Chemical effects on ices:
studies with a chemo-dynamical model

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Contents:

Very Low Luminosity Objects (VeLLOs, $L<0.1L_{\odot}$)

- Episodic accretion & Chemistry (Lee 2007)

CO_2 ice in Low Luminosity Objects ($L<1L_{\odot}$)

- Kim et al. (2012)
    - Lee et al. (2004)

      -chemo-dynamical model
    - Dunham et al. (2010)

      -luminosity model of episodic accretion

Other ices

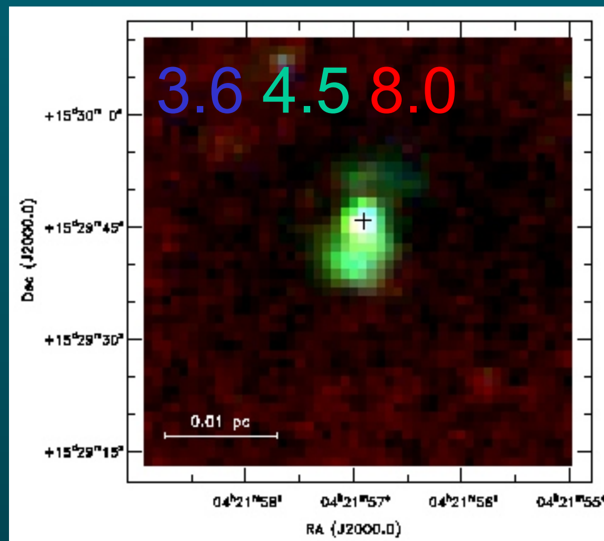
- Surface chemistry with the model of Lee (2007)

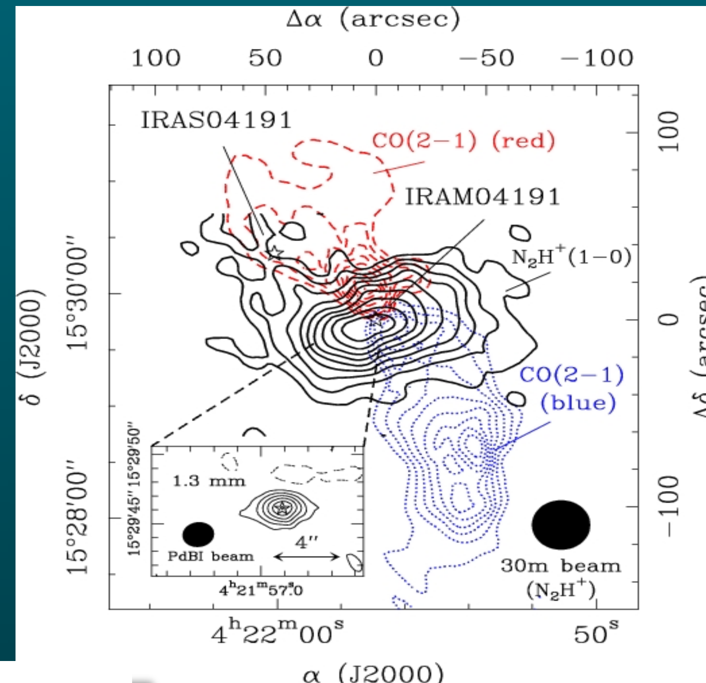
VeLLOs

Protostars in the quiescent phase or Proto-brown dwarfs?

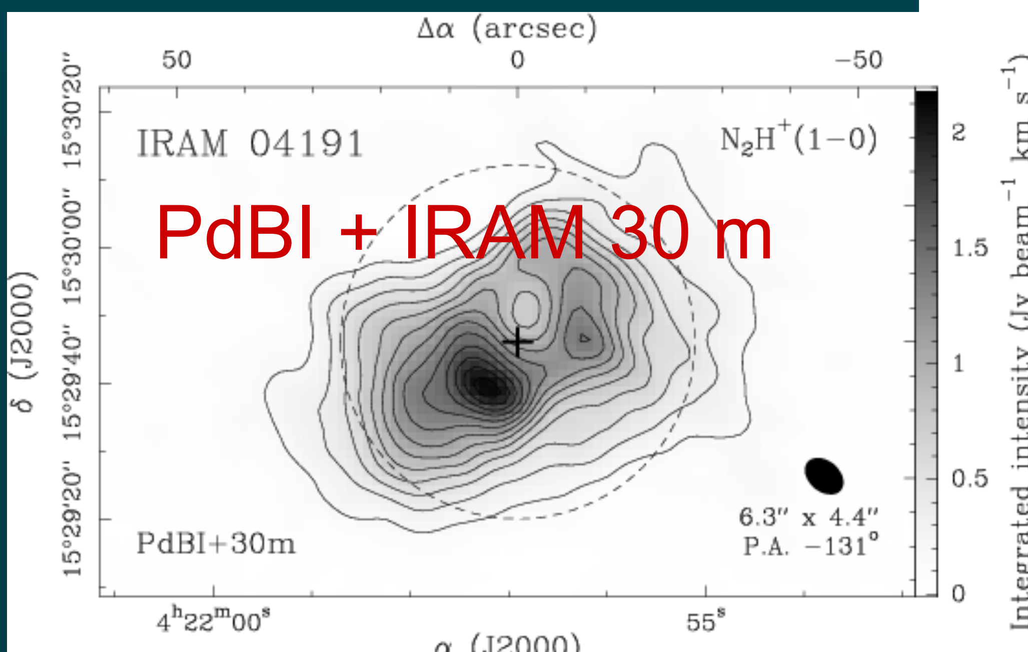
- If VeLLOs had a constant low accretion rate through their evolution, chemistry must be similar to that of starless cores
  - Depletion of CO, centrally peaked N_2H^+, high level of deuteration
- If VeLLOs are in their quiescent phase after accretion bursts, they will be different from either Class 0/I or starless cores in chemical distributions (Lee 2007, Visser & Bergin 2012)
- Therefore, ***chemistry can be used as a fingerprint of episodic accretion.***
- A possible example of episodic accretion – *IRAM 04191*

IRAM 04191 L~0.08 $L_\odot$





Strong Outflow
(Belloche et al. 2002)



N_2H^+ depletion at the continuum peak
(Belloche & Andre 2004)

Chemo-Dynamical Model

Evolution Model of Luminosity

n(r,t), v(r,t)
Shu's collapse model

$T_D(r,t)$
Continuum Radiative Transfer

$T_k(r,t)$
Gas Energetics

X(r′,t) → X(r,t)
Chemical evolution along infalling gas

Simulated line profile (r,t)
Line Radiative Tansfer

Lee, *et al* (2004)

Chemical evolution in episodic accretion (Lee 2007)

Chemical distributions for IRAM0419

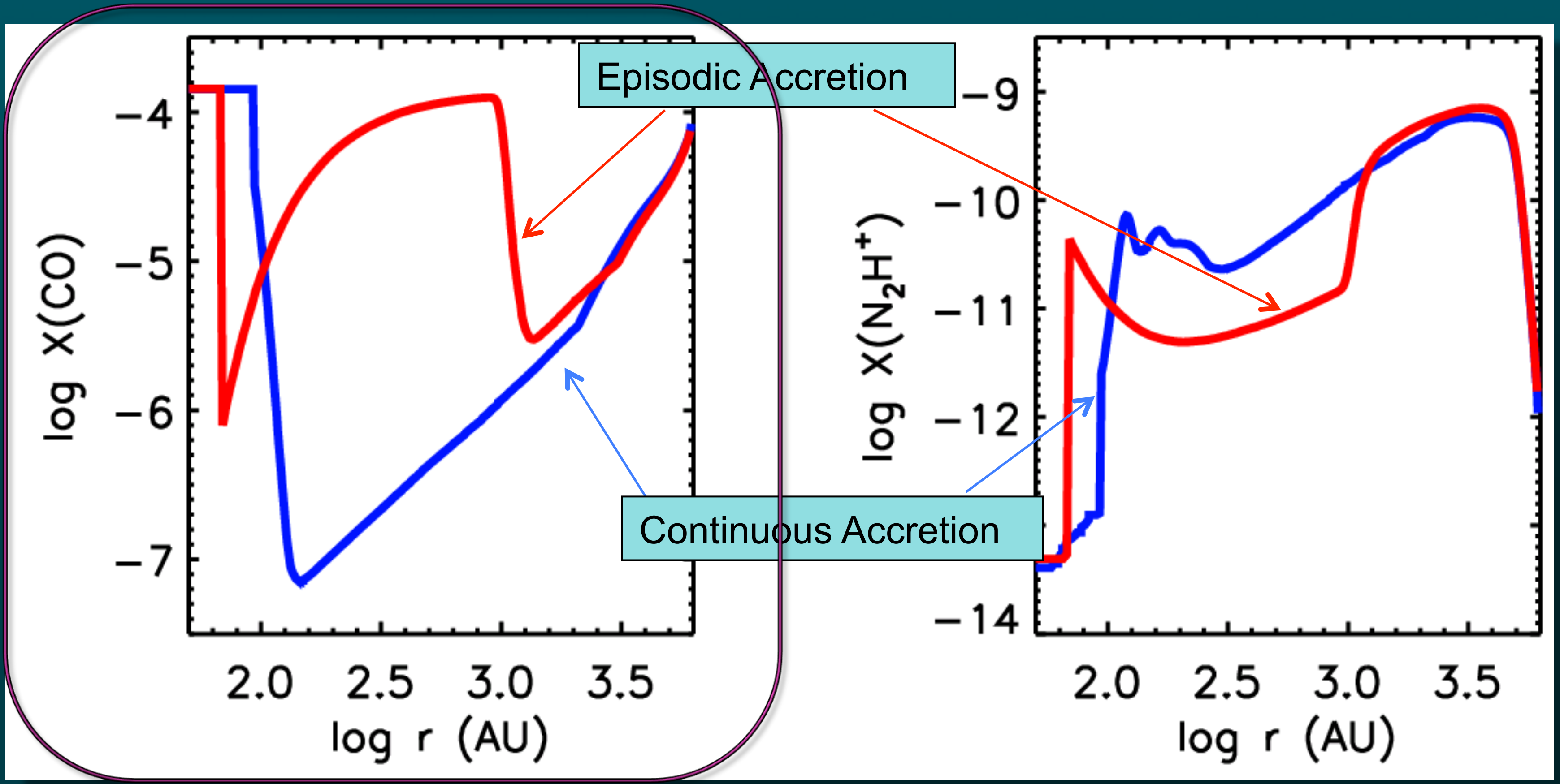
- assumptions:
  constant infall from envelope to disk
  episodic accretion from disk to star
  (accretion event every 10^4 yrs for 10^3 yrs)

- Model prameters:

Young and Evans (2004)
$M_{core} = 1\ M_{\odot}$
$R_{core} = 6200$ AU
normal accretion rate = $4.8 \times 10^{-6}\ M_{\odot}/yr$

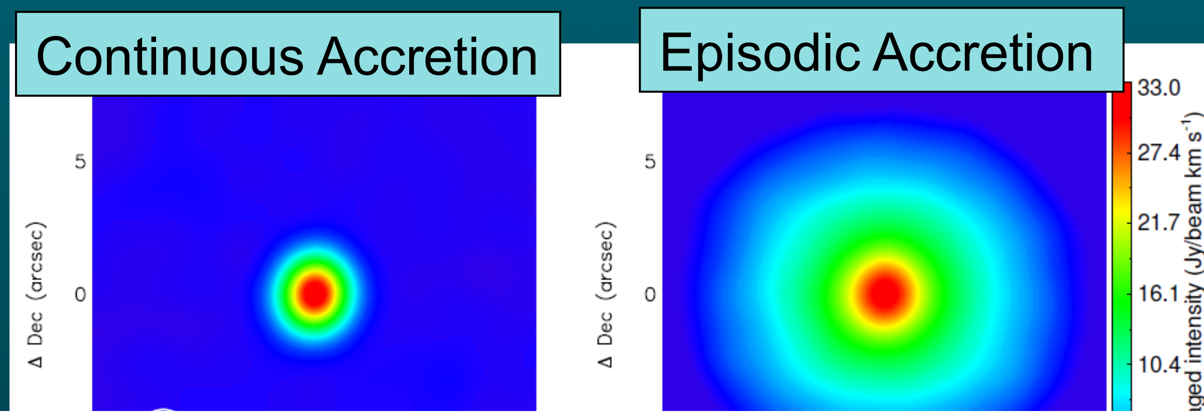
accretion rate (accretion phase) = 10 x normal rate
accretion rate (quiet phase) = 0.01 x normal rate

Difference between standard and episodic accretion models



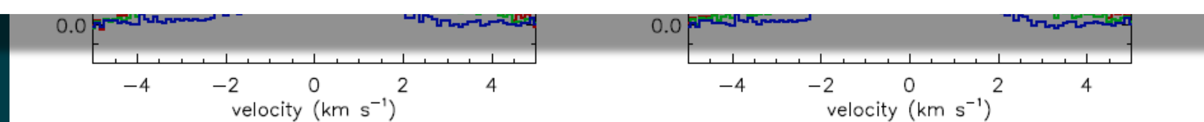
CO and N_2H^+ abundances

Expectation from ALMA



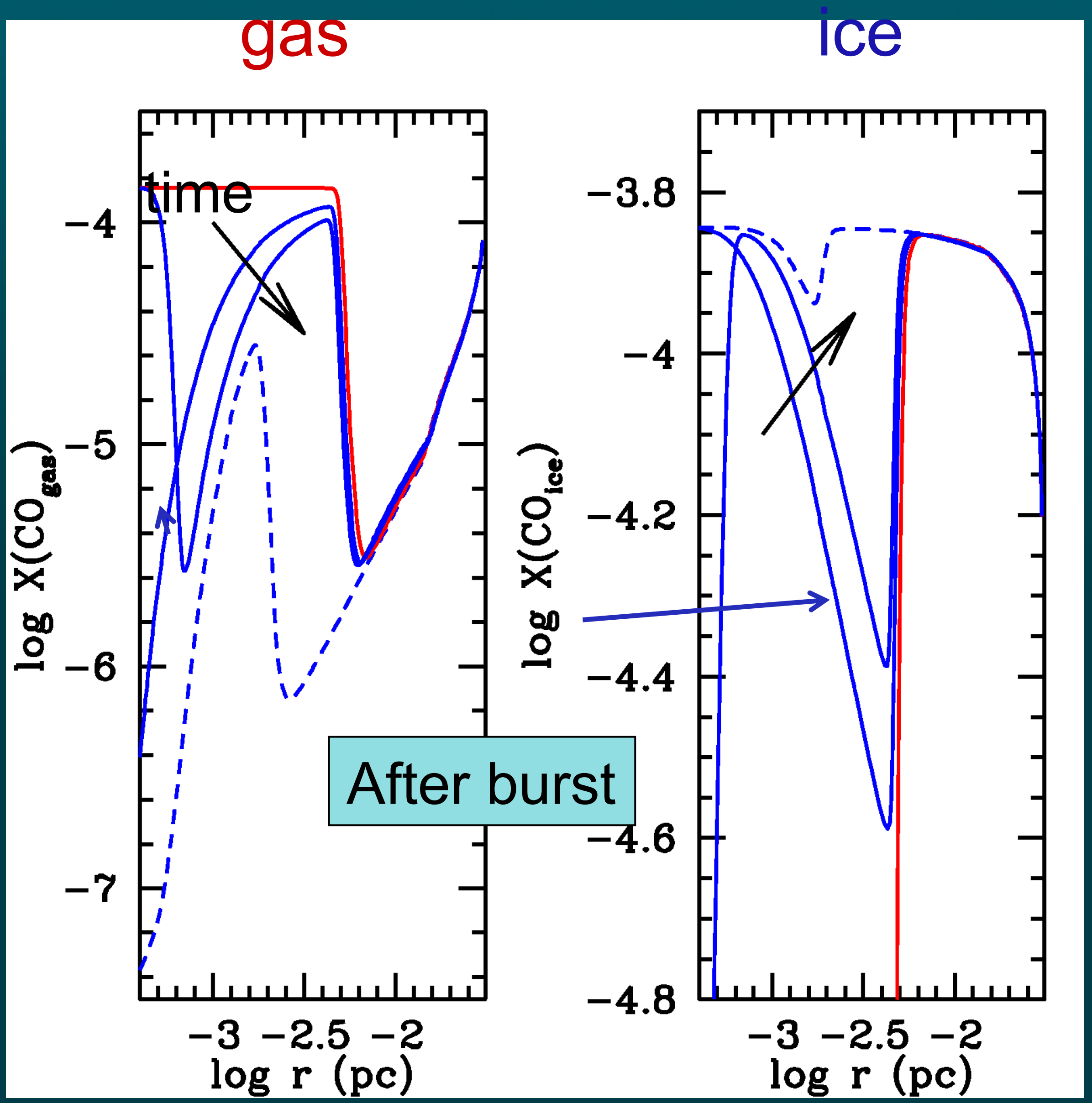
Cycle 2 ALMA targets

Source	RA	Dec	d (pc)	L_{bol} ($L_{\odot}$)	CO_2 pure ice	CO outflow
IRAM04191	$04^h\ 22^m\ 00.41^s$	$15°\ 30'\ 21.2''$	140	0.08	yes	yes
CB68	$16^h\ 57^m\ 19.63^s$	$-16°\ 09'\ 23.4''$	125	0.54	yes	yes
CB130-1	$18^h\ 16^m\ 16.39^s$	$-02°\ 32'\ 37.7''$	270	0.15	yes	no
L673-7	$19^h\ 21^m\ 34.82^s$	$11°\ 21'\ 23.4''$	300	0.04	–	yes



Simulation of observations in $C^{18}O$ J=2-1

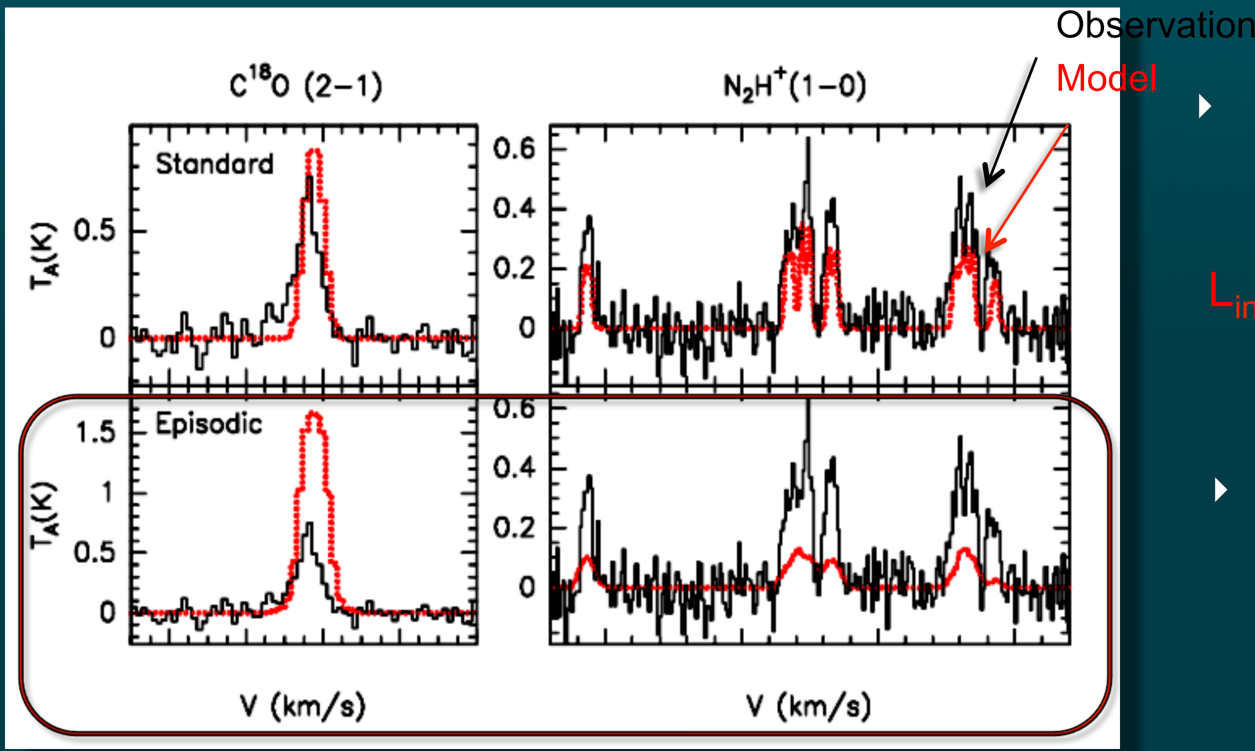
Constrain the time scale after a outburst



<u>Caveat</u>; No consideration of surface chemistry

Problem in $C^{18}O$ and N_2H^+

Standard and Episodic accretion models with the chemical network without surface chemistry cannot explain the observed luminosity or strength of $C^{18}O$ and N_2H^+ toward CB130-1.



- Continuous accretion model cannot match the source luminosity.

$L_{int\_mod} = 0.01\ L_\odot < L_{int\_obs} = 0.15\ L_\odot$

- Episodic accretion model has too strong $C^{18}O$ and too weak N_2H^+.

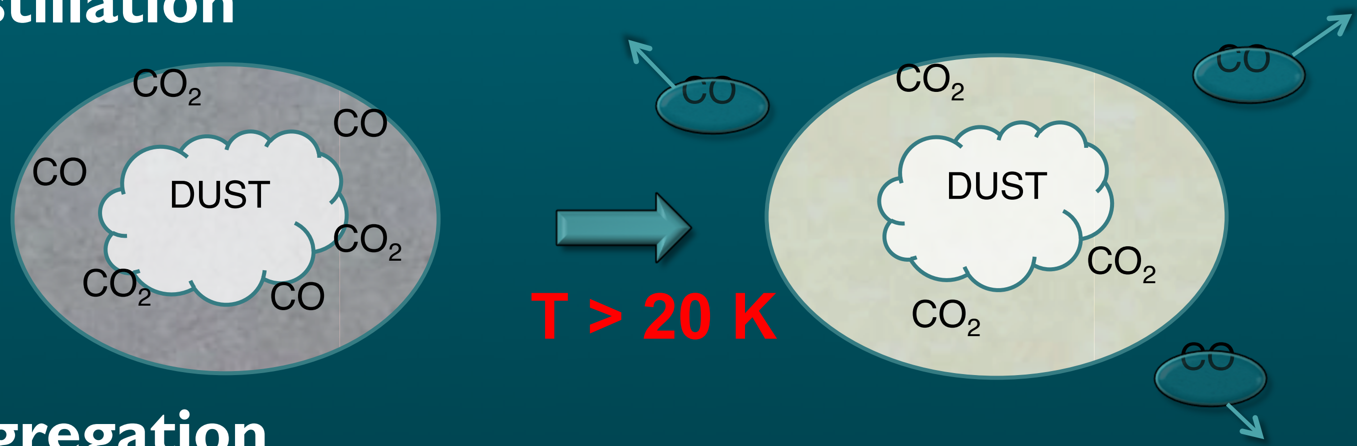
Kim *et al.*, 2011

<u>A possible solution</u>; part of CO gas gets converted to CO_2 ice when it is frozen on to grain surfaces.

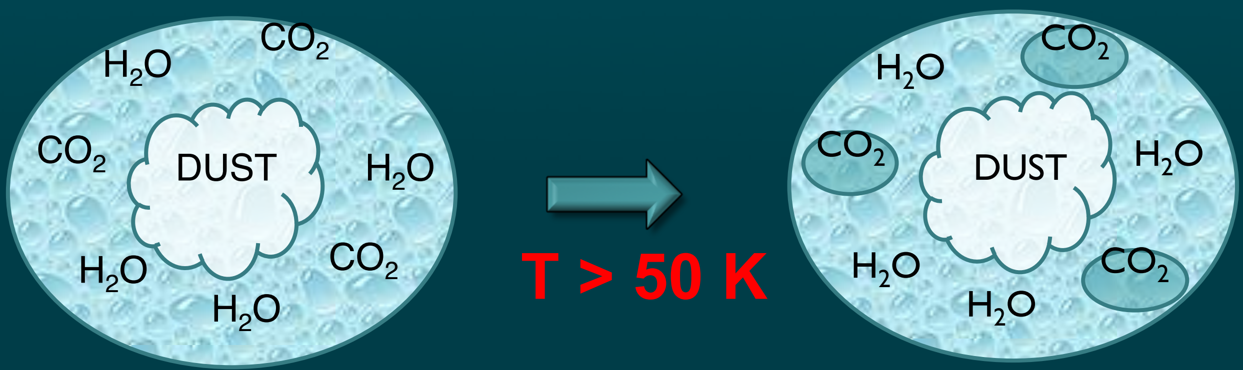
CO_2 is a useful constraint for episodic accretion because of its distinct pure ice feature.

Pure CO2 Ice Formation

Distillation



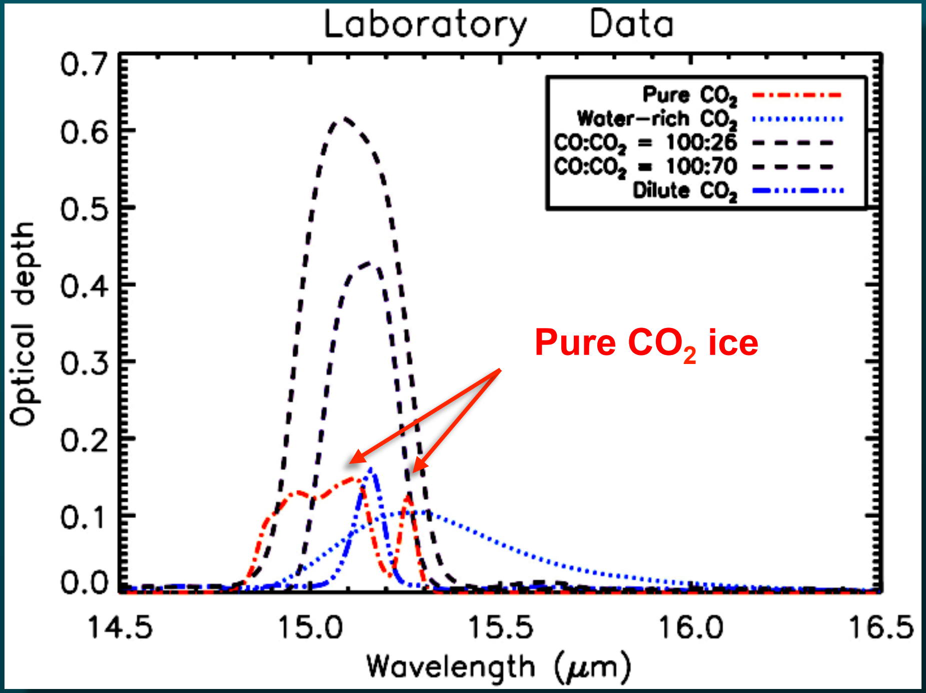
Segregation



- Formation of pure CO_2 ice requires at least 20 K.
- Pure CO_2 ice formation is an irreversible process.

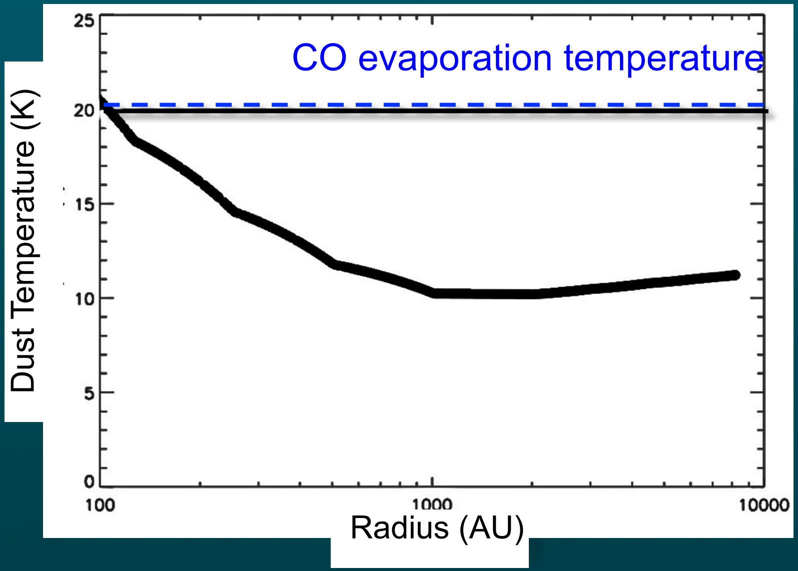
Laboratory Data

Laboratory data from Leiden Observatory data base.



- CO_2:H_2O mixture, CO:CO_2 mixture (Ehrenfreund et al. 1997)
- Only the pure CO_2 ice (van Broekhuizen et al. 2006) component has ***double peak.***

Dust Temperature is Too Low



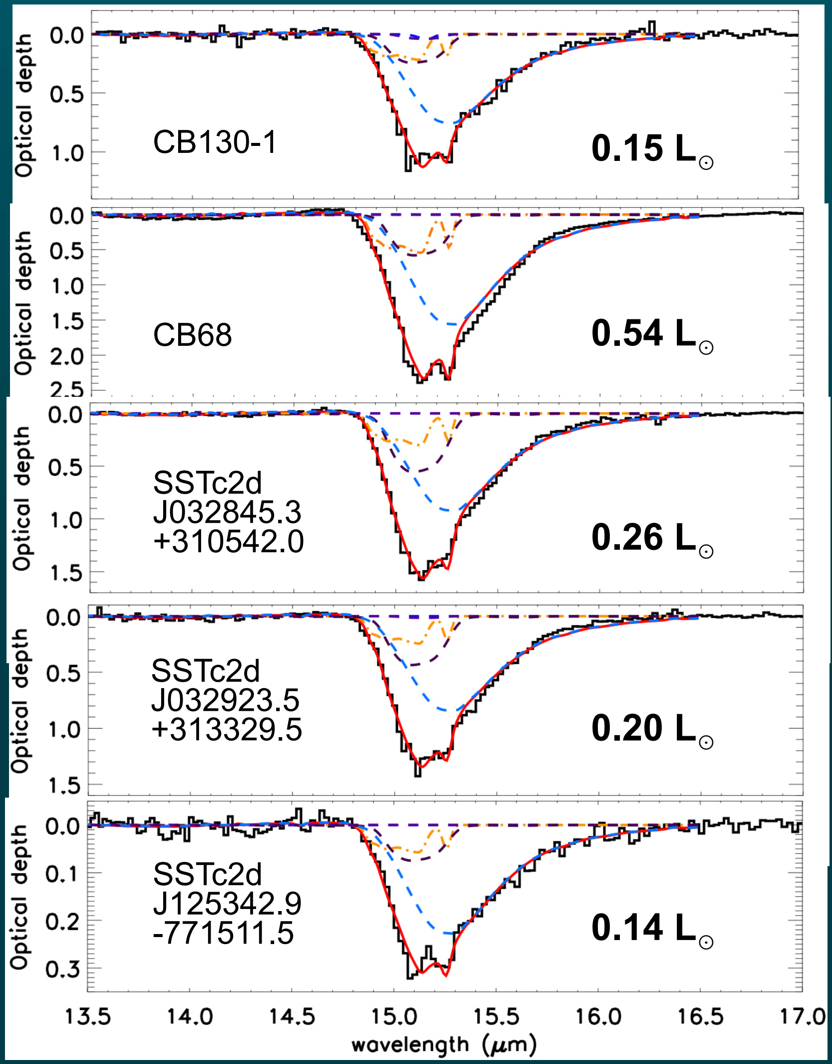
- The envelope around low luminosity protostars with 0.6 $L_{\odot}$ does *NOT* have a dust temperature higher than 20 K to form the pure CO_2 ice.
- If we can detect the pure CO_2 ice feature around low luminosity protostars, then it can be an evidence of the *past high accretion rate*!

Observation

- CO_2 ice with Spitzer/IRS SH mode (R=600)
  - 19 low luminosity protostars with $L_{int} < 0.7\ L_{\odot}$ (PI: M. Dunham)
    - 18 of them have $L_{int} < 0.6\ L_{\odot}$.
    - 3 of them have $L_{int} < 0.1\ L_{\odot}$.
  - 50 higher luminosity protostars with $L_{int} > 1\ L_{\odot}$ (c2d: Pontoppidan et al. 2008)
- $C^{18}O$ (J = 2→1; 219.560352 GHz) toward 11 low luminosity protostars at CSO.

Kim *et al.*, 2012

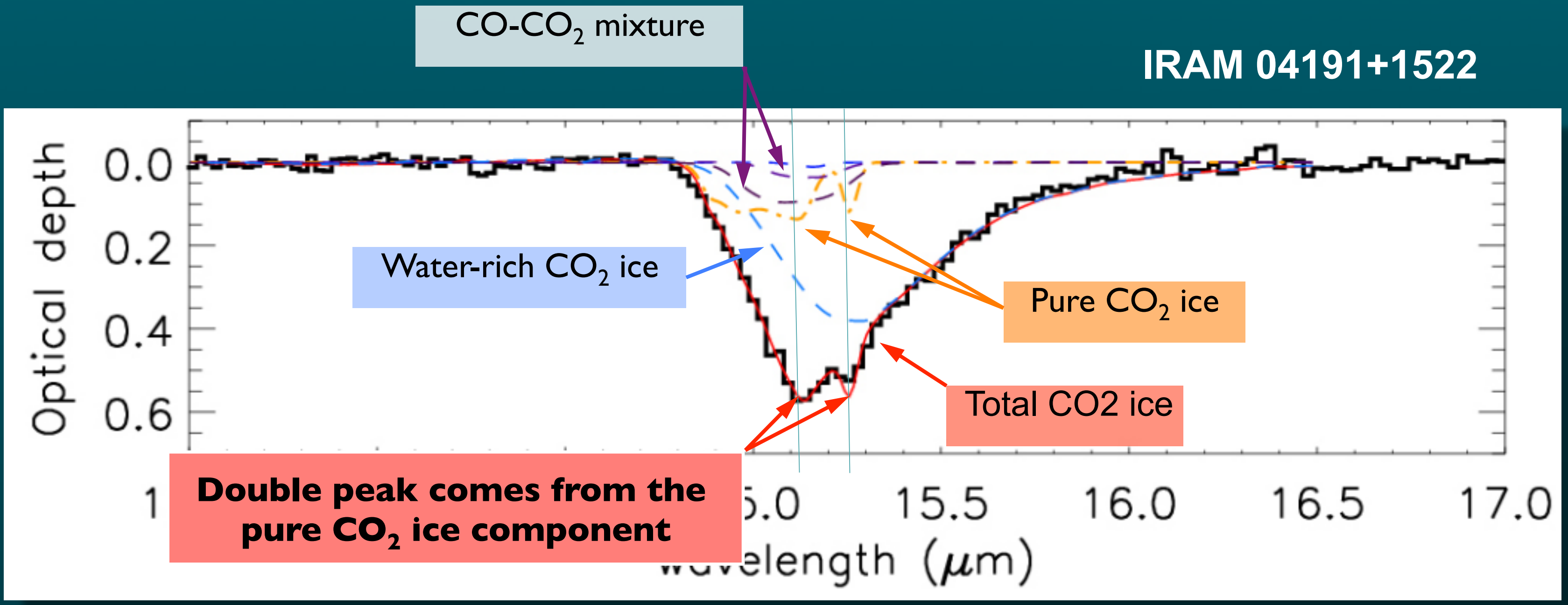
Pure CO_2 Ice Detections at Low Luminosity Protostars



- Six low luminosity embedded protostars show significant double peaks caused by the pure CO_2 ice .
- Three more sources show evidence of pure CO_2 ice.
- Column Density is calculated

$$N(\mathrm{CO_2}) = \int \tau(\nu) d\nu / A$$

Component Analysis with Laboratory Data



Internal luminosity of IRAM 04191+1522 is 0.08 $L_\odot$,
but it ***has*** the pure CO_2 ice component.

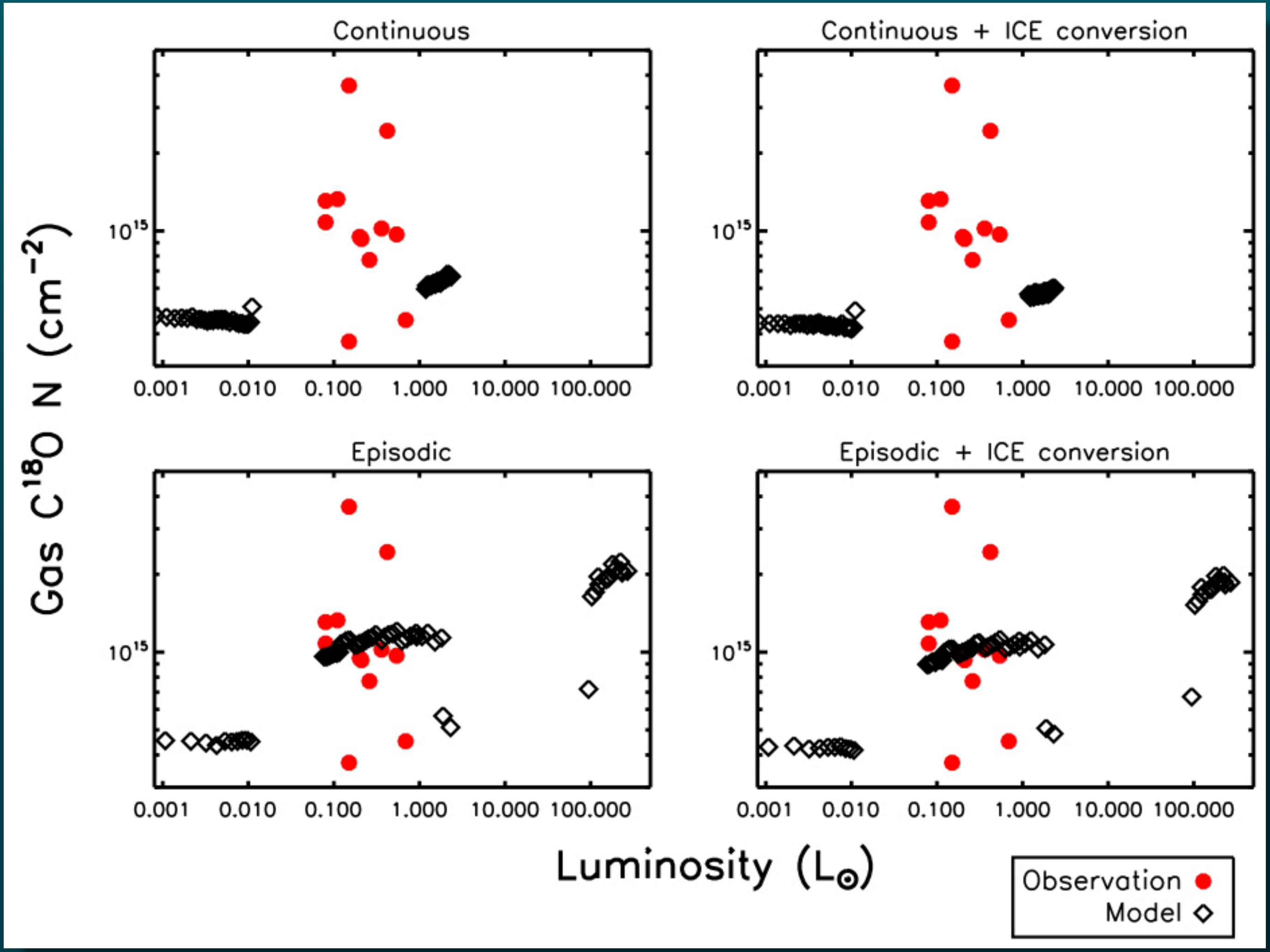
The source ***had*** higher temperatures than the dust temperature derived from the current SED.

Tests with Chemo-dynamical Models

- **Chemo-dynamical models**
  - Continuous accretion + chemical network without surface chemistry
  - Continuous accretion + CO to CO_2 ice conversion
  - Episodic accretion + chemical network without surface chemistry
  - Episodic accretion + CO to CO_2 ice conversion

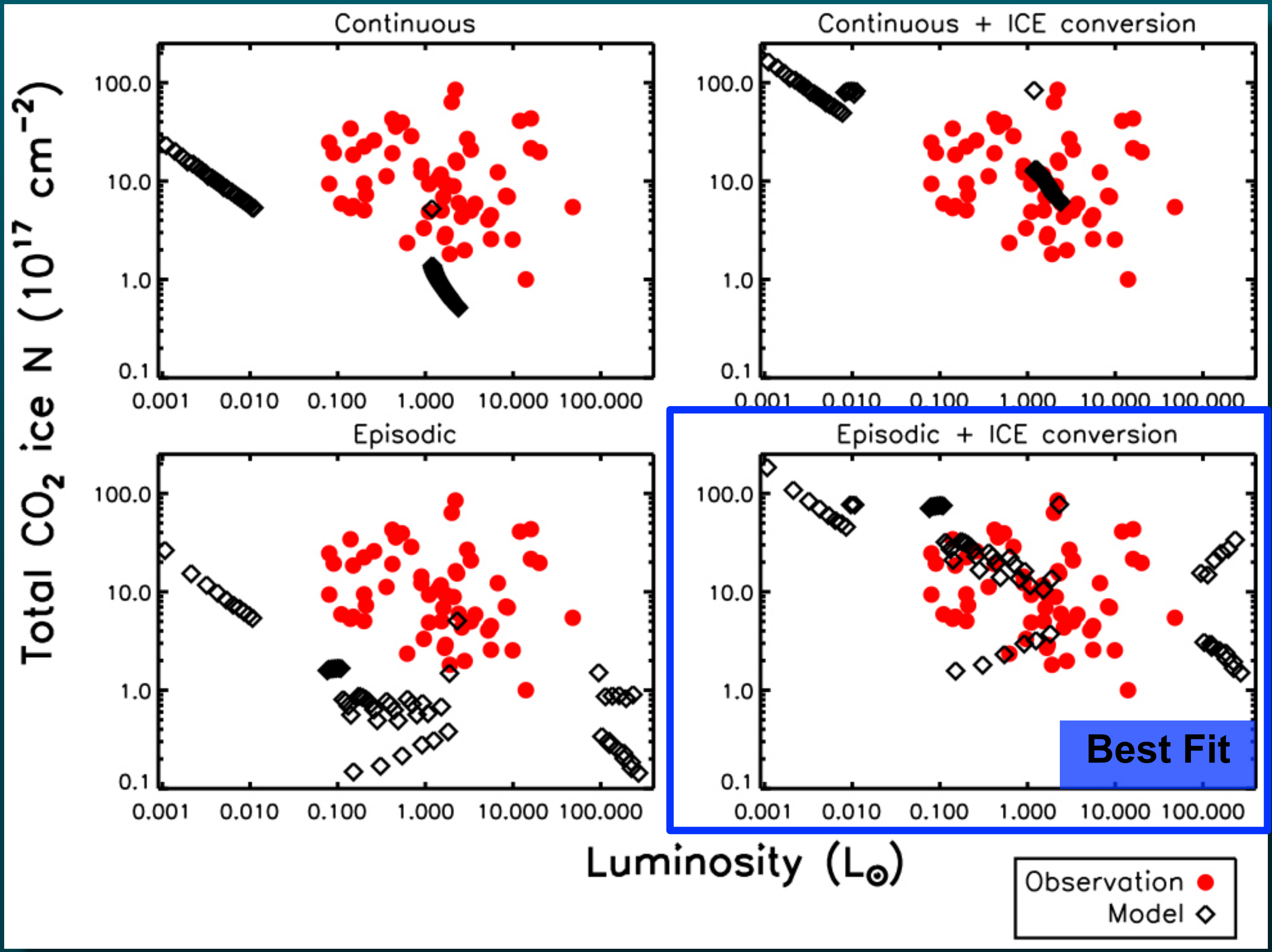
Kim *et al.*, 2012

Result: $C^{18}O$ gas



Kim *et al*., 2012

Result: CO_2 ice



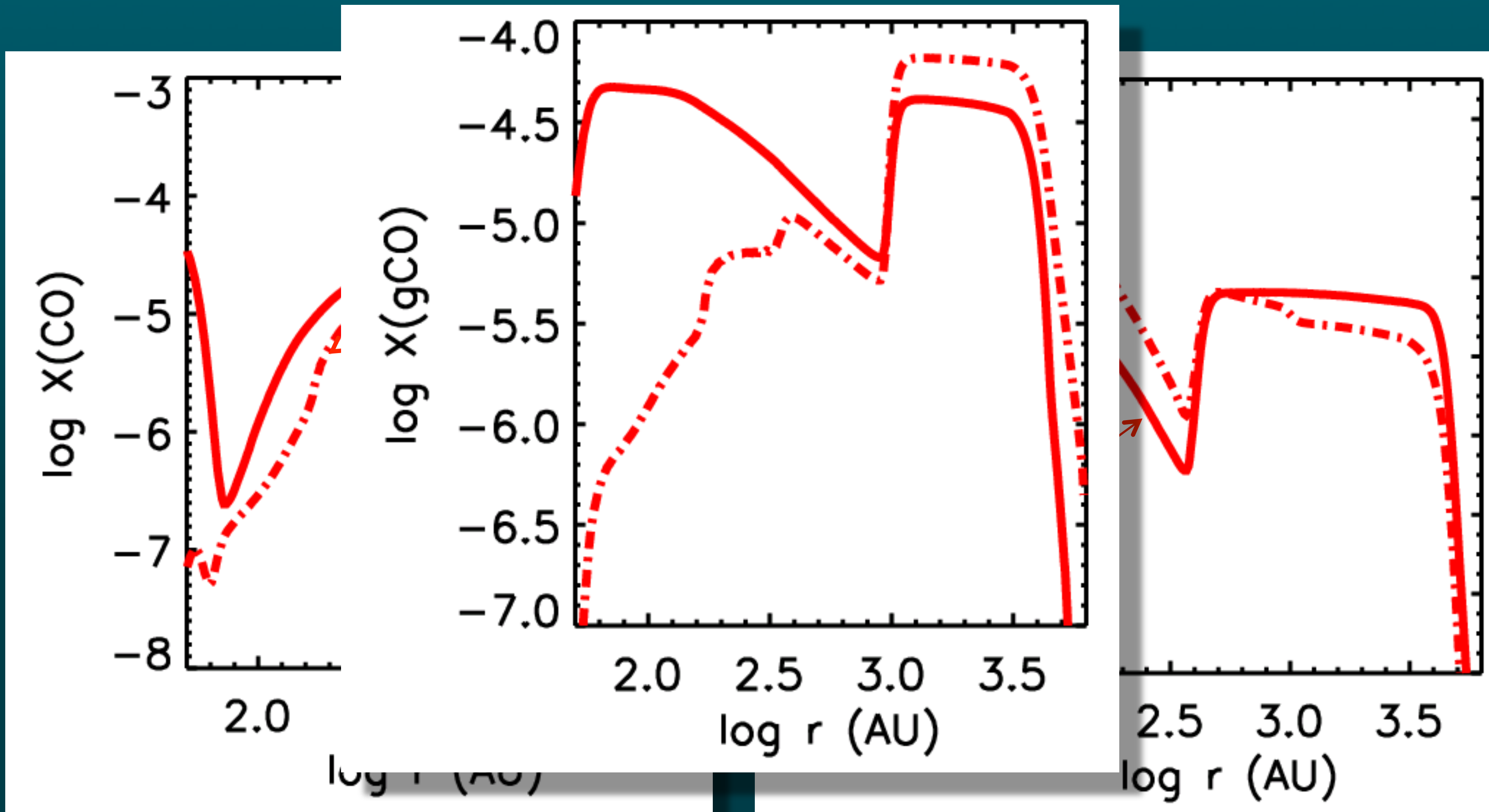
Kim *et al.*, 2012

Caveat; No explicit surface chemistry

Inclusion of surface chemistry explicitly using rate equations

- Willacy et al. (2006), Garrod and Herbst (2006), Dodson-Robinson et al. (2009), Yu et al. (in prep.)

ad hoc approximation vs. explicit surface chemistry



Branching ratio between CO ice and CO_2 ice = 0.5 : 0.5

CO + grain ➔ gCO (50%) or gCO_2 (50%)

AKARI spectrum of a low luminosity source

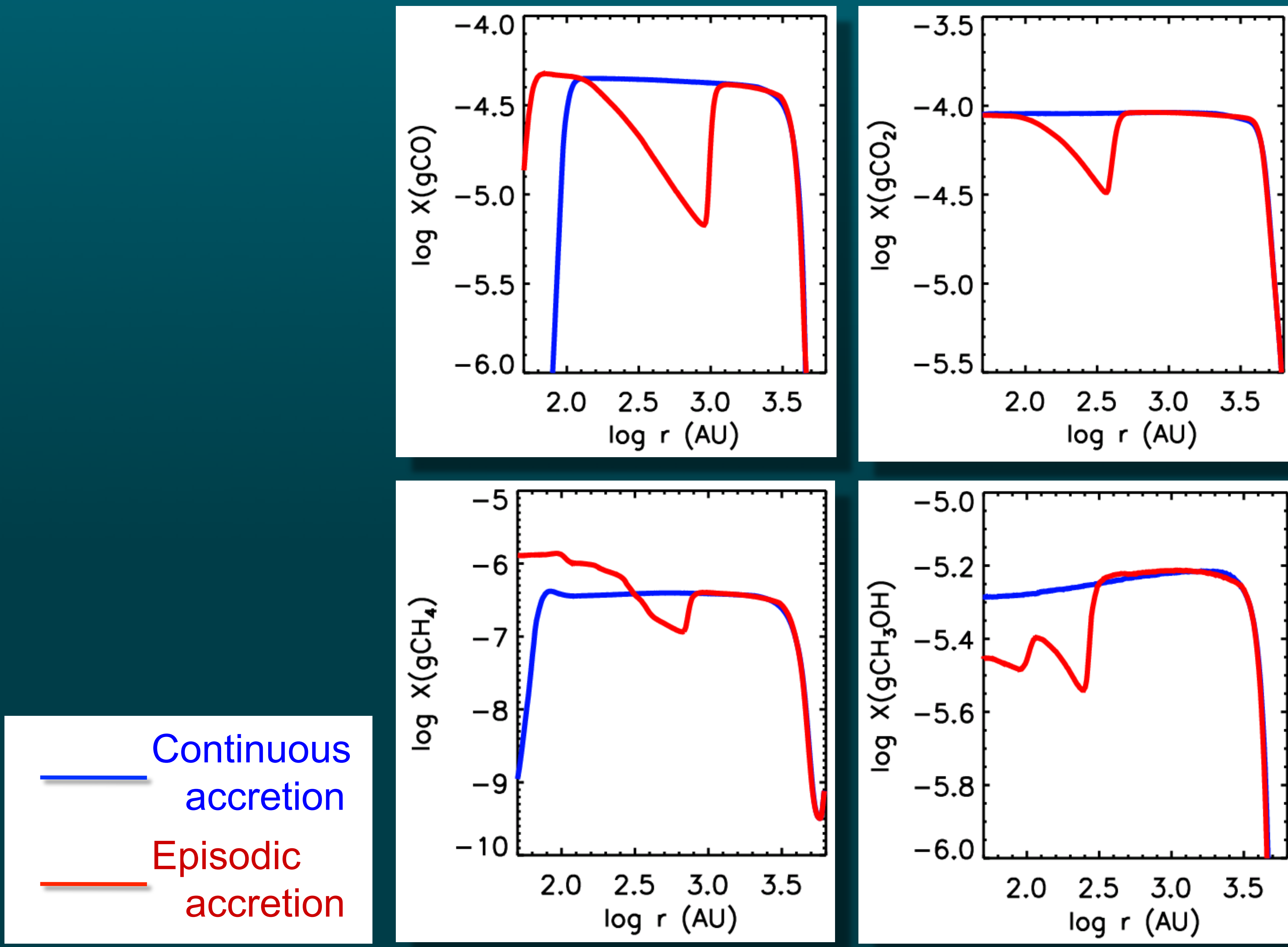
Table 5. Ice column densities

source name	$N(H_2O)$ $\times10^{17}(\mathrm{cm}^{-2})$	$N(CO_2)$ $\times10^{17}(\mathrm{cm}^{-2})$	$N(CO)$ $\times10^{17}(\mathrm{cm}^{-2})$	$N(XCN)$[a] $\times10^{17}(\mathrm{cm}^{-2})$
D060	70.10 ± 10.50	8.16 ± 1.10	18.89 ± 2.30	2.74
D090	19.16 ± 0.92	3.94 ± 0.28	2.98 ± 0.21	···
D104	34.11 ± 5.10	6.24 ± 0.60	11.81 ± 0.42	0.90

wavelength(μm)

J034351.02+320307.9 ($L=0.33\ L_\odot$, Dunham et al. 2008)

ICES



log X(gCO)
−4.0
−4.5
−5.0
−5.5
−6.0
2.0
2.5
3.0
3.5
log r (AU)
log X(gCO₂)
−3.5
−4.0
−4.5
−5.0
−5.5
2.0
2.5
3.0
3.5
log r (AU)
log X(gCH₄)
−5
−6
−7
−8
−9
−10
2.0
2.5
3.0
3.5
log r (AU)
log X(gCH₃OH)
−5.0
−5.2
−5.4
−5.6
−5.8
−6.0
2.0
2.5
3.0
3.5
log r (AU)
Continuous accretion
Episodic accretion

Further constraints for episodic accretion

- **ALMA observations for the distribution of gaseous molecules**
- **Other ices observed with Spitzer/IRS and AKARI**
  - e.g. Boogert et al. (2011)
  - e.g. Noble et al. (2013), Lee et al. (in prep.)

Summary

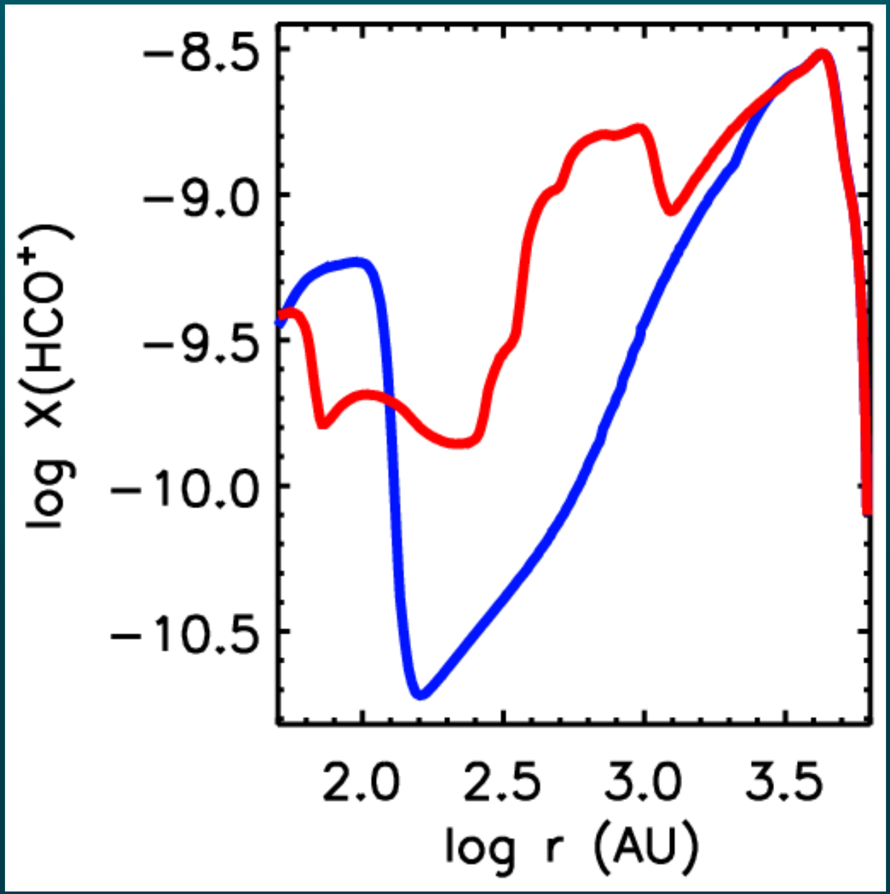
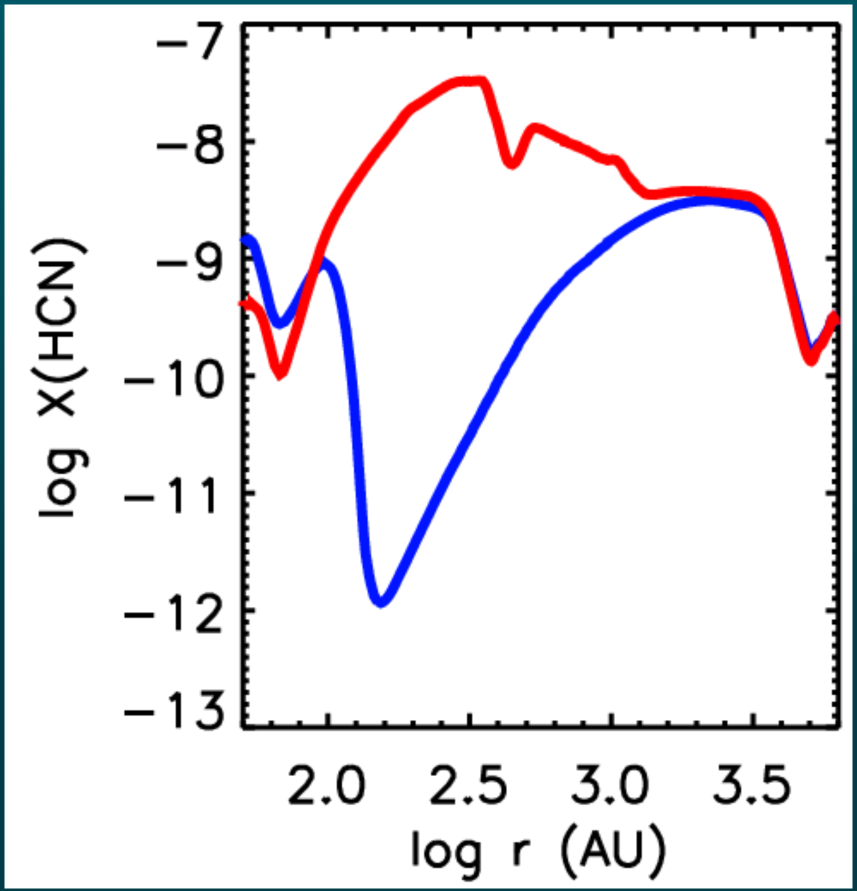
- ***Episodic Accretion Model*** **can explain**
  - presence of pure CO_2 ice in low luminosity protostars
  - low luminosity itself, strength of molecular lines, and total CO_2 ice column density with the ad hoc ice conversion of CO to CO_2
- ***Surface chemistry*** **must be included more** ***explicitly.***
- ***Chemo-Dynamical model for the episodic accretion model*** **could be constrained better by existing IR ice spectra and future ALMA observations.**

Thank you.

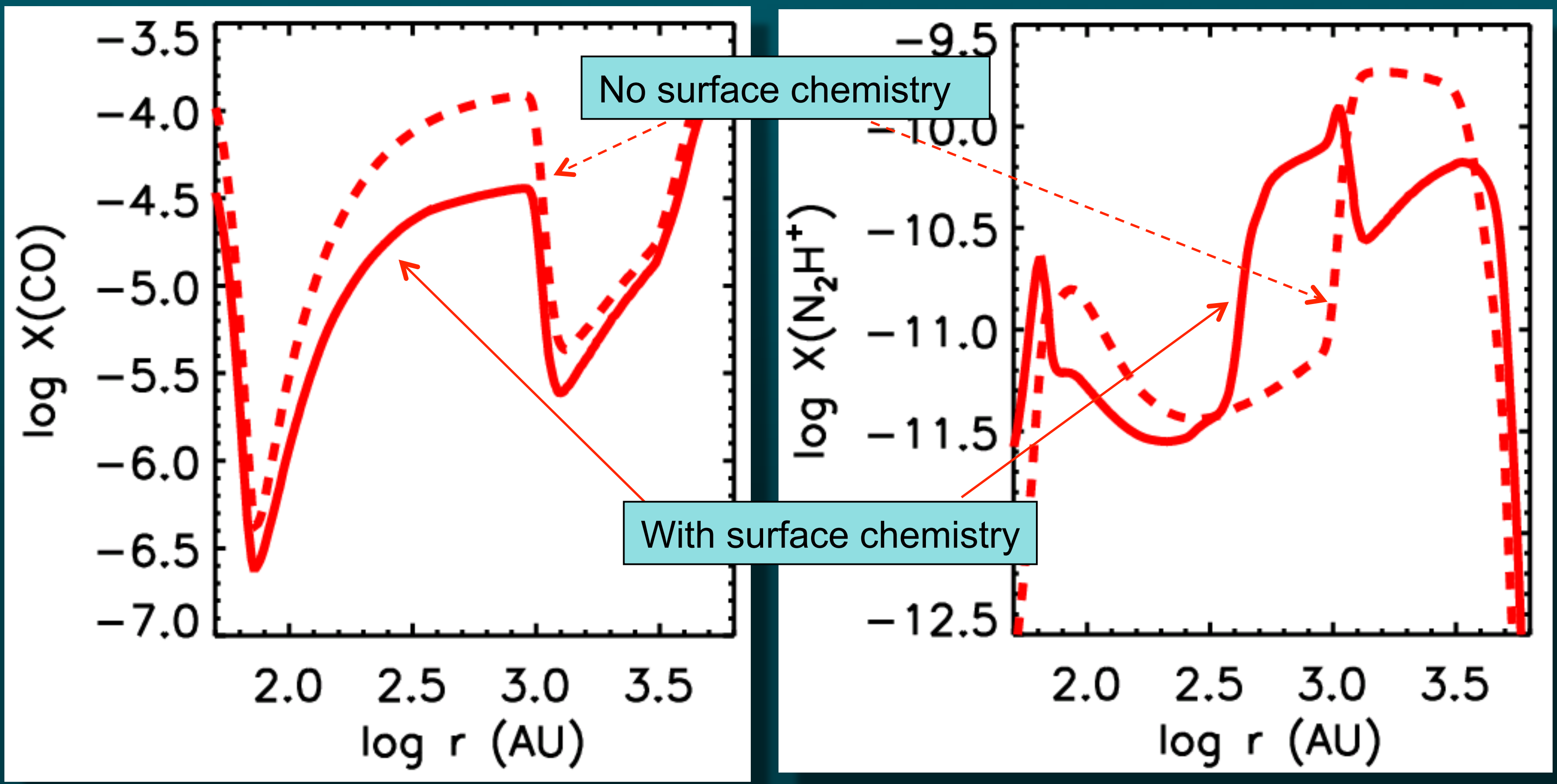
Table 7
Intrinsic Integrated Band Strengths

Molecule	Mode	A (cm molecule^{-1})	Reference
H_2O	3.0 μm stretch	2.0×10^{-16}	Hagen et al. (1981)
NH_4^+	6.8 μm deformation	4.4×10^{-17}	Schutte & Khanna (2003)
CO_2	15.0 μm bend	1.1×10^{-17}	Gerakines et al. (1995)
CH_3OH	3.53 μm C–H stretch	5.6×10^{-18}	Kerkhof et al. (1999)
CH_3OH	9.7 μm O–H stretch	1.6×10^{-17}	Kerkhof et al. (1999)
HCOOH	5.85 μm C=O stretch	6.7×10^{-17}	Schutte et al. (1999)
HCOOH	7.25 μm C–H deformation	2.6×10^{-18}	Schutte et al. (1999)
CH_4	7.68 μm deformation	7.3×10^{-18}	Boogert et al. (1997)
NH_3	8.9 μm umbrella	1.3×10^{-17}	Kerkhof et al. (1999)

Boogert *et al*., 2011


−8.5
−9.0
−9.5
−10.0
−10.5
log X(HCO⁺)
2.0
2.5
3.0
3.5
log r (AU)

−7
−8
−9
−10
−11
−12
−13
log X(HCN)
2.0
2.5
3.0
3.5
log r (AU)

Episodic accretion model with/without surface chemistry



CO and N_2H^+ abundances

- **GO + GCO → GCO_2**
- **GO + GHCO → GCO_2 + GH**
- **GOH + GCO → GCO_2 + GH**

- Assume ONLY GH, GC, GN, GO, GS, GH2, GCH, GOH, and GNH are mobile.

Grain surface reaction

$$k^{s2} = P\left(k_{\mathrm{diff}}(i) + k_{\mathrm{diff}}(j)\right)/n_{\mathrm{act}}$$

where P is the probability for reaction to occur and $k_{\mathrm{diff}}(i)$ is the thermal diffusion rate of species i,

$$k_{\mathrm{diff}}(i) = \nu_{\mathrm{s}} \exp(-E_{\mathrm{diff}}/T_{\mathrm{dust}})(\mathrm{s}^{-1})$$

where E_{diff} is the diffusion energy, which is typically $E_{\mathrm{b}}/3$

For exothermic reaction

- without an activation energy : P =1
- With an activation energy (E_a)

$$P_m = \exp(-E_a/T_{\rm dust})$$

$$P_{\rm tunn} = \exp\left[-\frac{2b}{\hbar}\sqrt{2k_b\mu_r E_a}\right]$$

b = 1 Å , μ_r = reduced mass

$$P = \frac{\nu_{\rm s} max[P_m, P_{\rm tunn}]}{\nu_{\rm s} max[P_m, P_{\rm tunn}] + k_{\rm diff}(i) + k_{\rm diff}(j)}$$