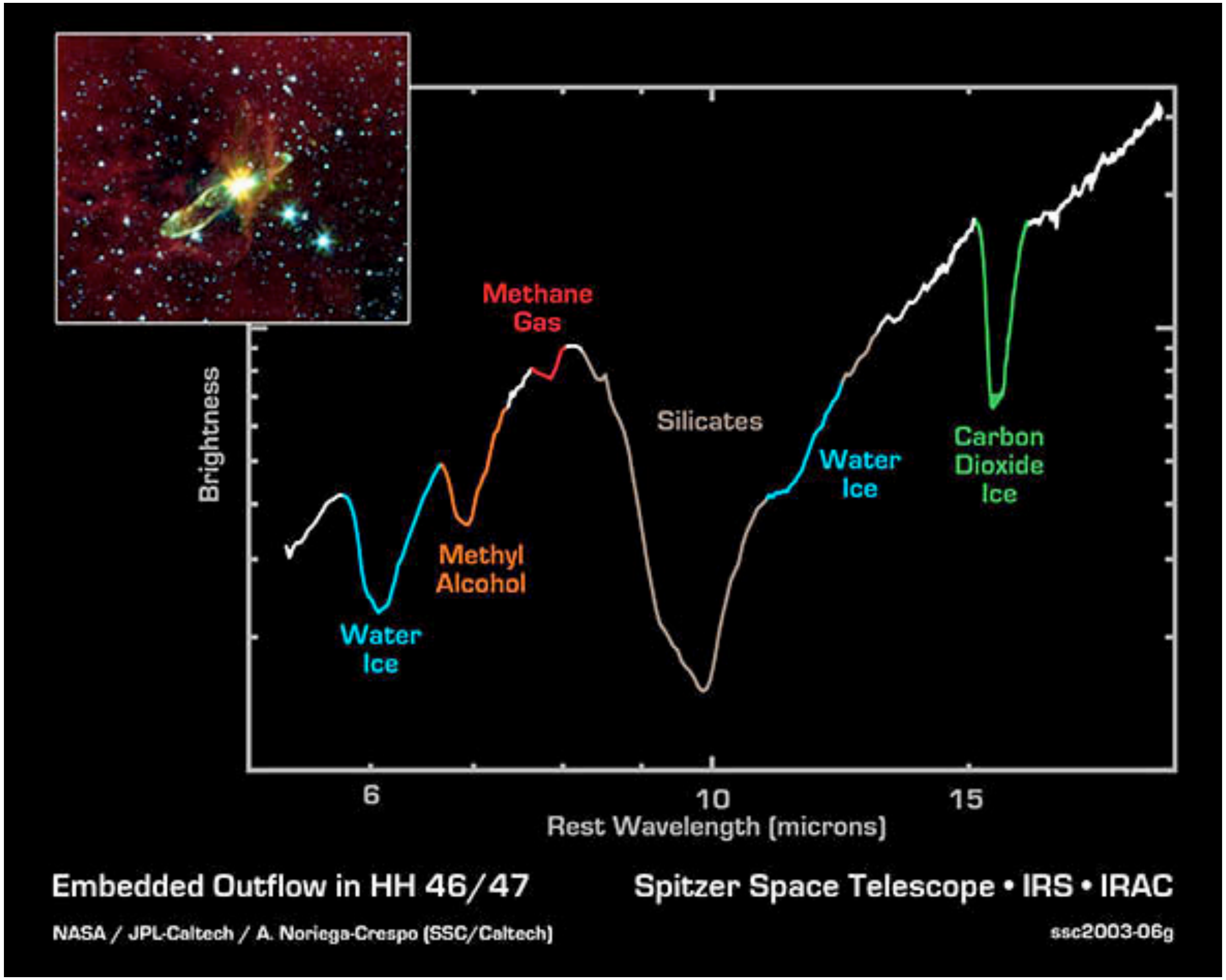
Vibrational transitions: H_2O



Detection of molecules

Infrared wavelengths: absorption





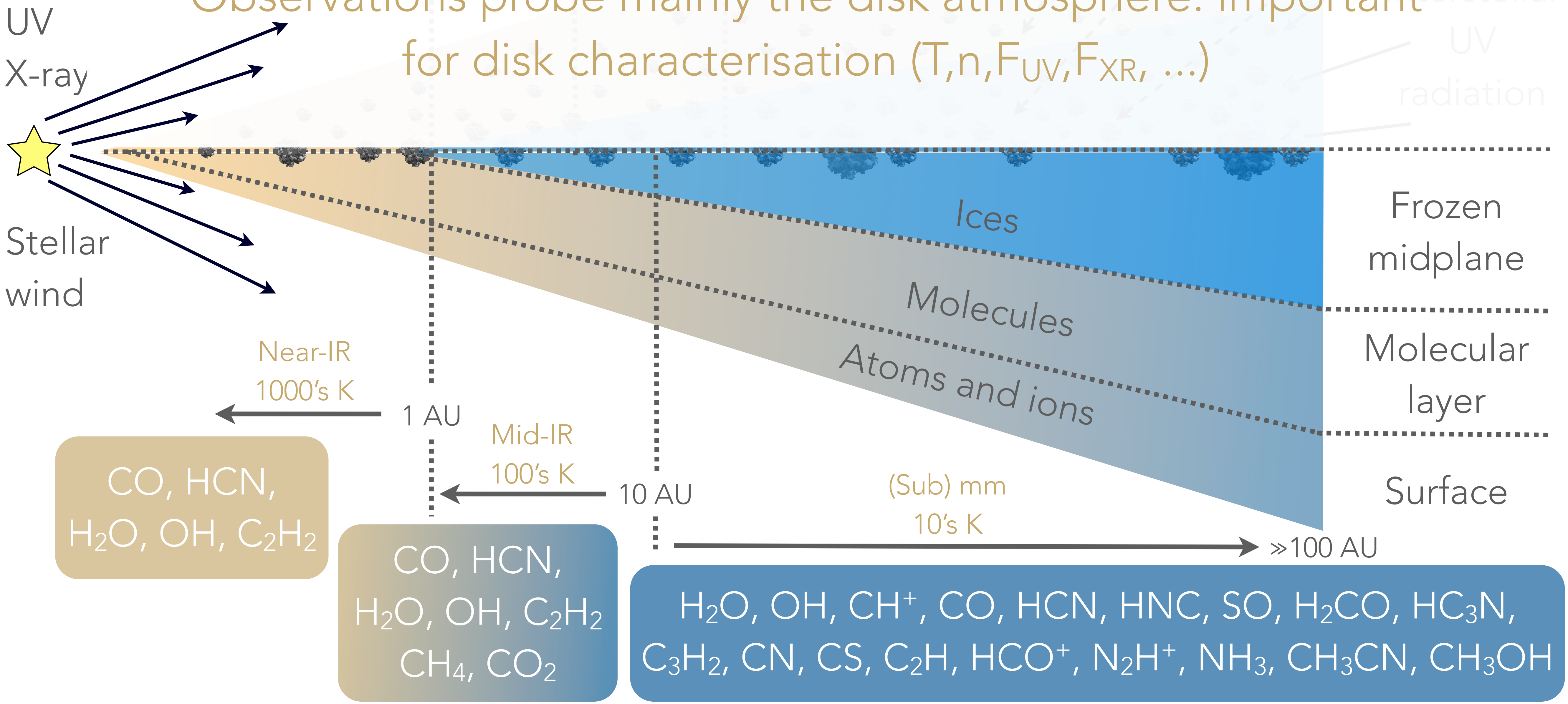
Detection of molecules

(Sub)millimeter wavelengths: emission

Chemical anatomy of a protoplanetary disk

Two phases of molecules/volatiles in protoplanetary disks: gas (H_2 dominated) and ice (H_2O dominated)

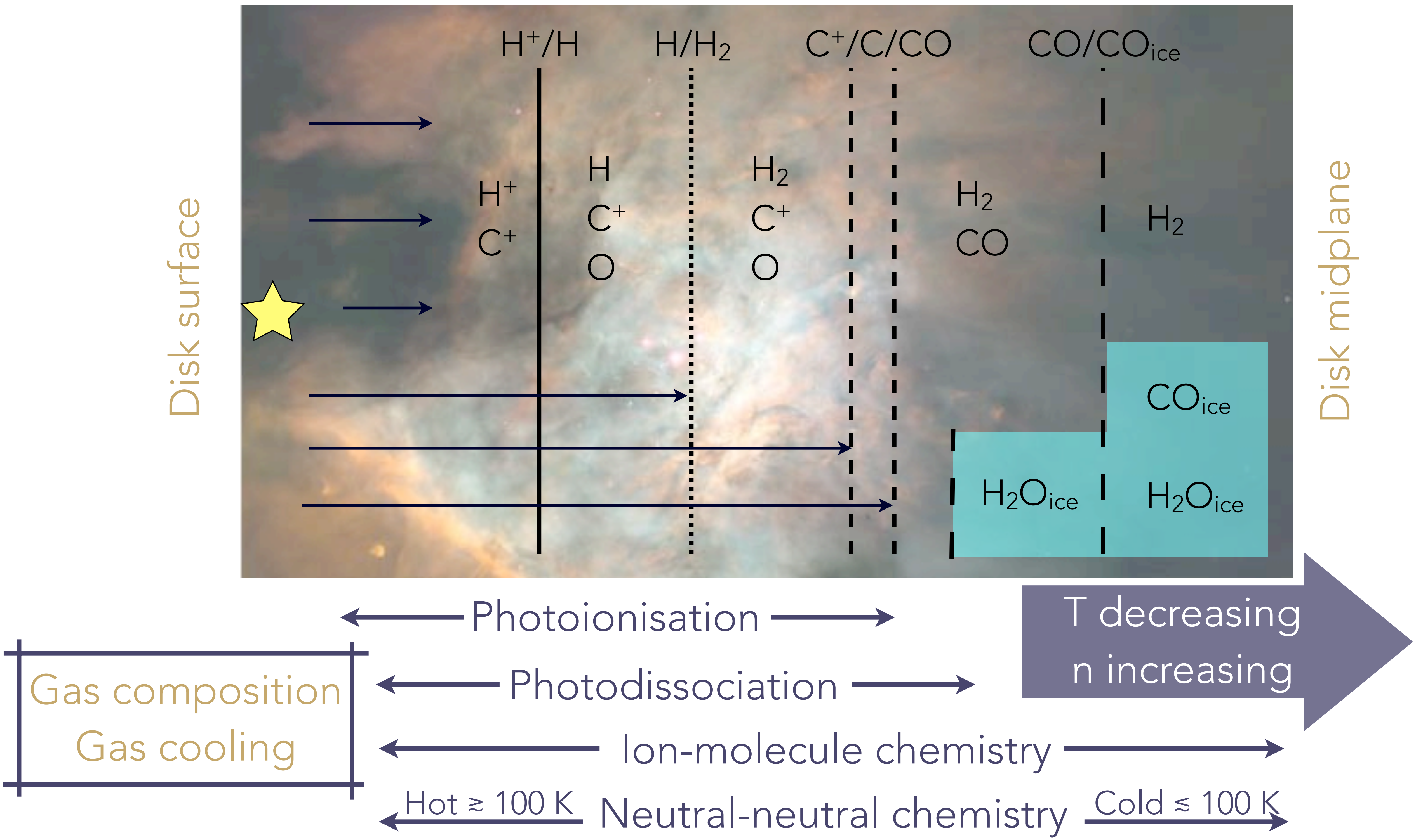
Observations probe mainly the disk atmosphere: important for disk characterisation (T, n, F_{UV}, F_{XR}, ...)



Pontoppidan+, Gibb+, Salyk+, van Dishoeck+, Dutrey+, Chapillon+, Qi+, Oberg+, Kastner+, Thi+, Carr+, Najita+, Hogerheijde+, Fedele+, Meeus+

What chemistry is important where and why?

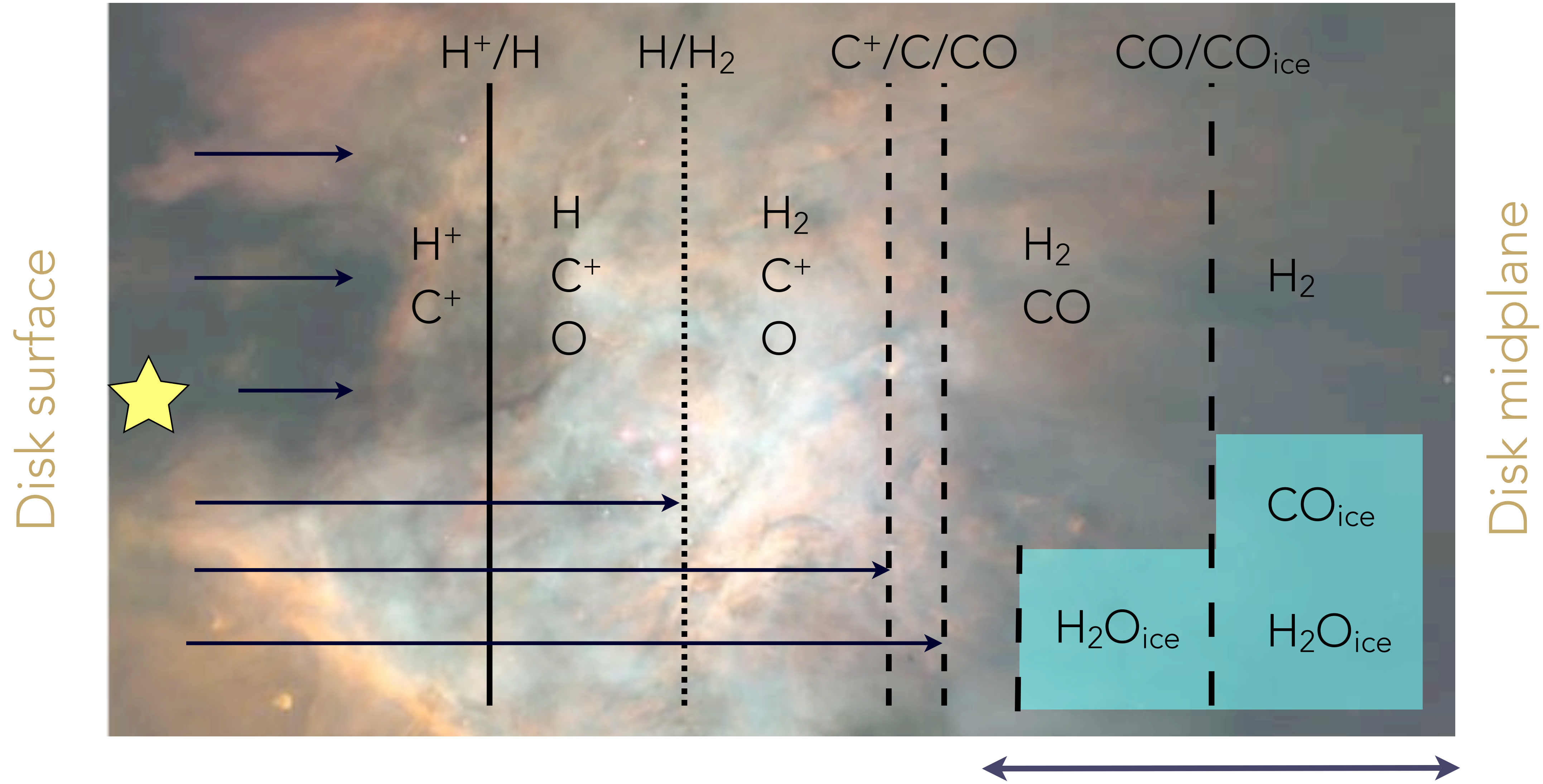
Protoplanetary disks are essentially 2/3D photon-dominated regions (PDRs)



Tielens, A. G. G. M. & Hollenbach, D. J.1994, ARA&A, 35, 179; Henning, Th. & Semenov, D. 2013, Chem. Rev., 113, 9016

What chemistry is important where and why?

Protoplanetary disks are essentially 2/3D photon-dominated regions (PDRs)



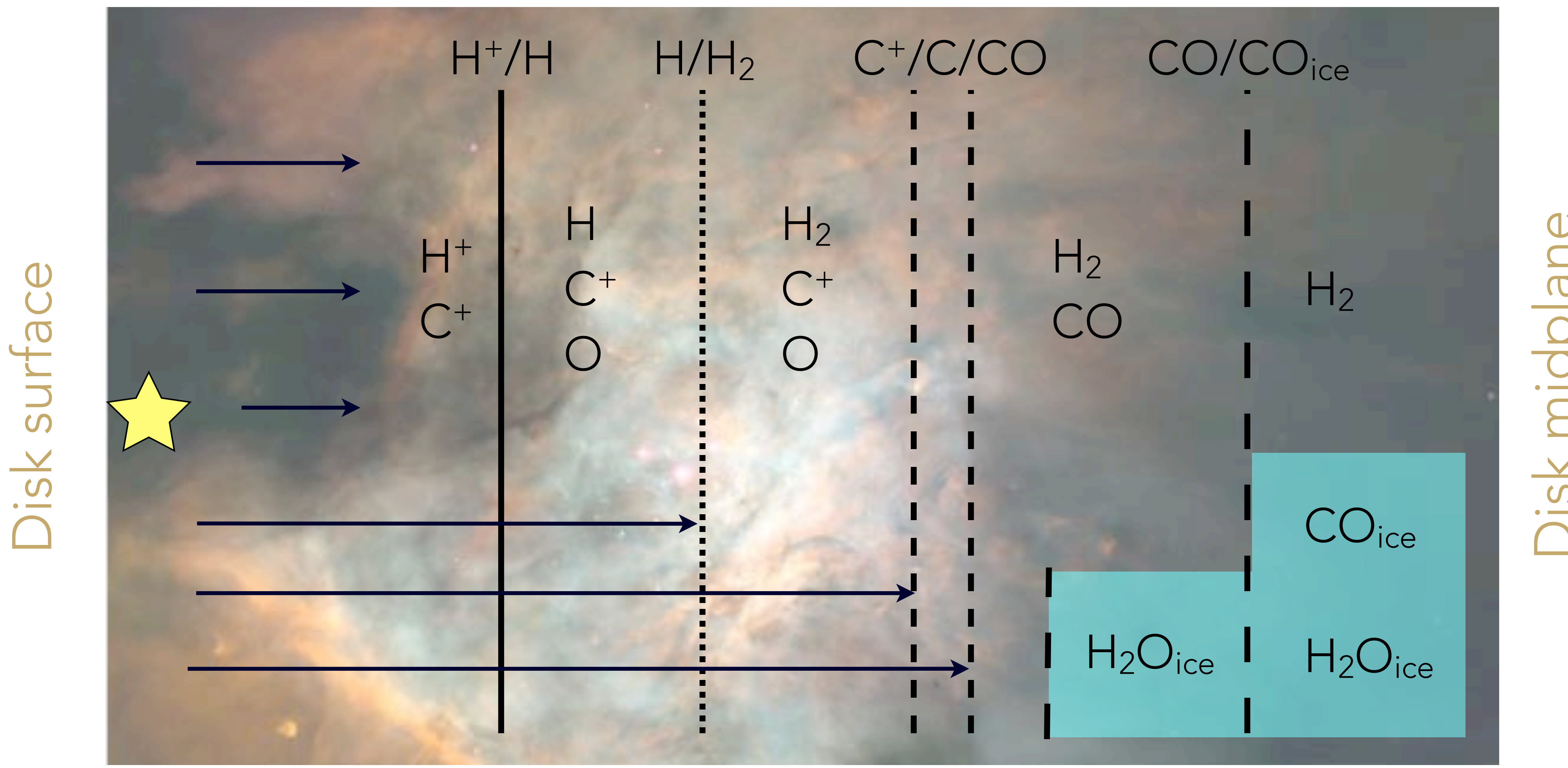
Gas composition
Ice composition
Snowlines

Freezeout
Desorption
Grain-surface chemistry

Tielens, A. G. G. M. & Hollenbach, D. J.1994, ARA&A, 35, 179; Henning, Th. & Semenov, D. 2013, Chem. Rev., 113, 9016

What chemistry is important where and why?

Protoplanetary disks are essentially 2/3D photon-dominated regions (PDRs)



← Photoionisation →

← X-ray ionisation →

← Cosmic-ray ionisation →

Gas composition
Ice composition
Ionisation fraction

Tielens, A. G. G. M. & Hollenbach, D. J.1994, ARA&A, 35, 179; Henning, Th. & Semenov, D. 2013, Chem. Rev., 113, 9016

Formation and destruction of molecules

Gas-phase chemistry

Bond formation

$X^+ + Y \rightarrow XY^+ + \gamma_{UV}$

$X^- + Y \rightarrow XY + e^-$

$X + Y + M \rightarrow XY + M$

Bond destruction

$XY + \gamma_{UV} \rightarrow X + Y$

$XY + \gamma_{XR} \rightarrow X + Y$

$XY + \gamma_{CR} \rightarrow X + Y$

$XY^+ + e^- \rightarrow X + Y$

$XY + M \rightarrow X + Y + M$

Bond rearrangement

$X^+ + YZ \rightarrow XY^+ + Z$

$X^+ + YZ \rightarrow X + YZ^+$

$X + YZ \rightarrow X + YZ$

Tielens, A. G. G. M. 2013, Rev. Mod. Phys., 85, 1021

Formation and destruction of molecules

Gas-phase chemistry

Bond formation

$X^+ + Y \rightarrow XY^+ + \gamma_{UV}$

$X^- + Y \rightarrow XY + e^-$

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$XY^+ + e^- \rightarrow X + Y$

$XY + M \rightarrow X + Y + M$

Bond rearrangement

$X^+ + YZ \rightarrow XY^+ + Z$

$X^+ + YZ \rightarrow X + YZ^+$

$X + YZ \rightarrow X + YZ$

Interstellar and circumstellar conditions: chemical kinetics dominate

Tielens, A. G. G. M. 2013, Rev. Mod. Phys., 85, 1021

Formation and destruction of molecules

Gas-phase chemistry

Bond formation

$X + Y + M \rightarrow XY + M$

Bond destruction

$XY + \gamma_{UV} \rightarrow X + Y$

$XY + \gamma_{XR} \rightarrow X + Y$

$XY + \gamma_{CR} \rightarrow X + Y$

$XY^{+} + e^{-} \rightarrow X + Y$

$XY + M \rightarrow X + Y + M$

Bond rearrangement

$X + YZ \rightarrow X + YZ$

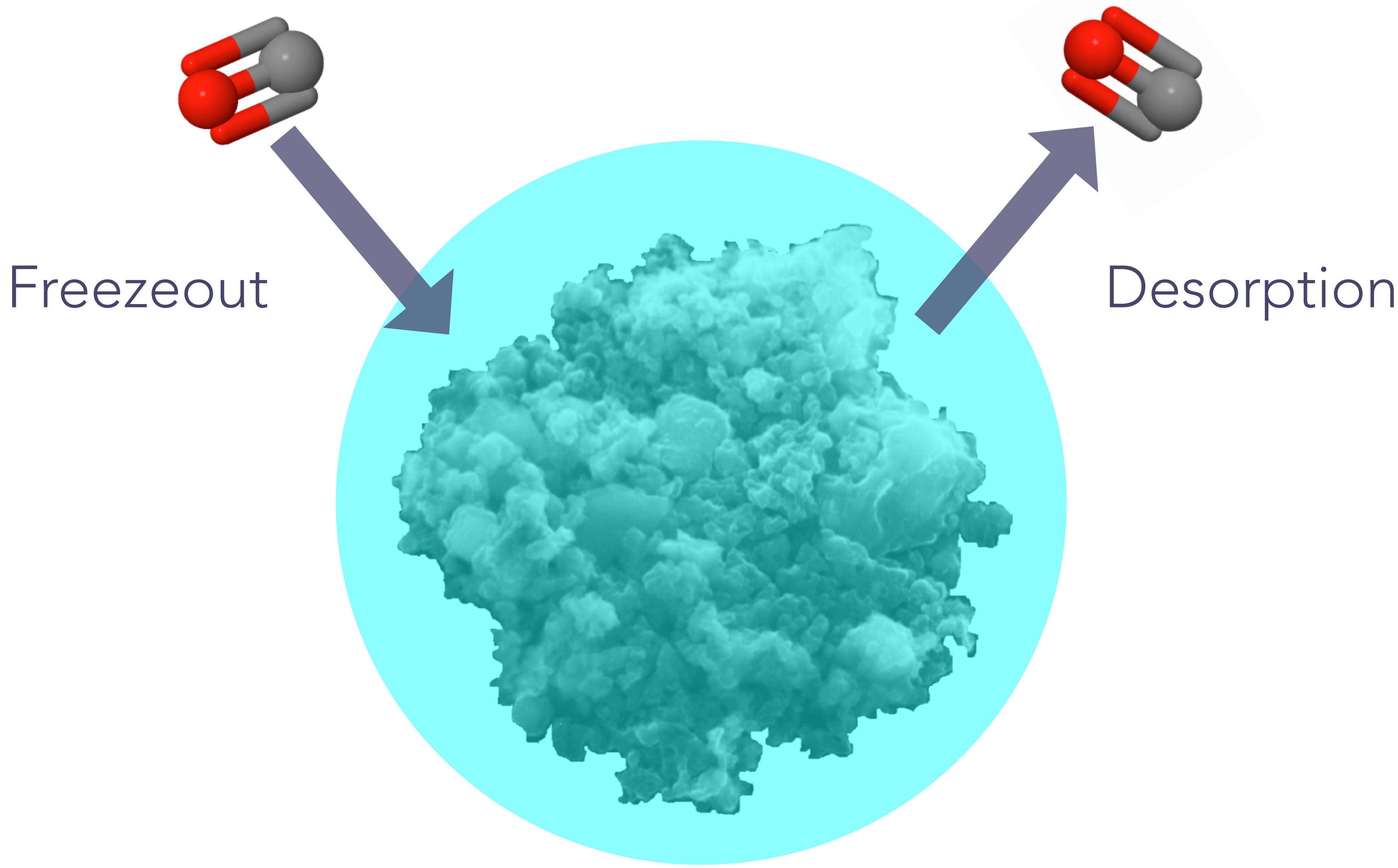
We know ion-molecule chemistry is important in disks because we see cations: CH^{+}, HCO^{+}, N_2H^{+}, DCO^{+}, N_2D^{+}

Interstellar and circumstellar conditions: chemical kinetics dominate

Tielens, A. G. G. M. 2013, Rev. Mod. Phys., 85, 1021

Formation and destruction of molecules

Grain-surface processes

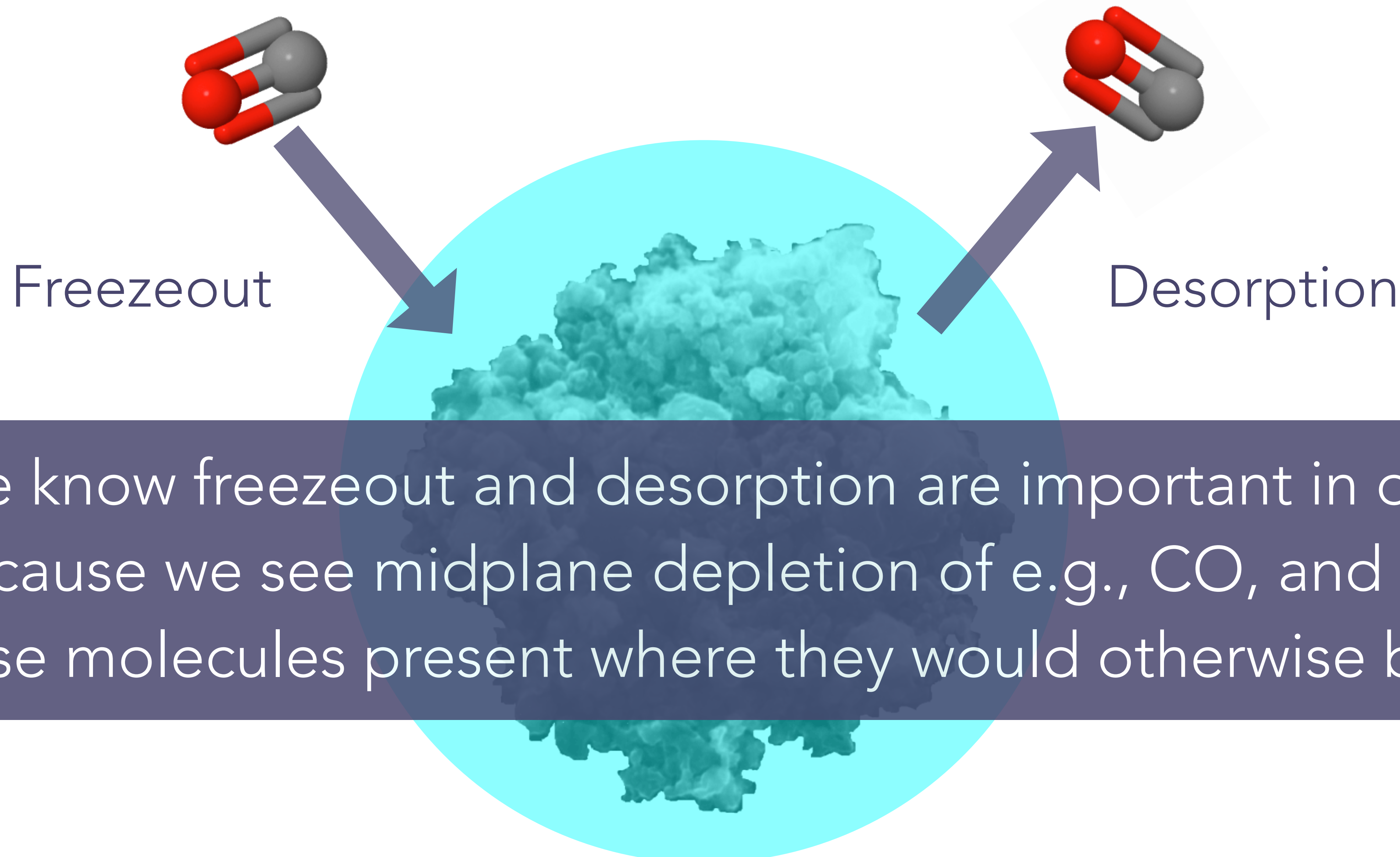


Dust grains act as a third body for association reactions

Herbst, E. & van Dishoeck, E. F. 2009, ARA&A, 47, 427; Hama, T. & Watanabe, N. 2013, Chem. Rev., 113, 8783; Cuppen, H., et al. 2016, Space Sci. Rev., in prep

Formation and destruction of molecules

Grain-surface processes



We know freezeout and desorption are important in disks because we see midplane depletion of e.g., CO, and gas-phase molecules present where they would otherwise be ice

Dust grains act as a third body for association reactions

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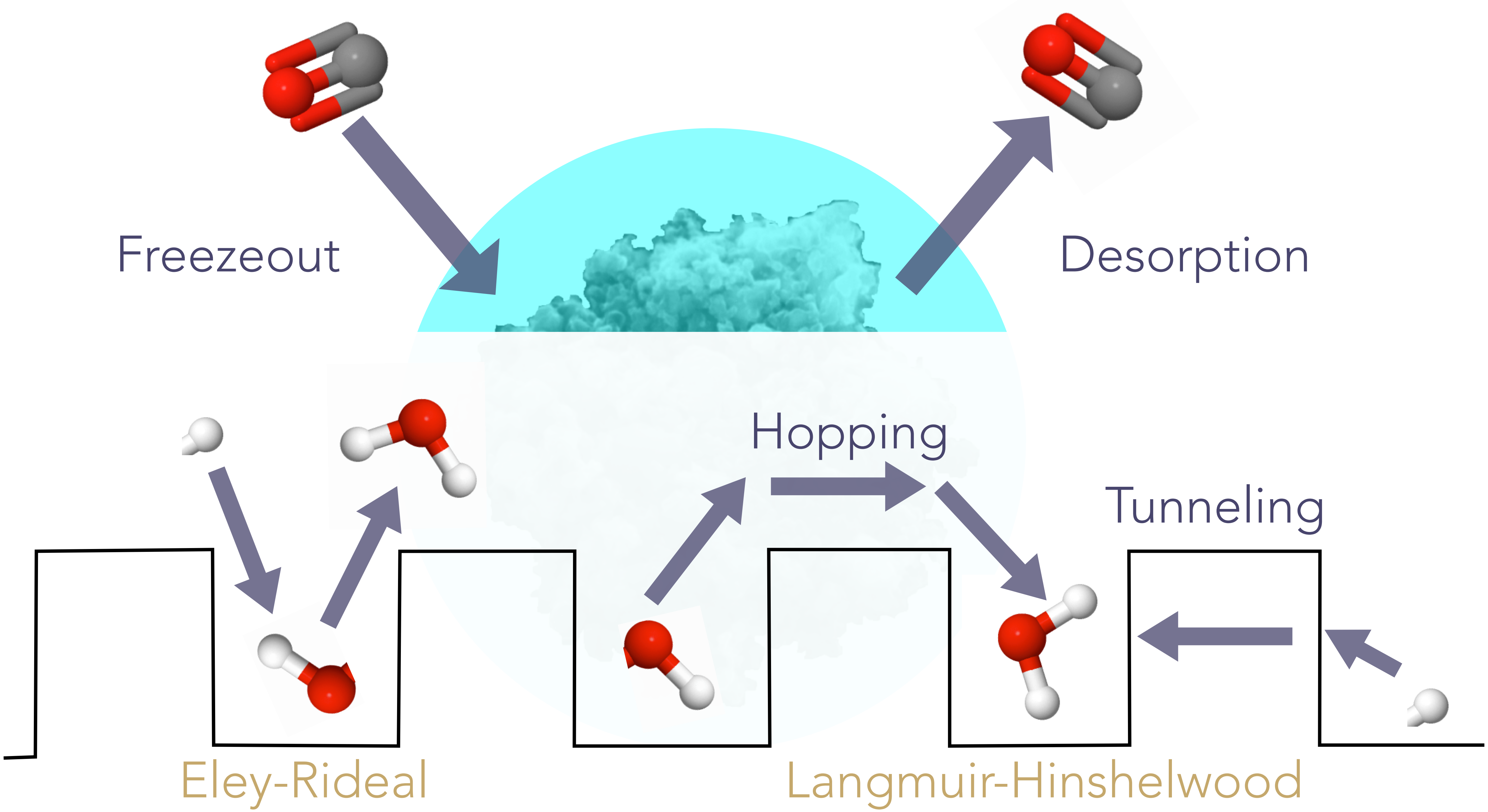
Formation and destruction of molecules

Grain-surface processes

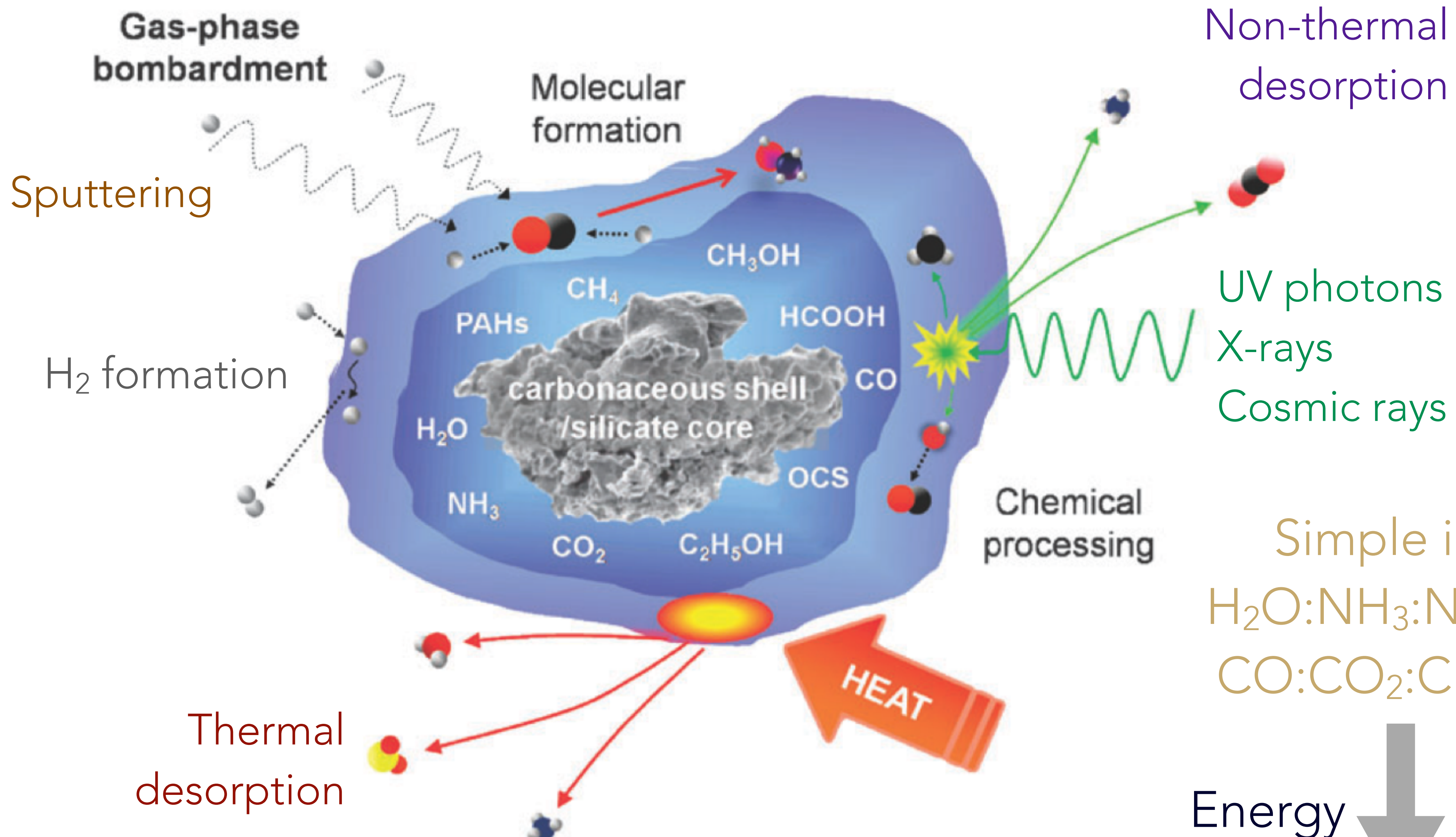


Dust grains act as a third body for association reactions

Herbst, E. & van Dishoeck, E. F. 2009, ARA&A, 47, 427; Hama, T. & Watanabe, N. 2013, Chem. Rev., 113, 8783; Cuppen, H., et al. 2016, Space Sci. Rev., in prep

Formation and destruction of molecules

Grain-surface processes



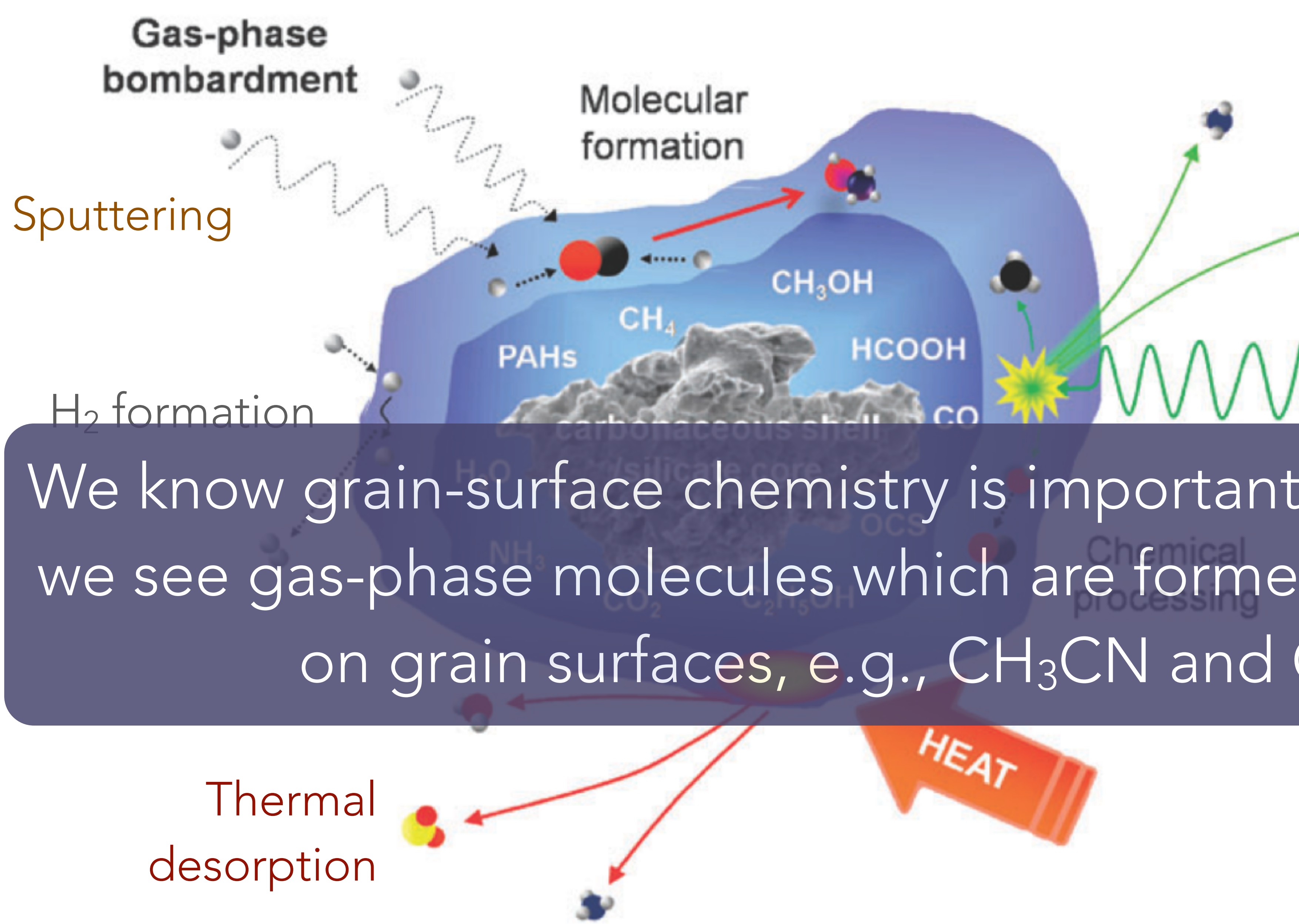
Simple ices
H_2O:NH_3:N_2:CH_4:
CO:CO_2:CH_3OH

Energy ↓ Heat

Complex molecules

Formation and destruction of molecules

Grain-surface processes



We know grain-surface chemistry is important in disks because we see gas-phase molecules which are formed partly or solely on grain surfaces, e.g., CH_3CN and CH_3OH

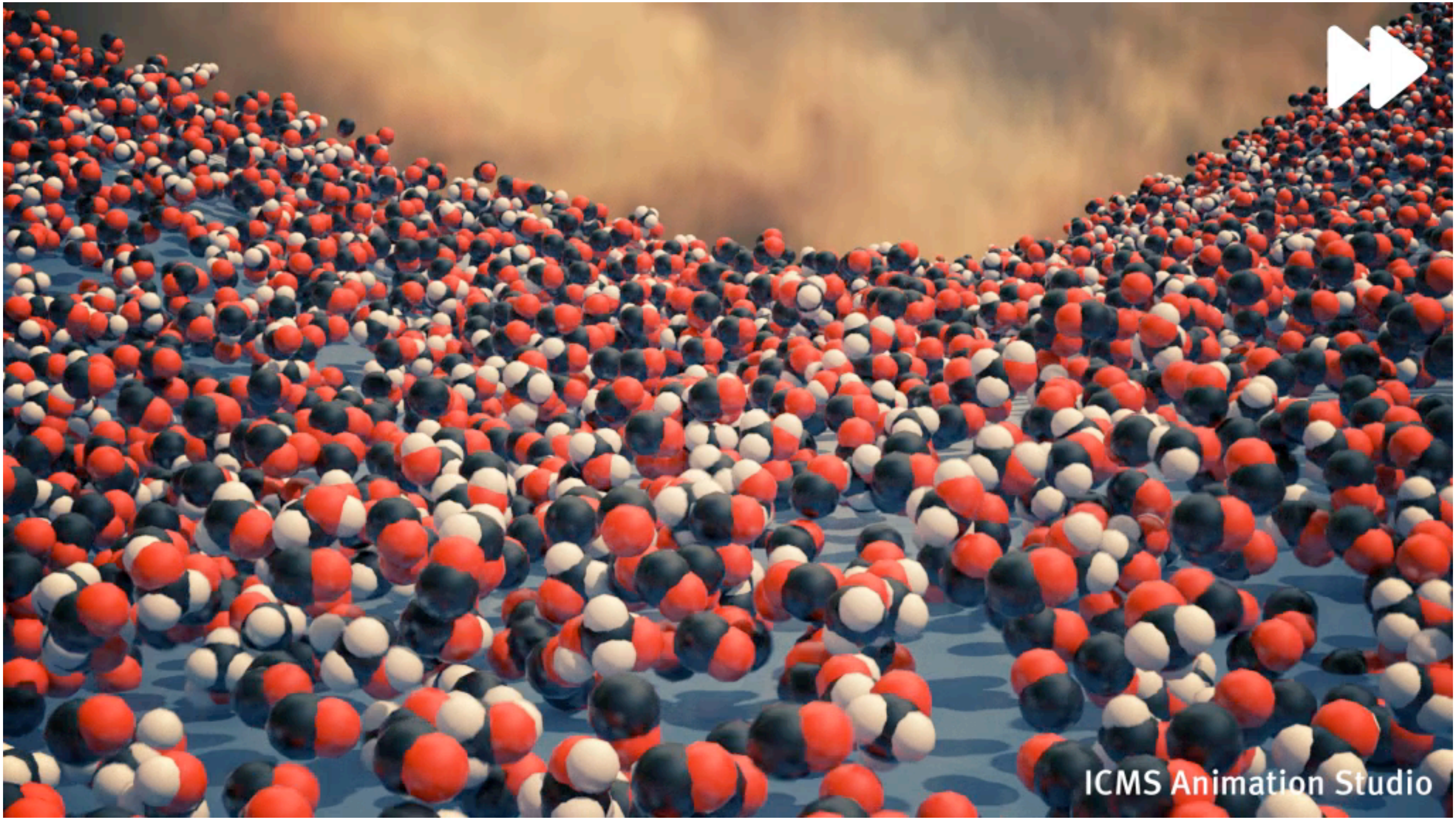
Simple ices
$H_2O:NH_3:N_2:CH_4:CO:CO_2:CH_3OH$

Energy ↓ Heat

Complex molecules

Grain-surface chemistry increases complexity

Grain-surface chemistry increases complexity



Fuchs, G., et al. 2009, A&A, 505, 629; Oberg, K. I., et al. 2009, ApJ, 504, 891; Fedoseev, G., et al. 2015, MNRAS, 448, 1288

Calculating the chemistry

Molecular abundances are a function of disk conditions and time

$$n_{\mathrm{X}} = F\left[T_{\mathrm{gas}}, T_{\mathrm{dust}}, n_{\mathrm{gas}}, F_{\mathrm{UV}}(\lambda), F_{\mathrm{XR}}(E_{\mathrm{XR}}), \zeta_{\mathrm{CR}}, \sigma_{\mathrm{dust}}\right]$$

$$\frac{dn_{\mathrm{X}}}{dt} = \mathrm{F_X} - \mathrm{D_X}$$

$$\frac{dn_{\mathrm{X}}}{ds} = \mathrm{F_X} - \mathrm{D_X}$$

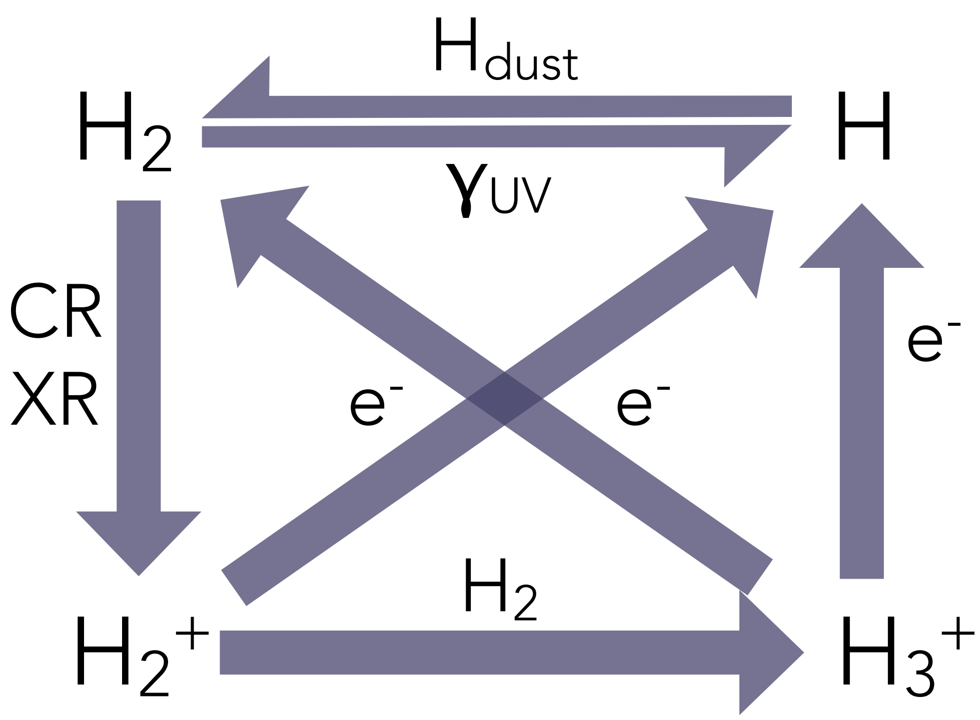
$$s = (r, z) \quad \text{or} \quad (\rho, \phi, z)$$

Chemistry in disks is not in equilibrium: steady state is possible

A "simple" chemical network: H_2

Dense gas:
Av ≫ 1 mag

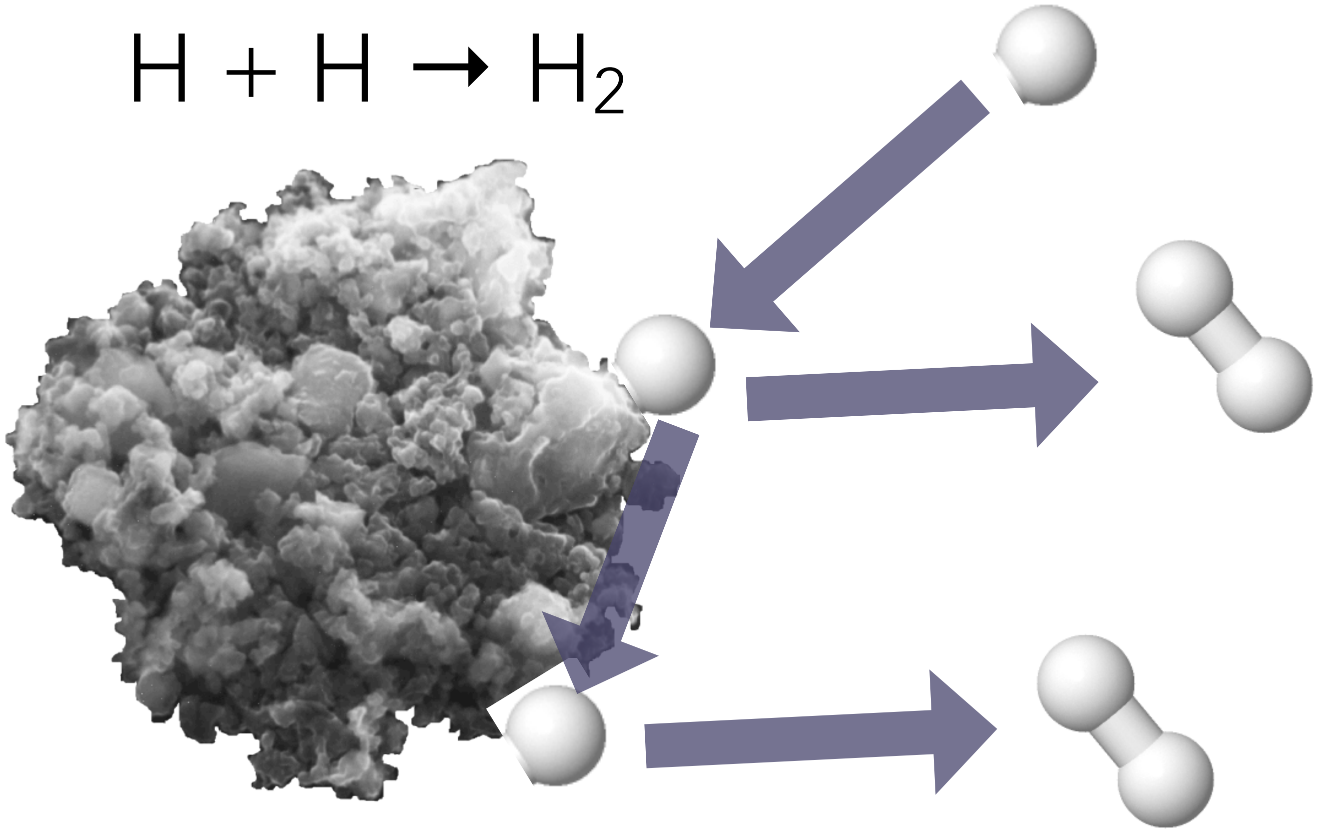
$$H_2 + CR/XR \rightarrow H_2^+ + e^-$$



Irradiated gas:
Av < 1 mag

$$H_2 + \gamma_{UV} \rightarrow H + H$$

$$H + H \rightarrow H_2$$



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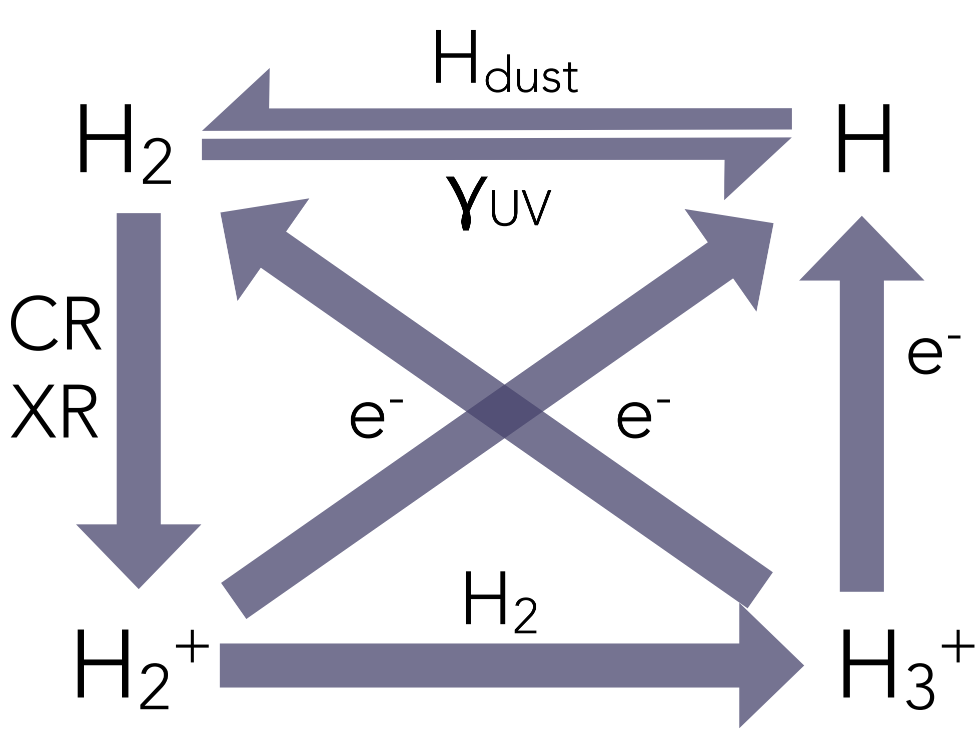
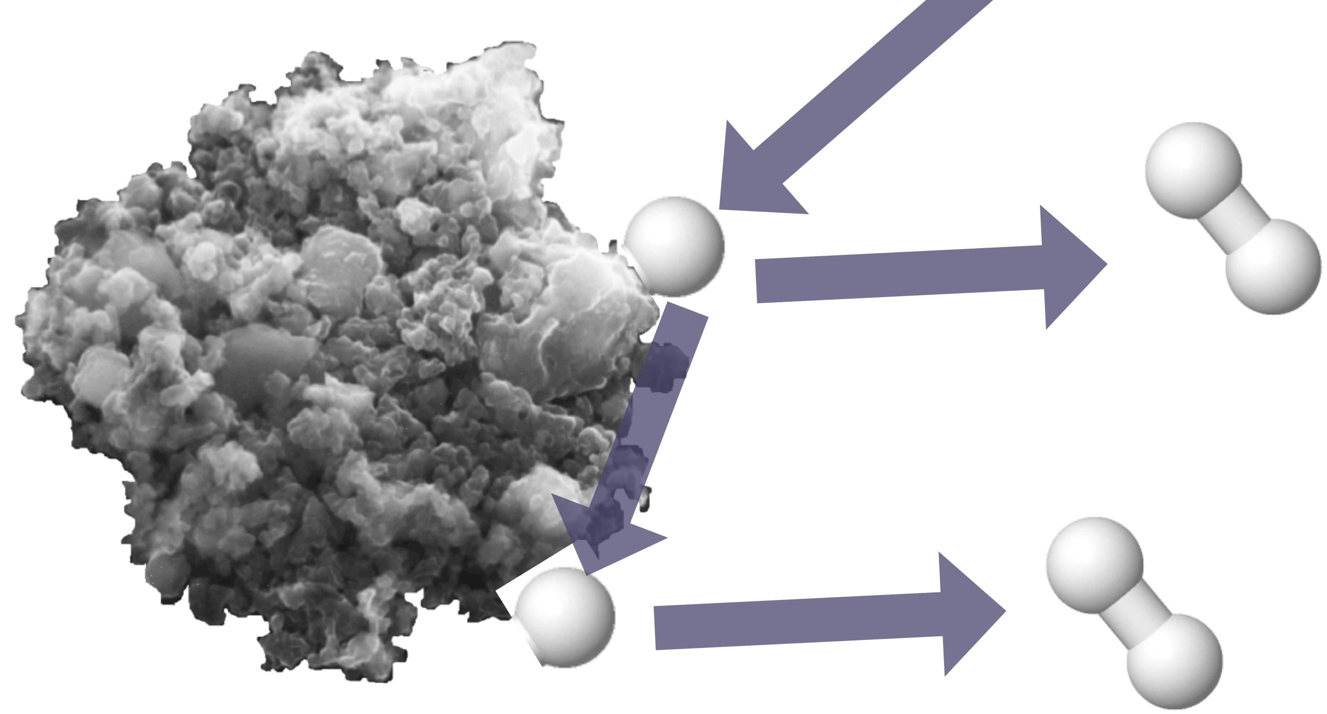
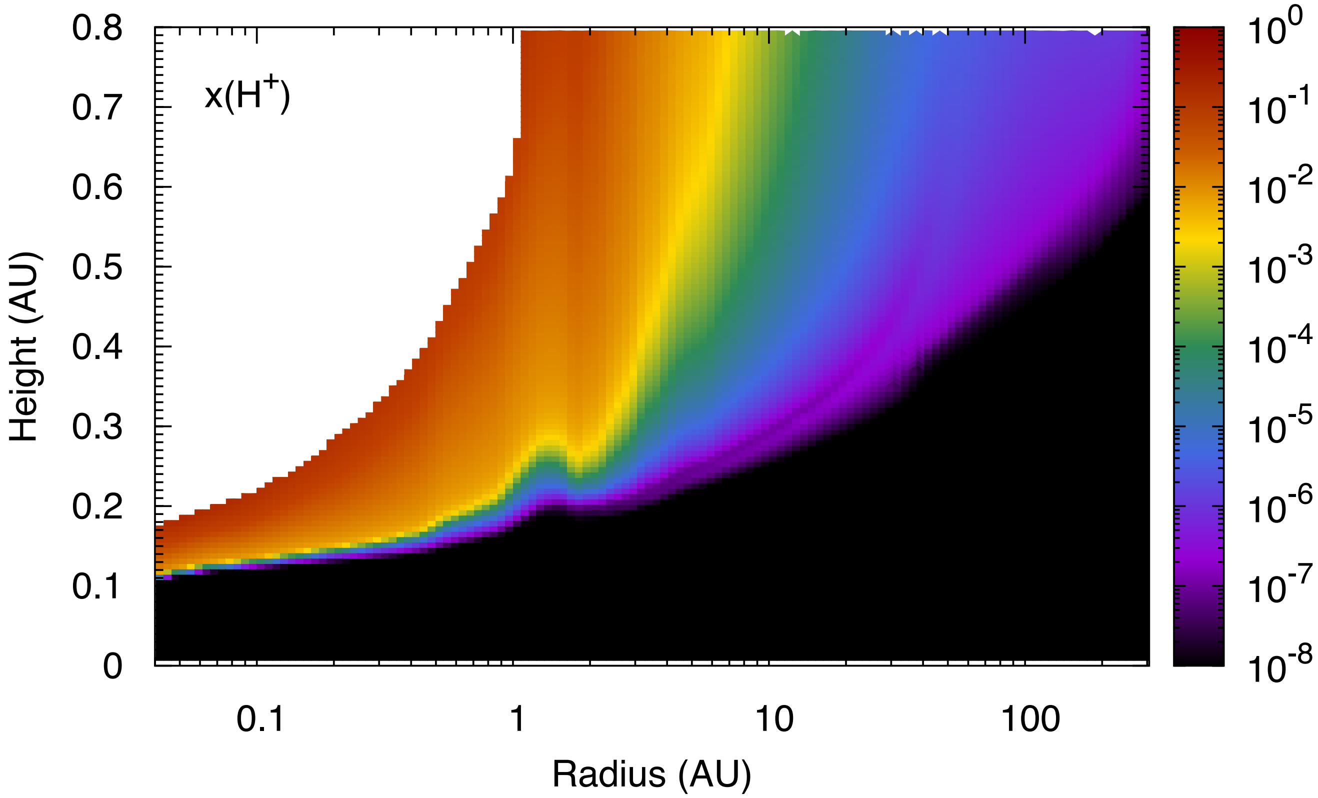


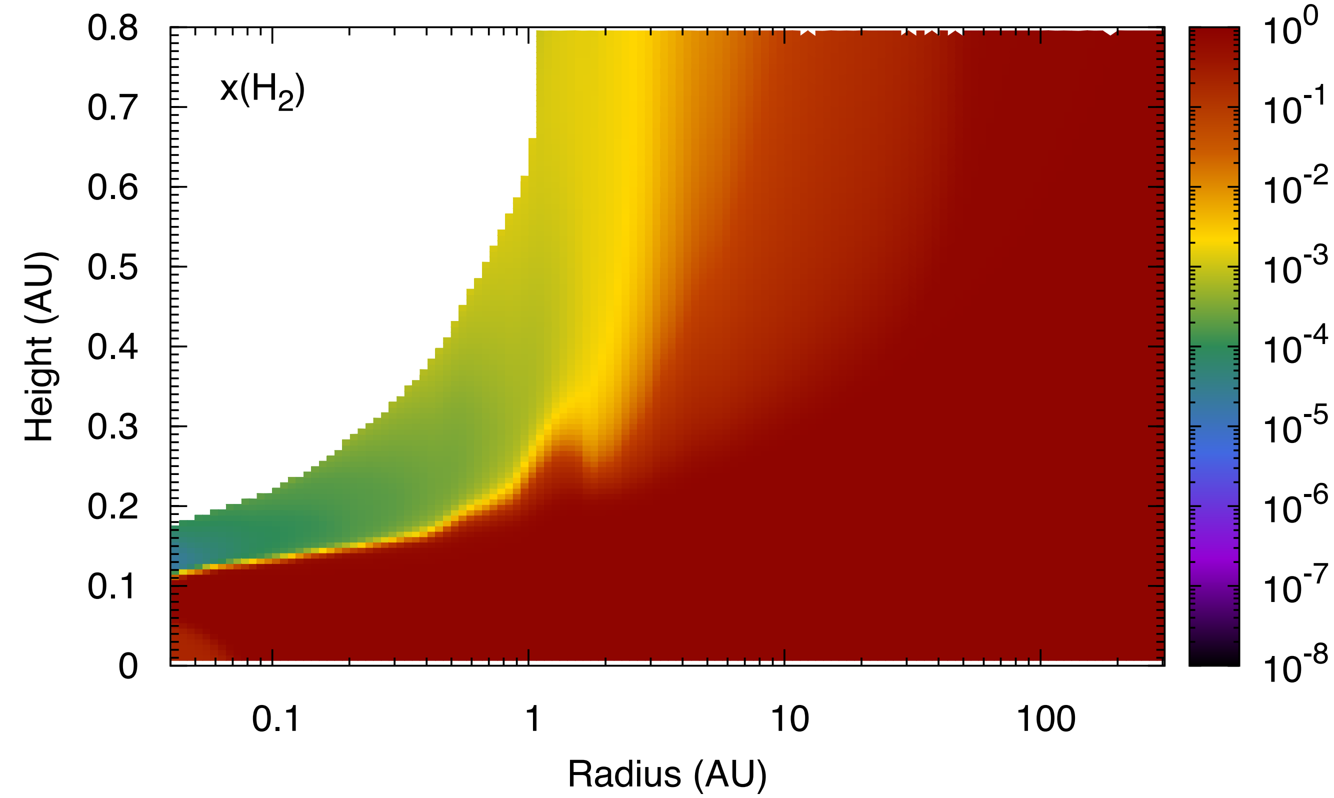
$$H + H \rightarrow H_2$$

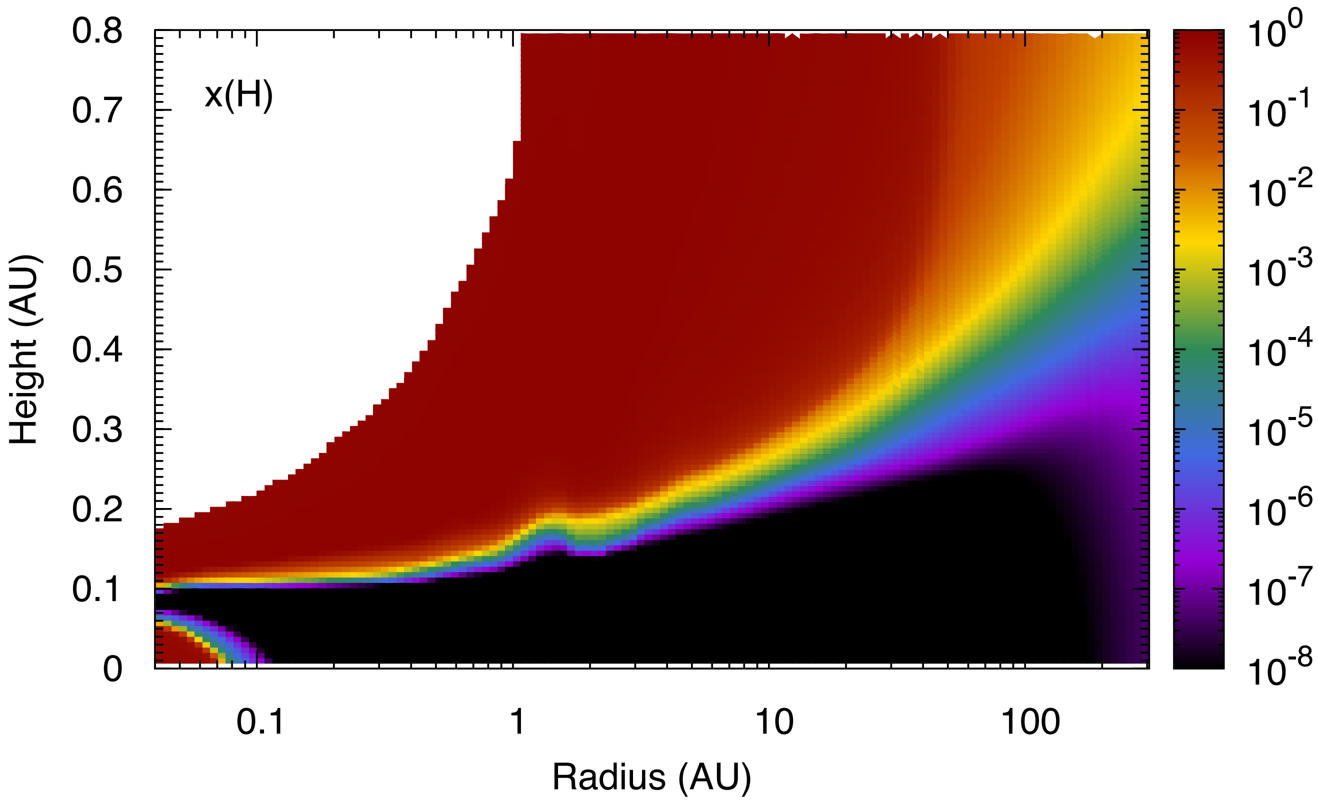


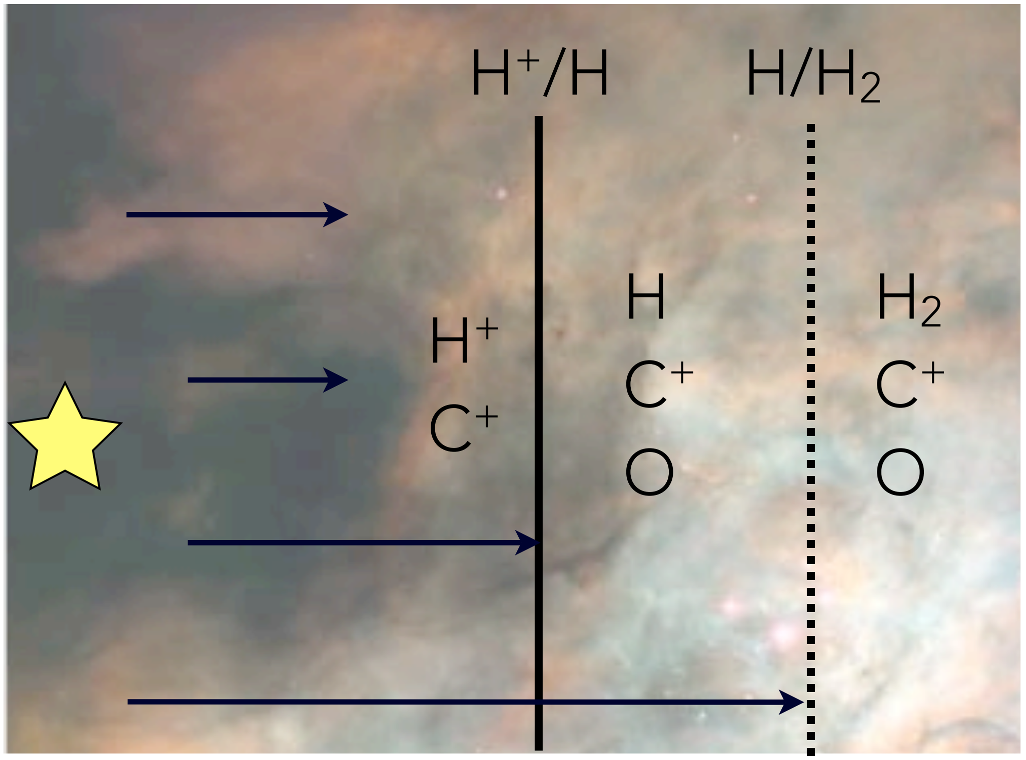
H_2 forms almost exclusively on dust grains

$H^+/H/H_2$ in protoplanetary disks









Nomura, H., et al. 2007, ApJ, 661, 334; Walsh, C., et al. 2012, ApJ, 747, 114

$H^+/H/H_2$ in protoplanetary disks

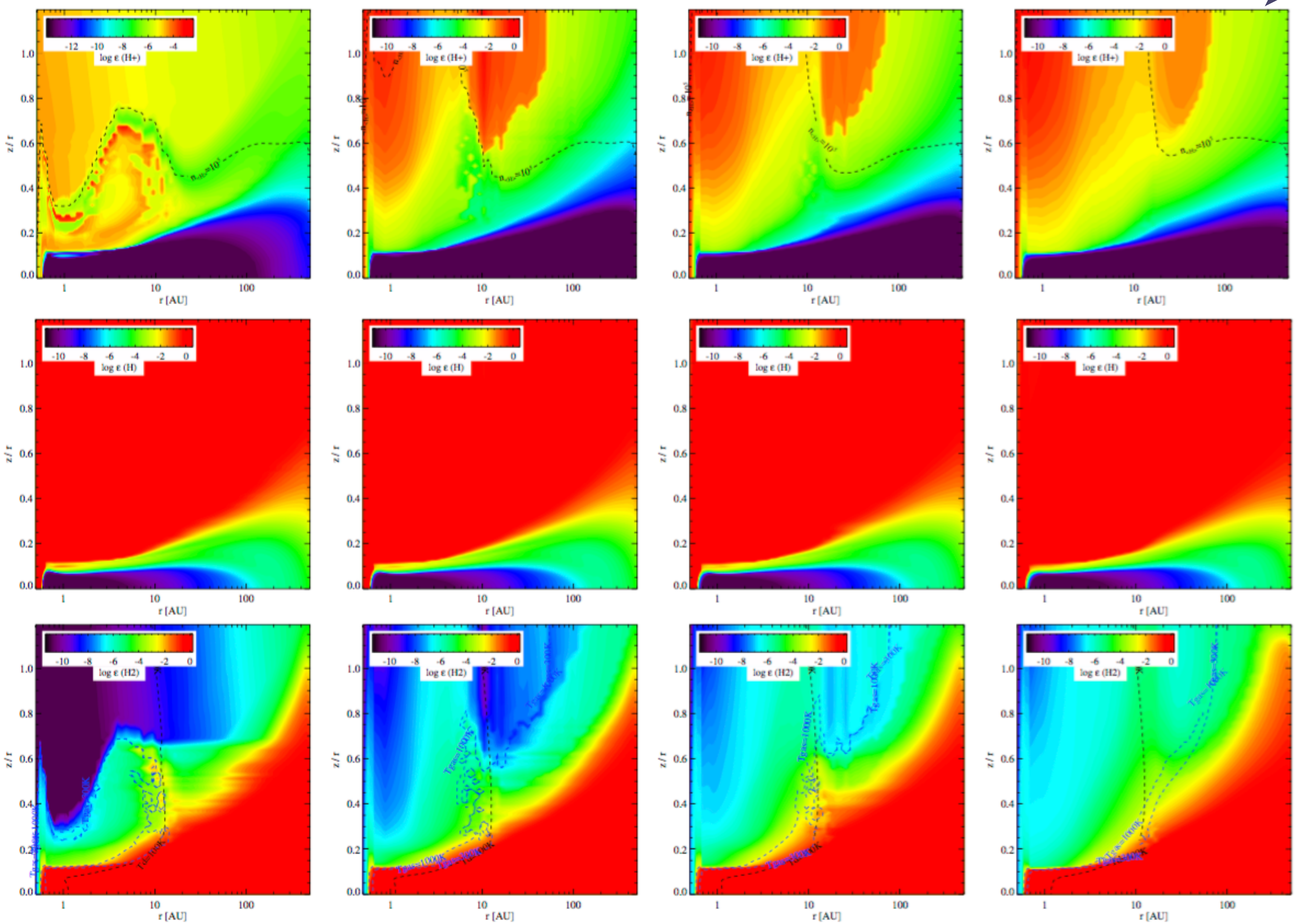
X-rays also influence the $H^+/H/H_2$ transition regions

Increasing X-ray luminosity →

H^+

H

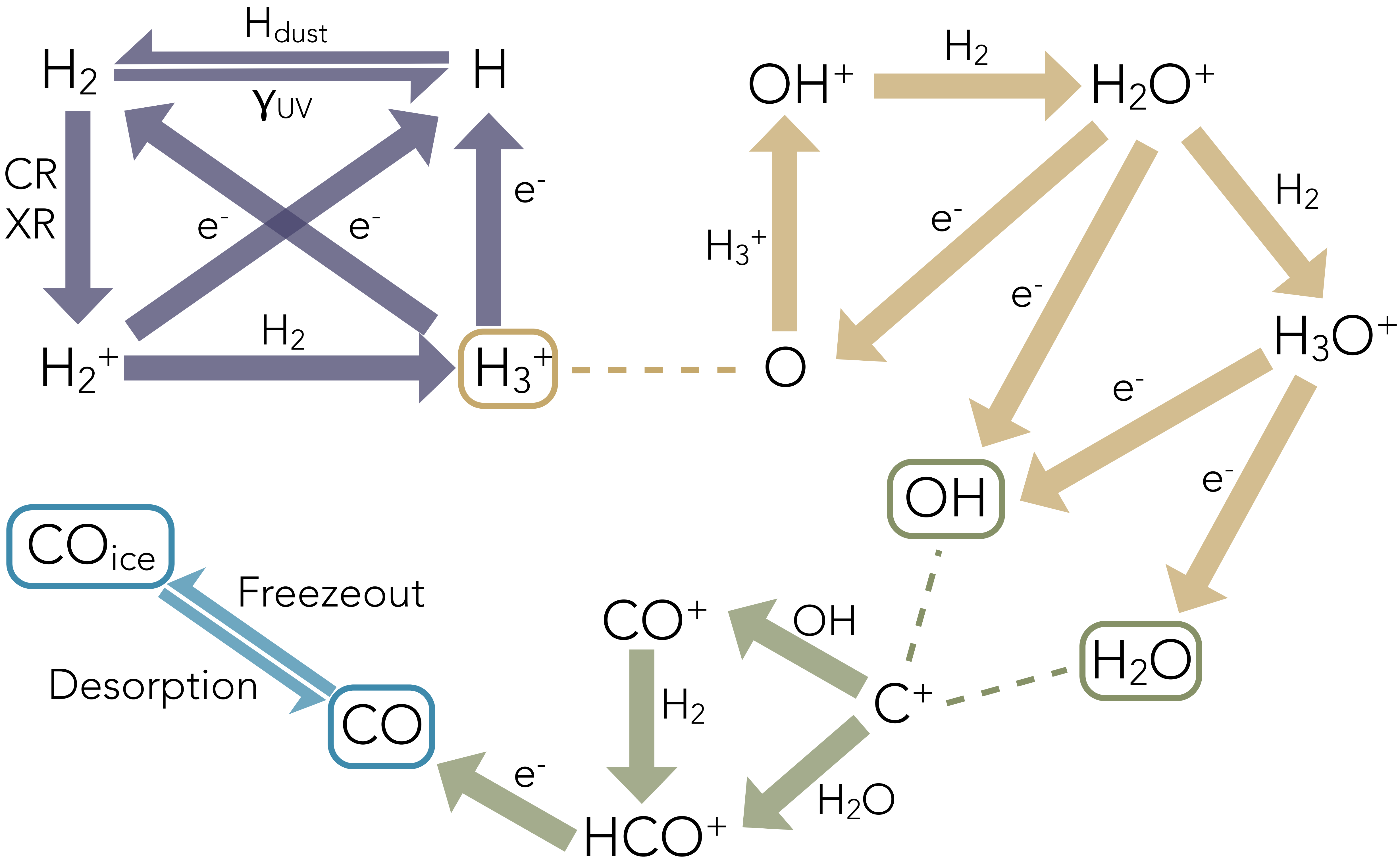
H_2



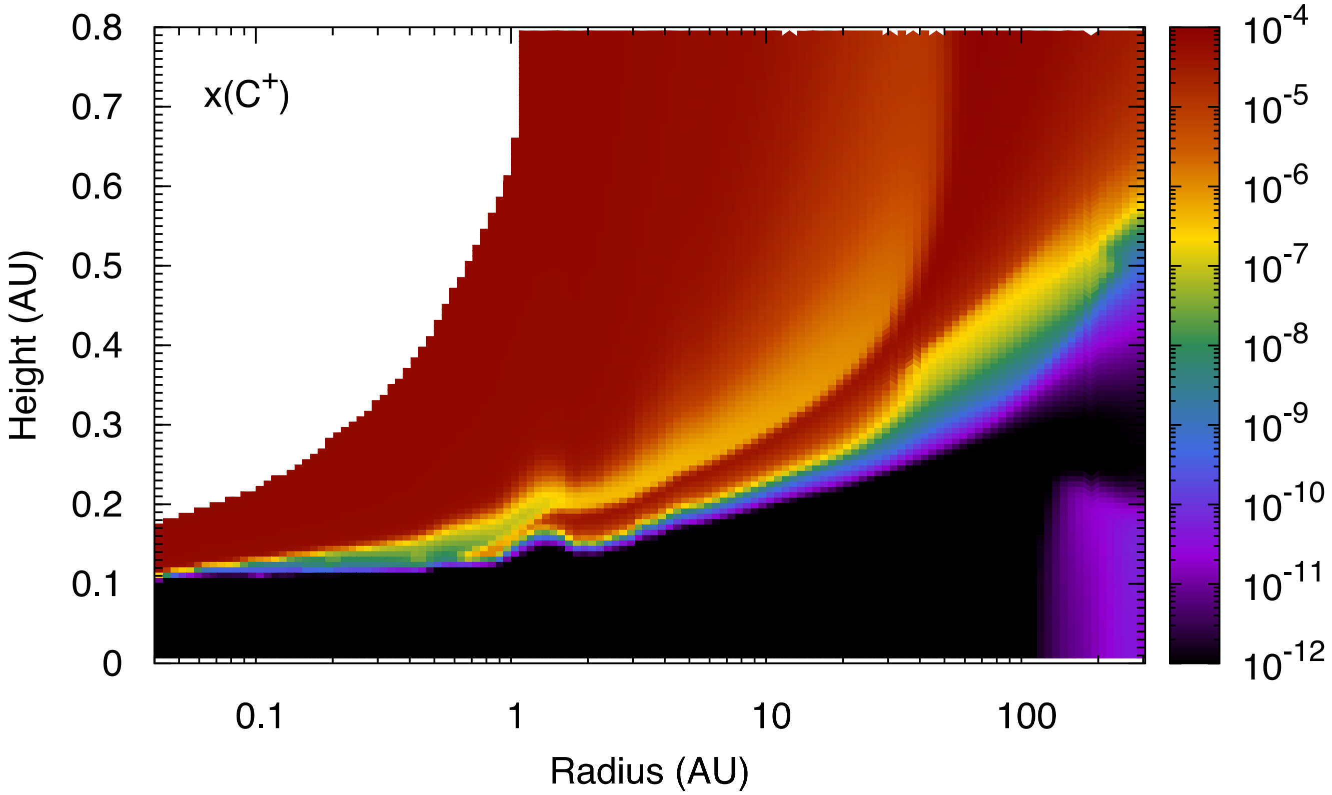
Increase in H^+

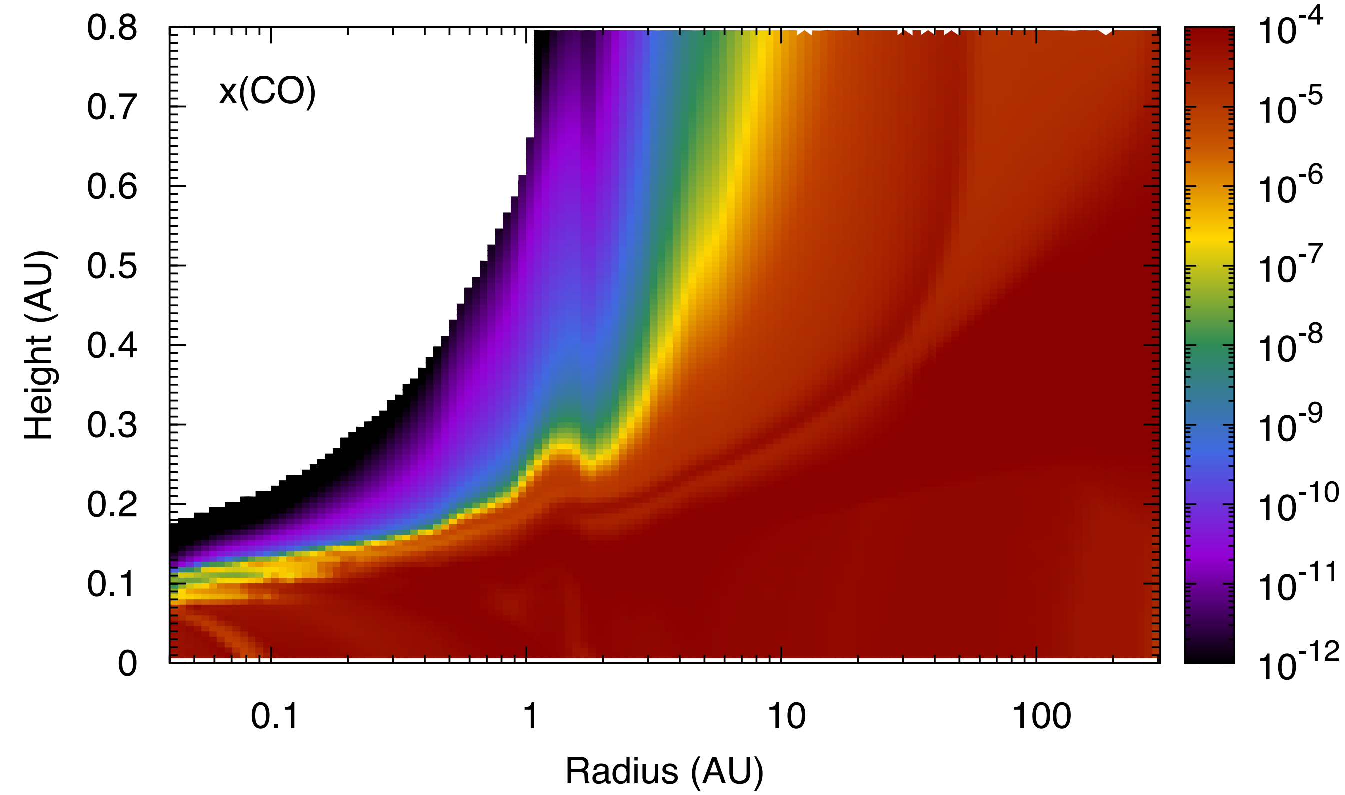
Increase in H_2

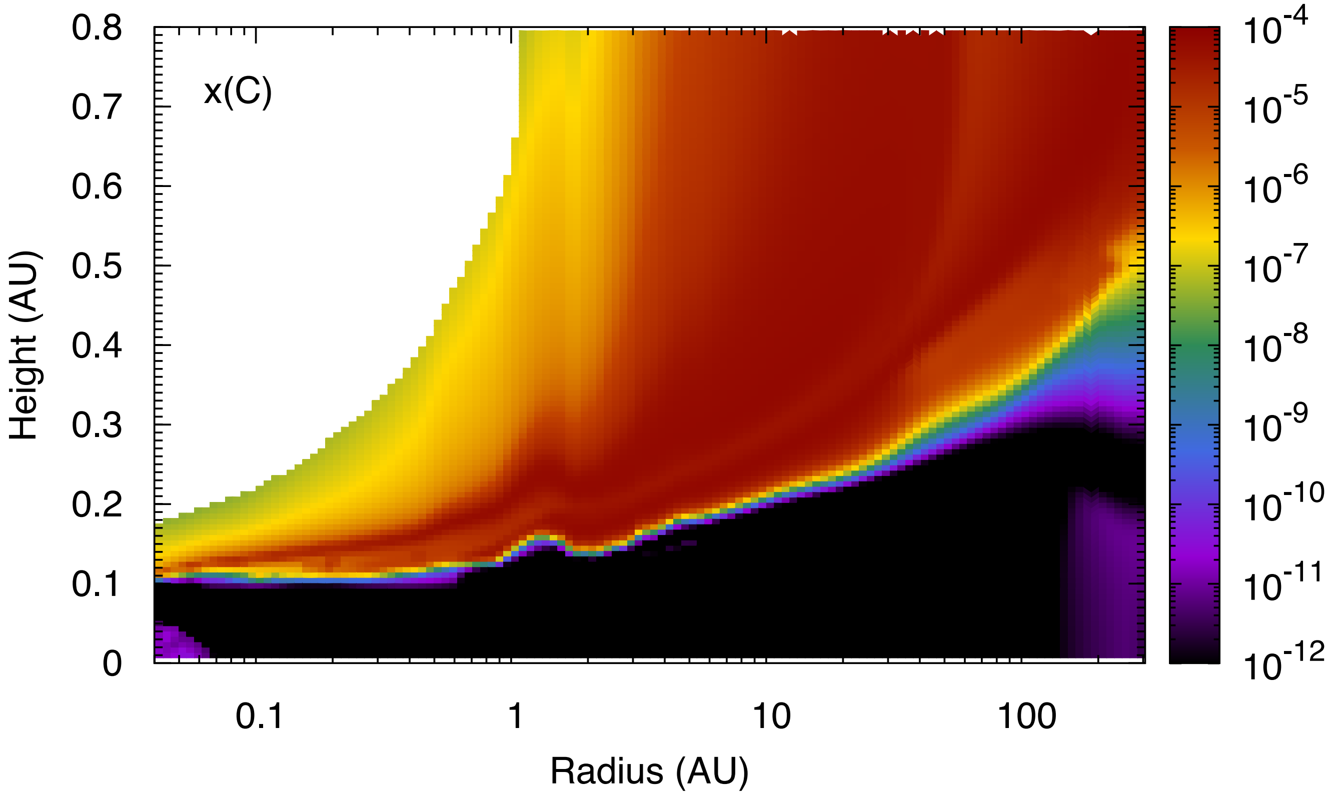
A more complicated network: CO

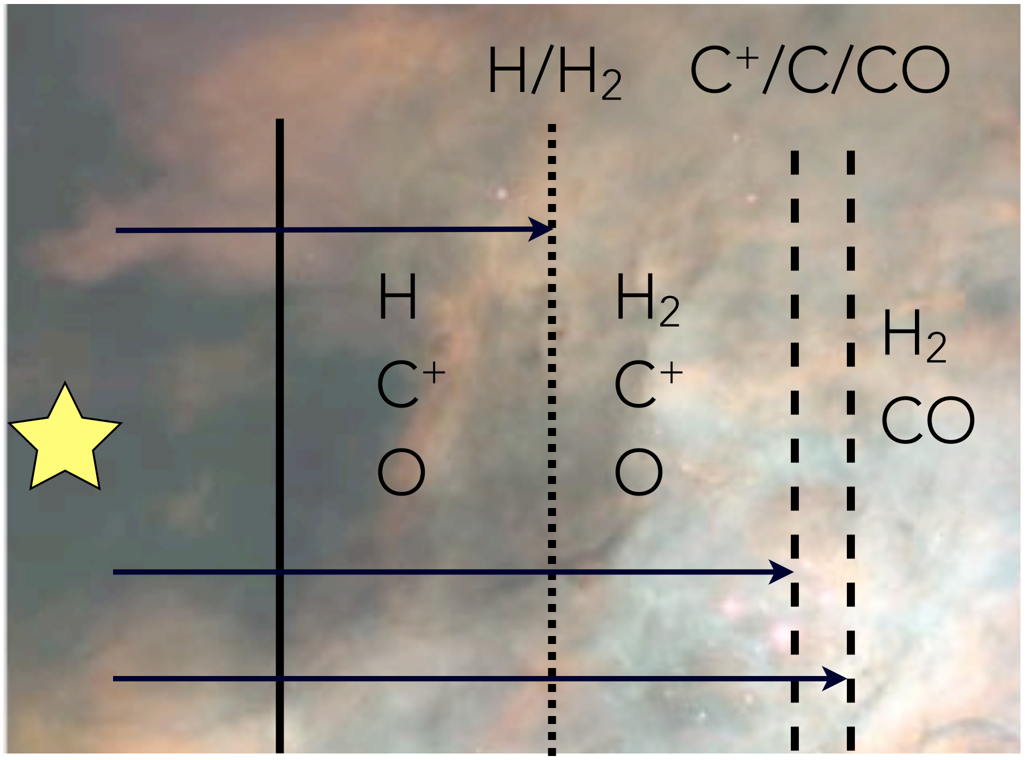


$C^+/C/CO$ in protoplanetary disks



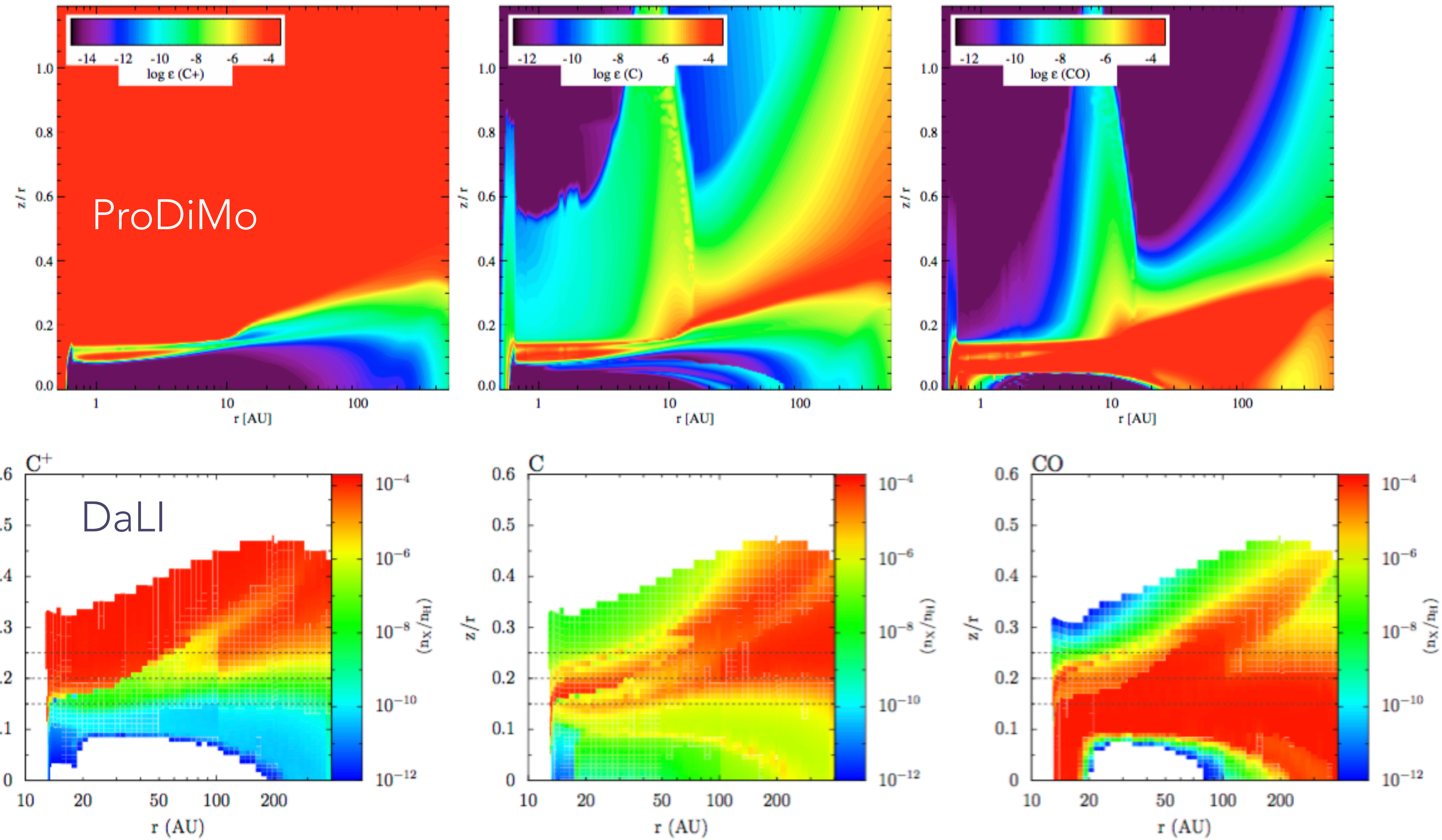






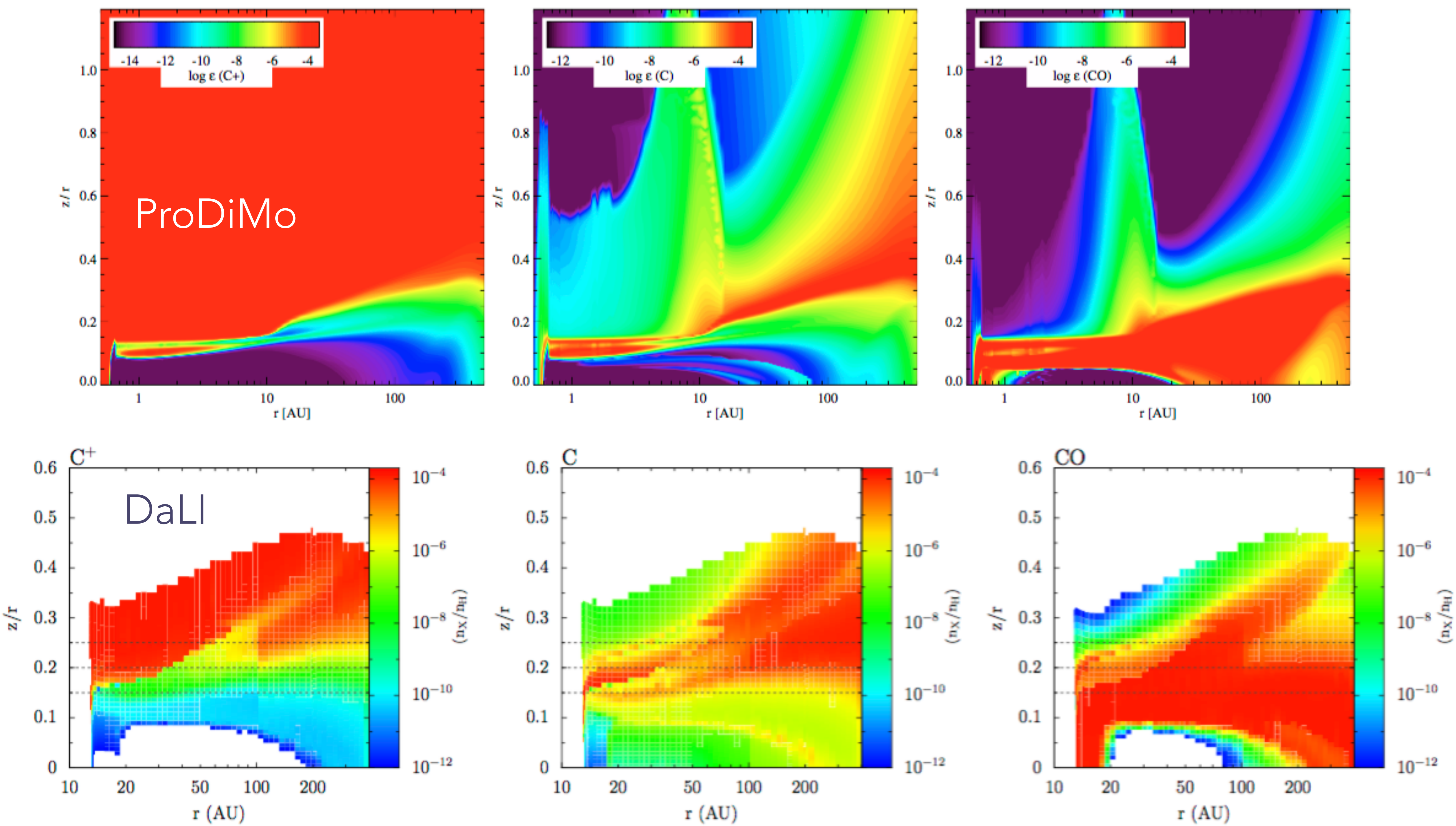
Nomura, H., et al. 2007, ApJ, 661, 334; Walsh, C., et al. 2012, ApJ, 747, 114

C^+/C/CO in protoplanetary disks



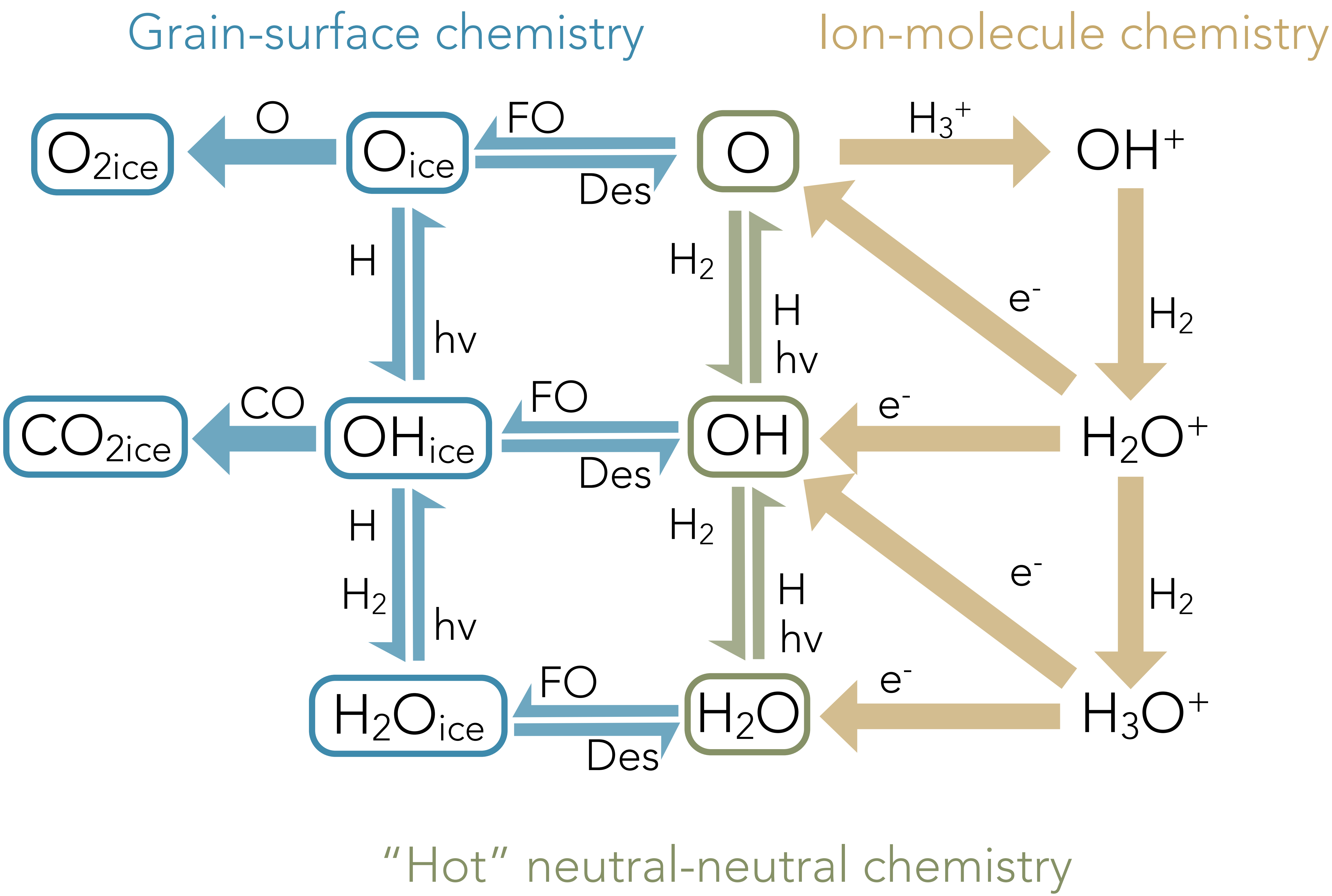
C^+/C/CO in protoplanetary disks

Similar stratification is seen in numerous physico-chemical models



Woitke, P., et al. 2009, A&A, 501, 383; Bruderer, S., et al. 2012, A&A, 541, 91

An even more complicated network: H_2O

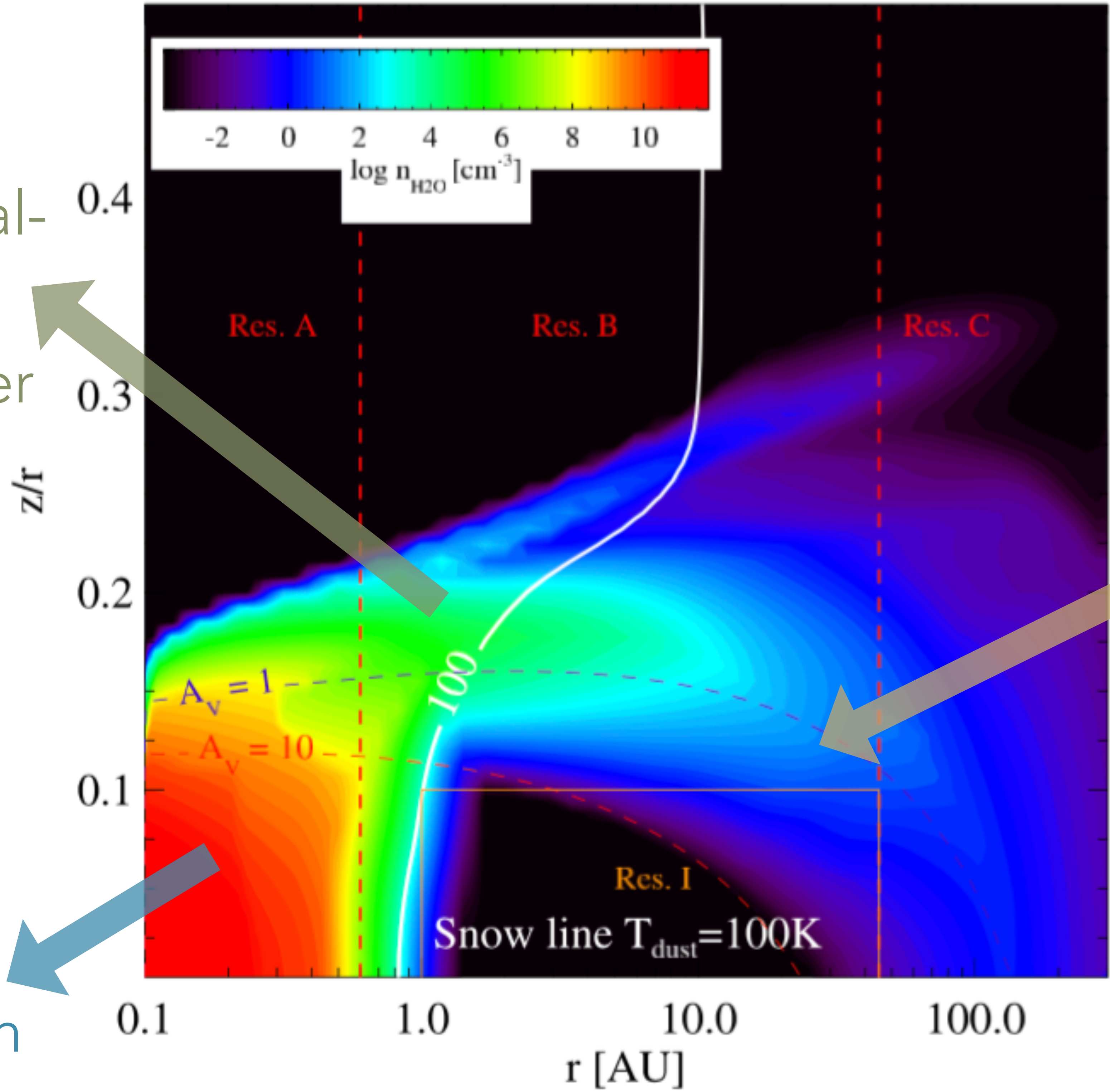


Water in protoplanetary disks

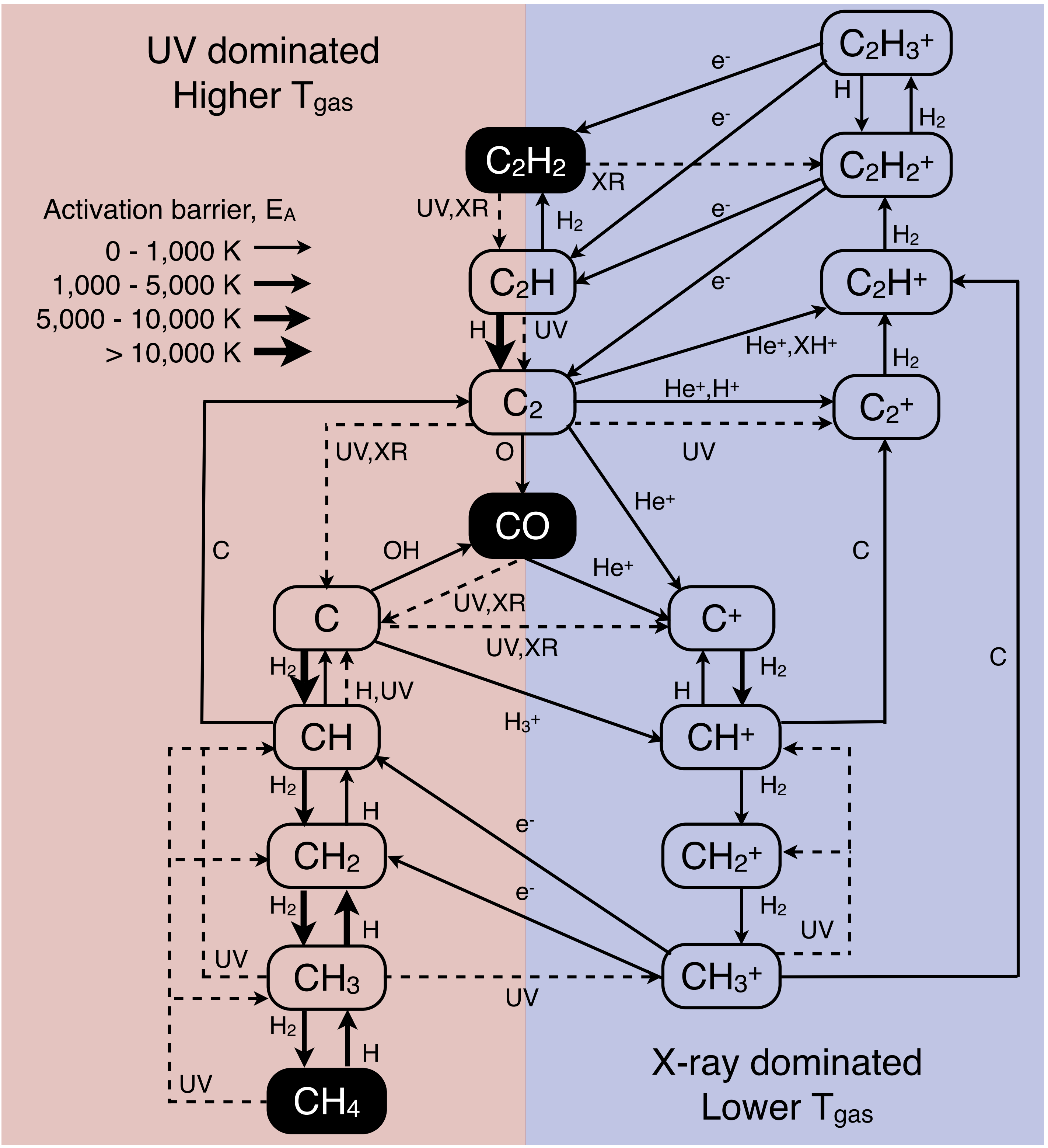
“Hot” neutral-neutral formed water

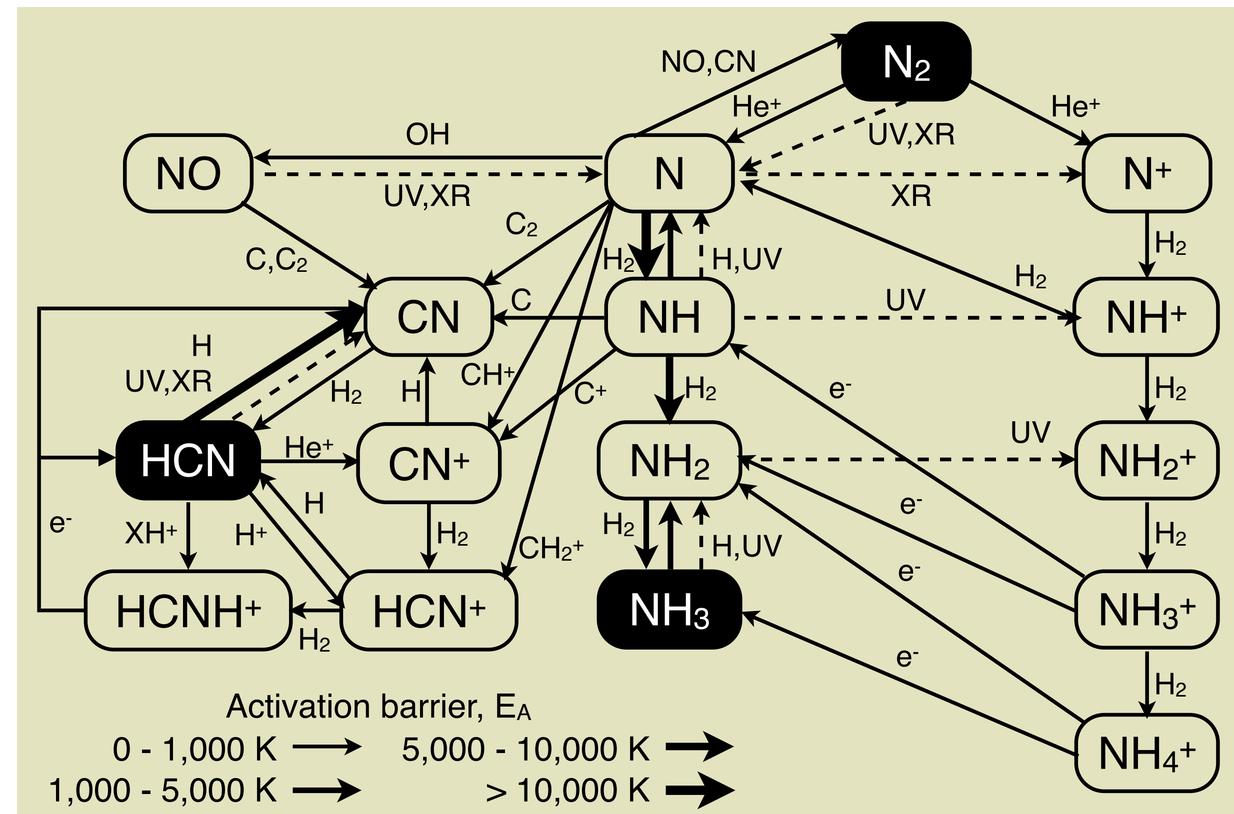
“Cold” ion-molecule/ photo-desorbed water

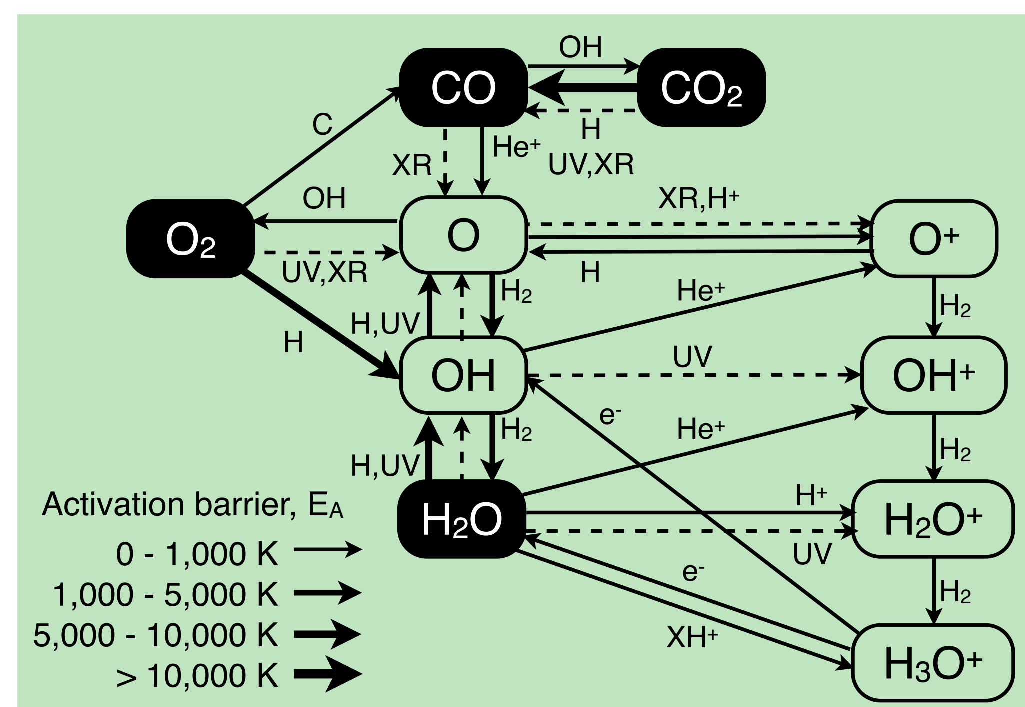
Thermal desorption



Networks can quickly become complicated!

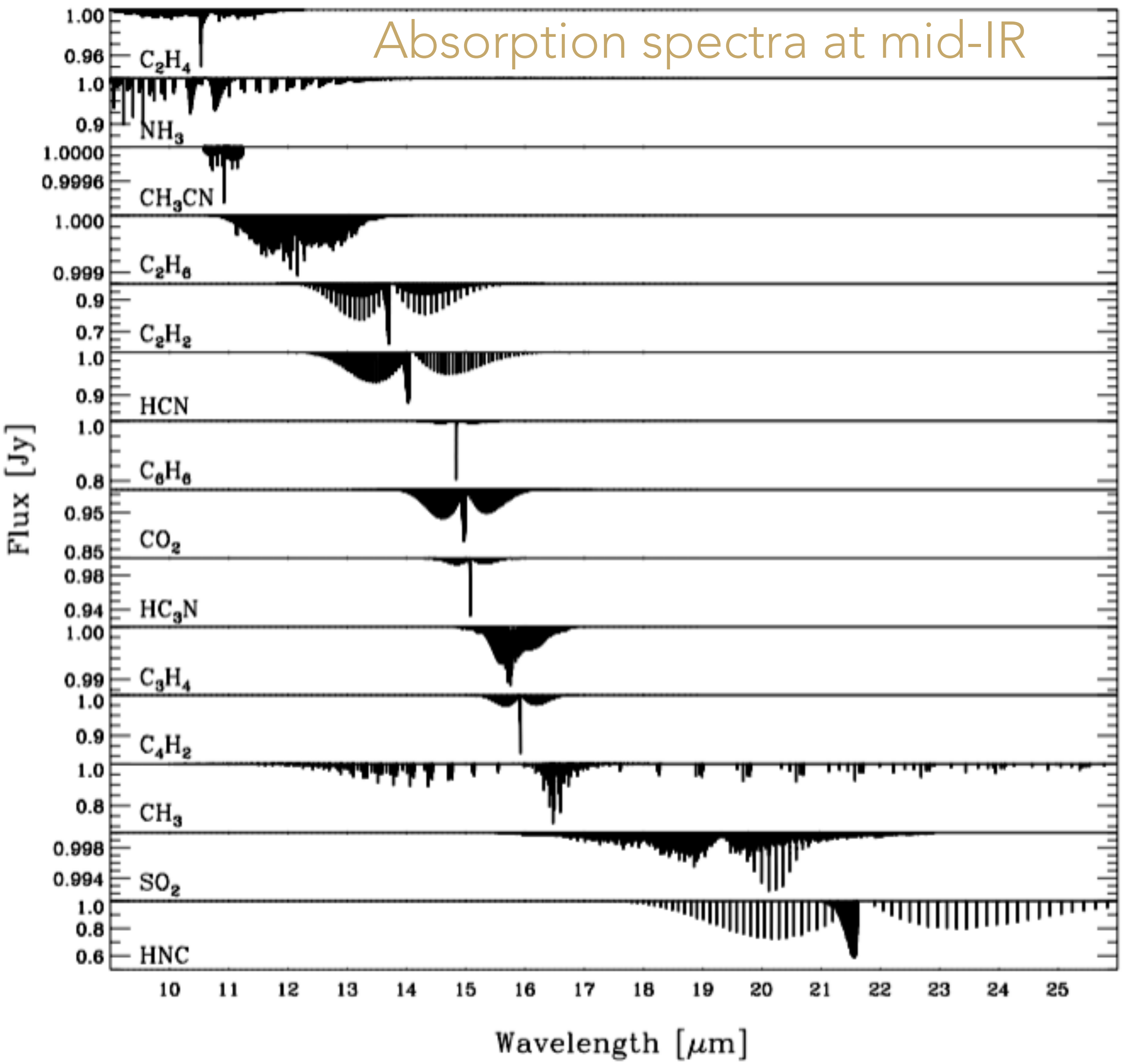


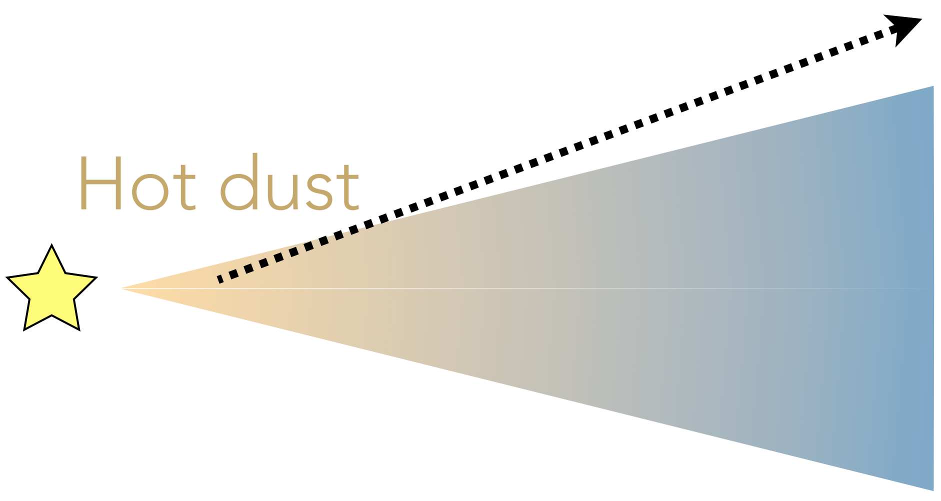




Walsh, C. et al. 2015, A&A, 582, A88

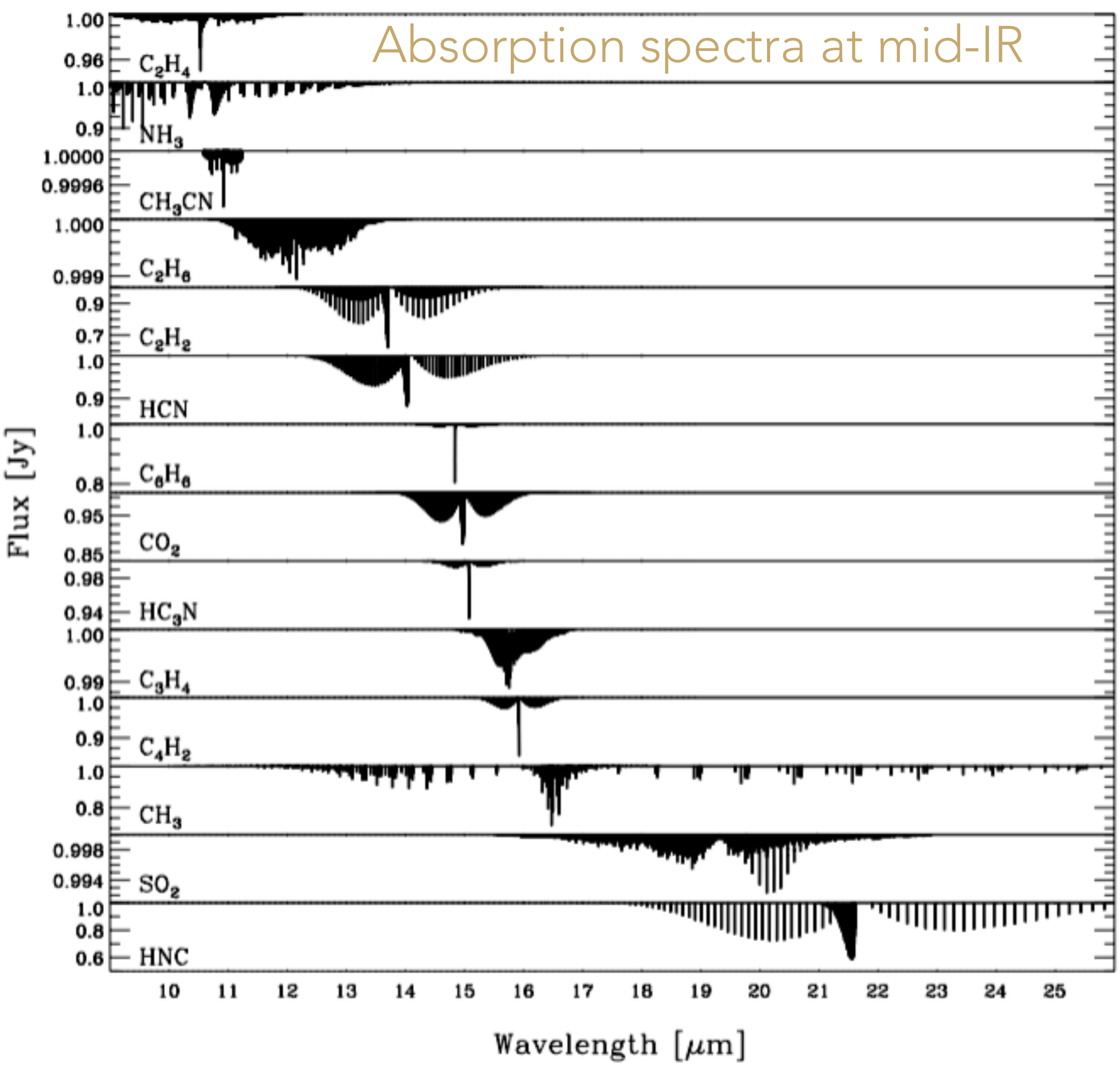
Creating synthetic observations



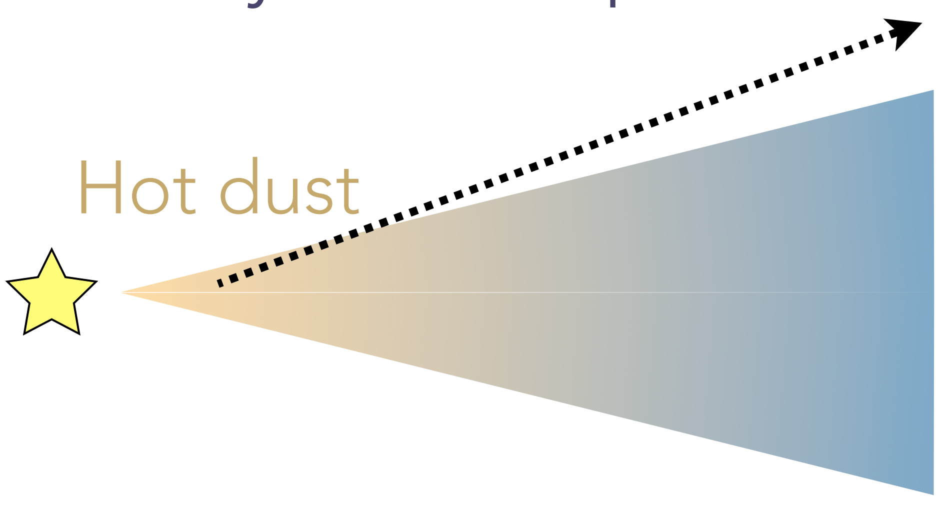


Bast, J., et al. 2013, A&A, 551, 118

Creating synthetic observations

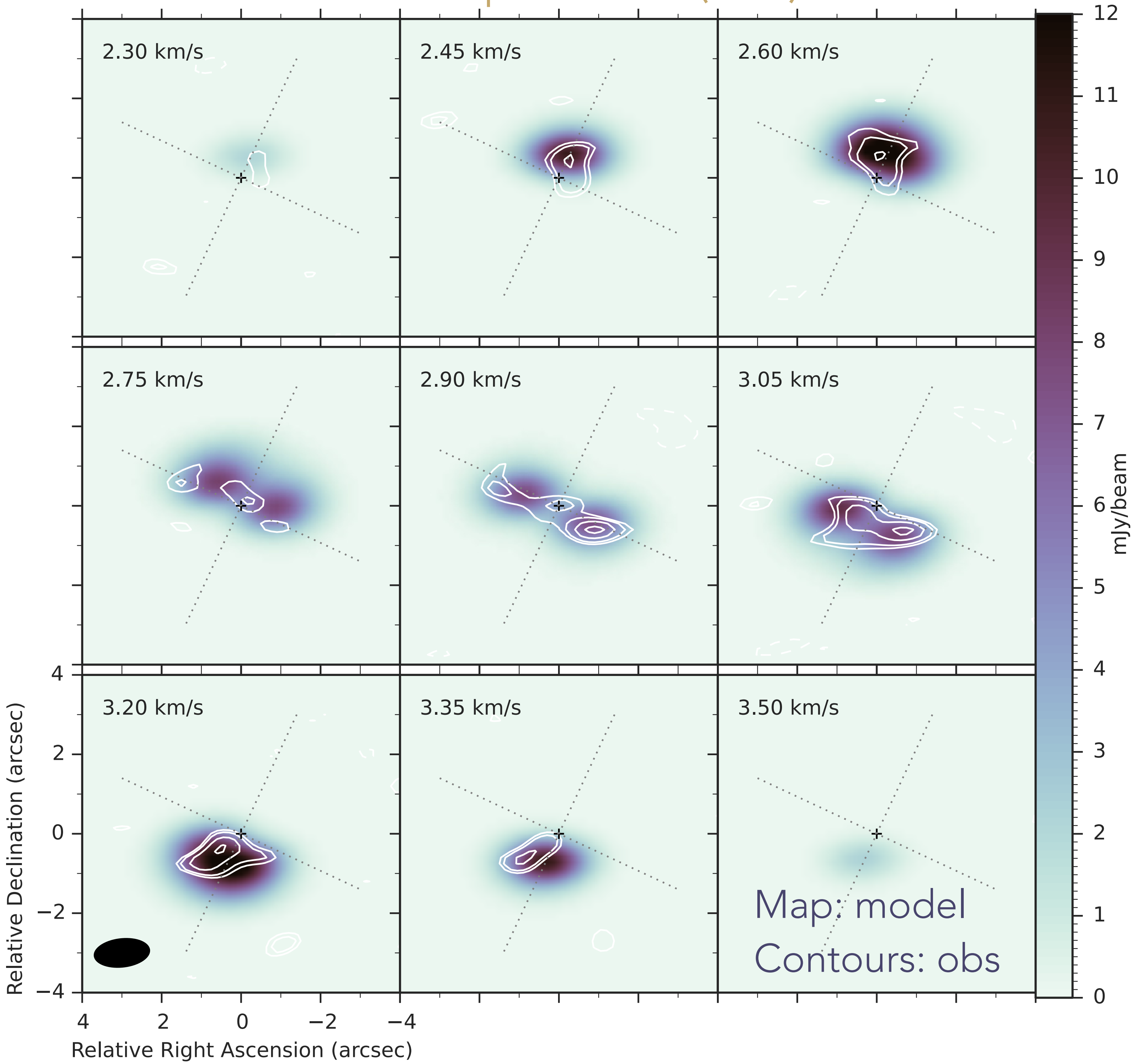


Radiative transfer codes (dust continuum and lines) are used along with molecular data to create synthetic spectra

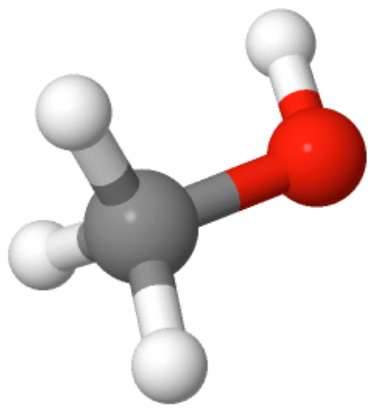


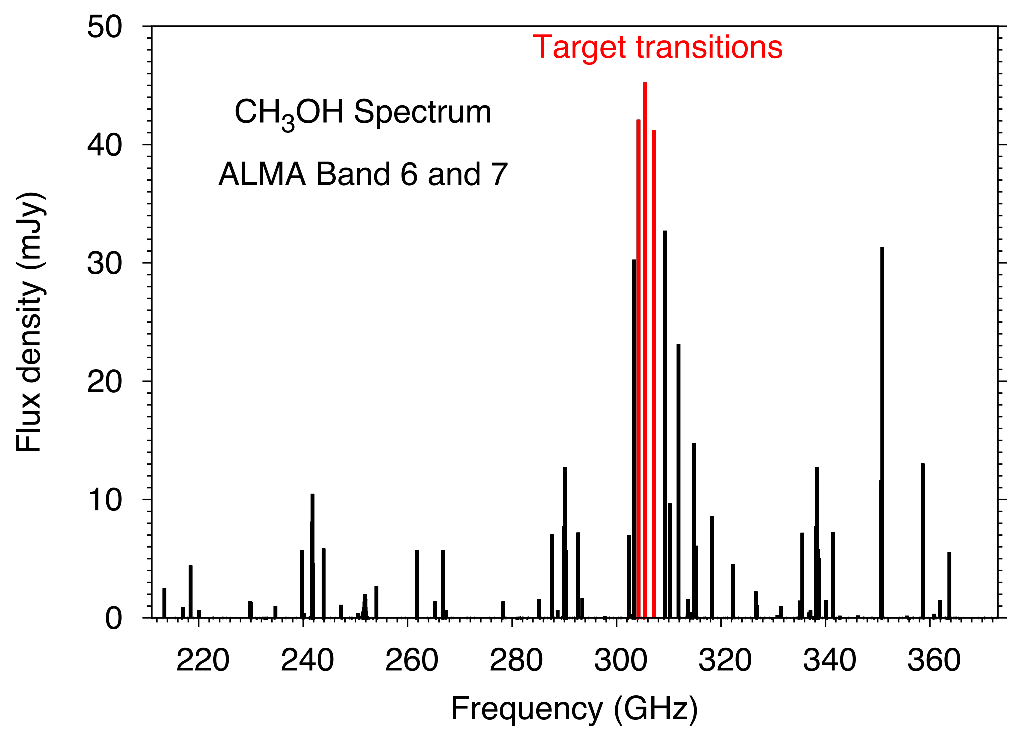
Creating synthetic observations

Emission spectra at (sub)mm



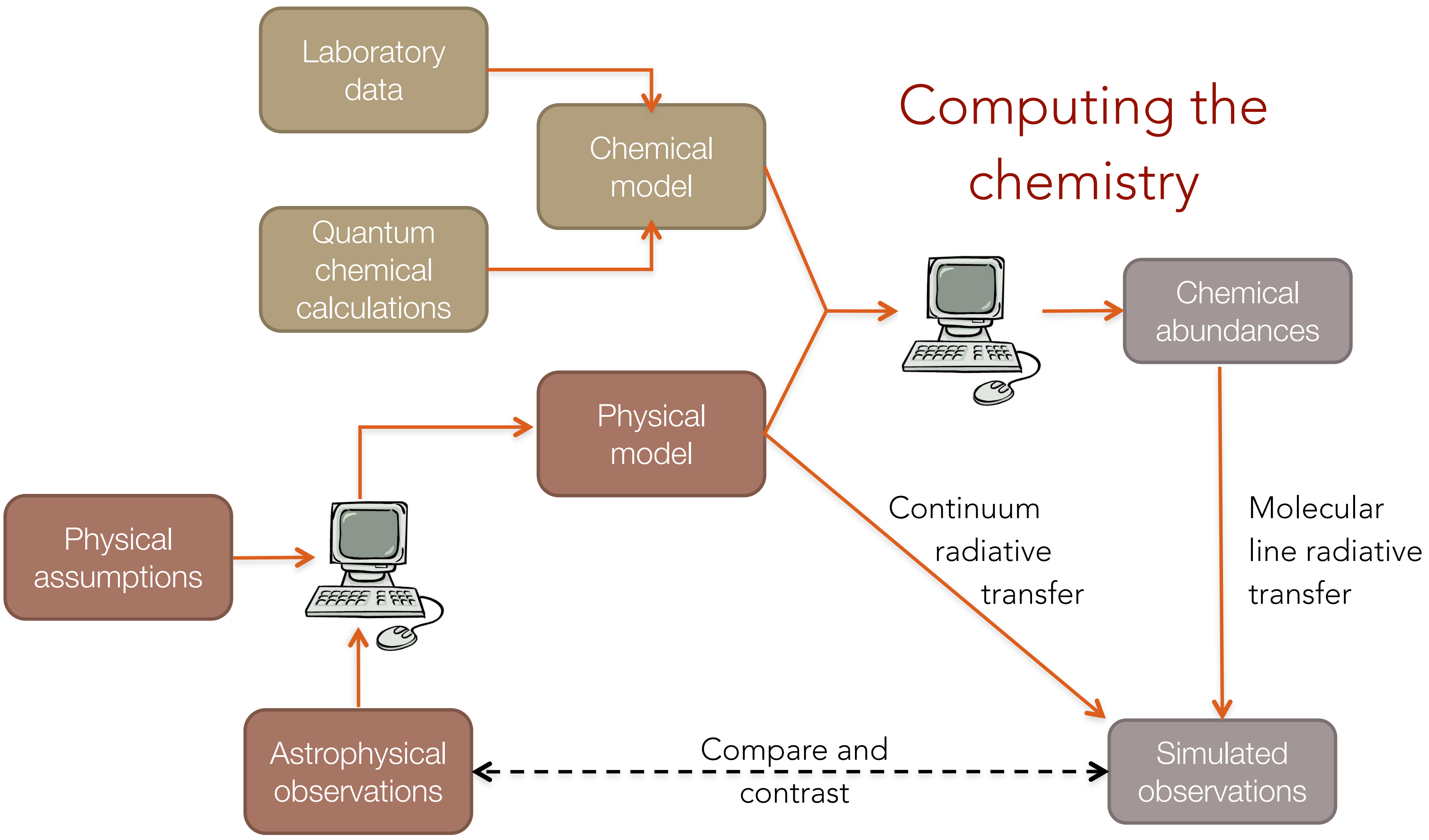
First detection of methanol (CH_3OH) in the disk around TW Hya





Walsh, C., et al. 2014, A&A, 2014; Walsh, C., et al. 2016, ApJ, 2016

General outline of a physico-chemical model



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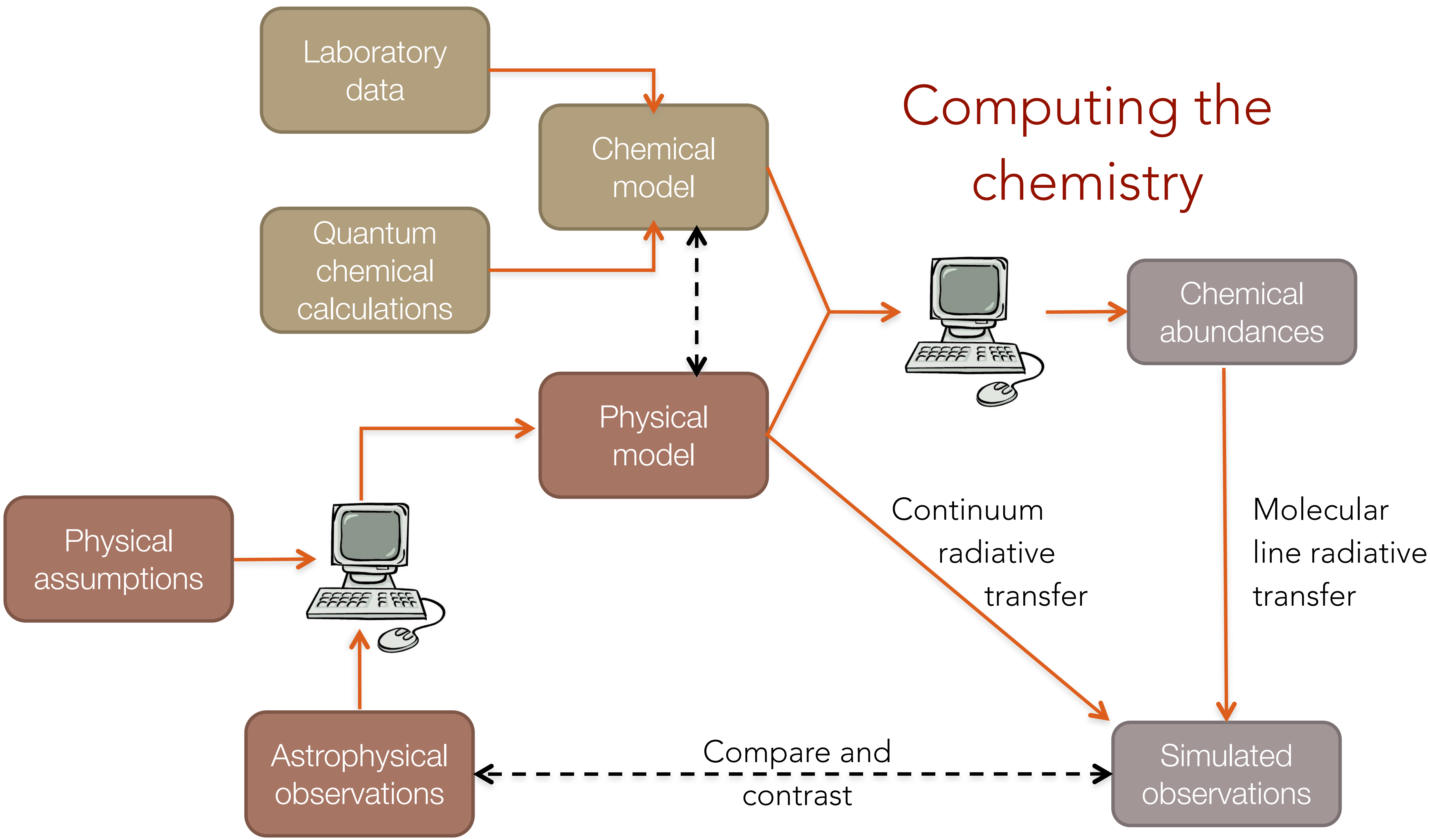
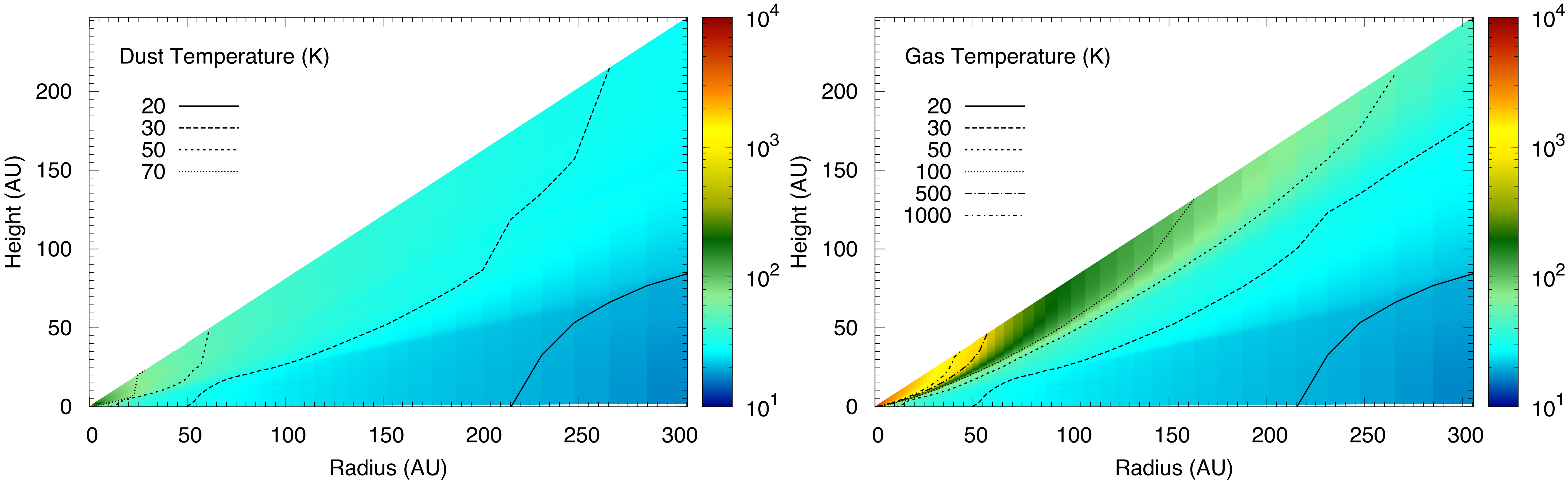


T_{gas} and T_{dust} decouple in disk atmosphere

At low densities and high ultraviolet fluxes, gas-grain collisions are inefficient and gas cools radiatively (which is slow)



Gas temperature calculation needs to be coupled with small chemical network to compute self-consistently the abundances of the main coolants: [CI], [OI], CO, H_2O

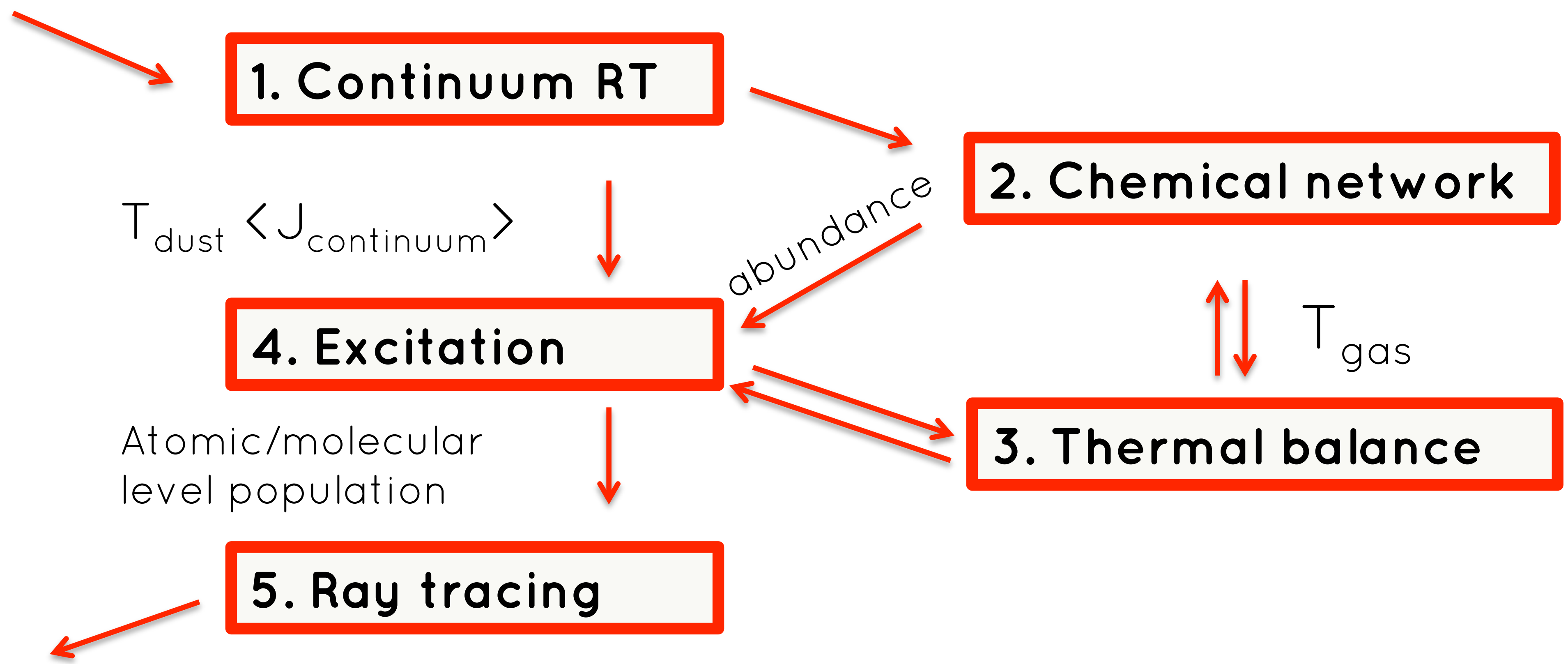
Nomura, H. & Millar, T. J., 2005, A&A, 438; Woitke, P., et al. 2009, A&A, 501, 383; Walsh, C., et al. 2010, ApJ, 722, 1607; Bruderer, S 2013, A&A, 559, A46

Coupled physico-chemical models

DALI

Bruderer et al. (2012); Bruderer (2013)

INPUTS
- Density structure
- Stellar spectrum



OUTPUTS
- Spectra
  Image cubes

See also, ProDiMo (Woitke et al. 2009, A&A, 501, 383)

Chemical networks for astrochemistry

Talk to an astrochemist!

Gas-phase chemistry

http://www.udfa.net/

http://kida.obs.u-bordeaux1.fr/

http://kinetics.nist.gov/kinetics/index.jsp

Photoionisation/photodissociation

http://home.strw.leidenuniv.nl/~ewine/photo/

http://phidrates.space.swri.edu/

Freezeout/desorption

Grain-surface chemistry

http://kida.obs.u-bordeaux1.fr/

http://faculty.virginia.edu/ericherb/research.html

McElroy, D., et al. 2013, A&A, 550, A36; Wakelam, V., et al. ApJS, 2015, 217, 20; Garrod, R. T. & Herbst, E., A&A, 457, 927; van Dishoeck, E. F., et al. 2006, Farad. Disk., 133, 231; Heays, A., et al. 2016, ApJS, in prep.; Huebner, W. F. & Mukherjee, J. 2015, Plan. Space. Sci., 106, 11; Cuppen, H., et al. 2016, Space Sci. Rev., in prep.

Molecular data

Talk to an astrochemist!

LAMDA: Leiden Atomic and Molecular Database
http://home.strw.leidenuniv.nl/~moldata/

Cologne Database for Molecular Spectroscopy
http://www.astro.uni-koeln.de/cdms/

JPL Molecular Spectroscopy
http://spec.jpl.nasa.gov/

HITRAN/HITEMP
http://hitran.org/

ExoMol
http://www.exomol.com/

Radiative transfer codes

Talk to an astrochemist!

RADMC2D/3D
dust and lines
http://www.ita.uni-heidelberg.de/~dullemond/software/radmc-3d/

TORUS
dust and lines
https://www.astro.ex.ac.uk/people/th2/torus_html/homepage.html

HYPERION
dust
http://www.hyperion-rt.org/

RATRAN
lines
https://personal.sron.nl/~vdtak/ratran/frames.html

LIME
dust and lines
http://www.nbi.dk/~brinch/lime.php

Radiative transfer codes

Talk to an astrochemist!

RADMC2D/3D
dust and lines
http://www.ita.uni-heidelberg.de/~dullemond/software/radmc-3d/

TORUS
dust and lines
https://www.astro.ex.ac.uk/people/th2/torus_html/homepage.html

HJPDOC
Dust optical constants
http://www.mpia.de/HJPDOC/

HYPERION
dust
http://www.hyperion-rt.org/

RATRAN
lines
https://personal.sron.nl/~vdtak/ratran/frames.html

LIME
dust and lines
http://www.nbi.dk/~brinch/lime.php

Future outlook

- Coupling dust evolution models with thermo-chemical and complex chemistry models: dust models are inherently 1D
- Correct treatment of viscous effects on disk structure and chemistry
- Large-scale mixing: connection with the solar system
- Breaking axisymmetry: creation of vortices, dust traps, and corresponding chemical effects
- Using molecular lines to distinguish between different models to explain dust morphology as observed with ALMA
- Chemistry in evolving disks: fingerprints of early conditions