

# Physics 224

# The Interstellar Medium

Lecture #17: More molecular clouds!

# Outline

- Part I: Virial Equation, Bonnor-Ebert Mass, Magnetic Sub-/Super-critical Clouds
- Part II: Molecular Gas Chemistry
- Part III: Tracing Molecular Gas
- Part IV: Observations of Molecular Gas

# Chemistry in Molecular Gas

List of molecules that have been detected in the ISM:

2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	>12 atoms
H <sub>2</sub>	C <sub>3</sub> <sup>+</sup>	<i>c</i> -C <sub>3</sub> H	C <sub>5</sub> <sup>+</sup>	C <sub>5</sub> H	C <sub>6</sub> H	CH <sub>3</sub> C <sub>3</sub> N	CH <sub>3</sub> C <sub>4</sub> H	CH <sub>3</sub> C <sub>5</sub> N	HC <sub>9</sub> N	<i>c</i> -C <sub>6</sub> H <sub>6</sub> <sup>+</sup>	HC <sub>11</sub> N
AlF	C <sub>2</sub> H	<i>i</i> -C <sub>3</sub> H	C <sub>4</sub> H	<i>i</i> -H <sub>2</sub> C <sub>4</sub>	CH <sub>2</sub> CHCN	HC(O)OCH <sub>3</sub>	CH <sub>3</sub> CH <sub>2</sub> CN	(CH <sub>3</sub> ) <sub>2</sub> CO	CH <sub>3</sub> C <sub>6</sub> H	<i>n</i> -C <sub>3</sub> H <sub>7</sub> CN	C <sub>60</sub> <sup>+</sup>
AlCl	C <sub>2</sub> O	C <sub>3</sub> N	C <sub>4</sub> Si	C <sub>2</sub> H <sub>4</sub> <sup>+</sup>	CH <sub>3</sub> C <sub>2</sub> H	CH <sub>3</sub> COOH	(CH <sub>3</sub> ) <sub>2</sub> O	(CH <sub>2</sub> OH) <sub>2</sub>	C <sub>2</sub> H <sub>5</sub> OCHO	<i>i</i> -C <sub>3</sub> H <sub>7</sub> CN	C <sub>70</sub> <sup>+</sup>
C <sub>2</sub> <sup>++</sup>	C <sub>2</sub> S	C <sub>3</sub> O	<i>i</i> -C <sub>3</sub> H <sub>2</sub>	CH <sub>3</sub> CN	HC <sub>5</sub> N	C <sub>7</sub> H	CH <sub>3</sub> CH <sub>2</sub> OH	CH <sub>3</sub> CH <sub>2</sub> CHO	CH <sub>3</sub> OC(O)CH <sub>3</sub>	C <sub>2</sub> H <sub>5</sub> OCH <sub>3</sub> ?	C <sub>60</sub> <sup>++</sup>
CH	CH <sub>2</sub>	C <sub>3</sub> S	<i>c</i> -C <sub>3</sub> H <sub>2</sub>	CH <sub>3</sub> NC	CH <sub>3</sub> CHO	C <sub>6</sub> H <sub>2</sub>	HC <sub>7</sub> N				
CH <sup>+</sup>	HCN	C <sub>2</sub> H <sub>2</sub> <sup>+</sup>	H <sub>2</sub> CCN	CH <sub>3</sub> OH	CH <sub>3</sub> NH <sub>2</sub>	CH <sub>2</sub> OHCHO	C <sub>8</sub> H				
CN	HCO	NH <sub>3</sub>	CH <sub>4</sub> <sup>+</sup>	CH <sub>3</sub> SH	<i>c</i> -C <sub>2</sub> H <sub>4</sub> O	<i>i</i> -HC <sub>6</sub> H <sup>+</sup>	CH <sub>3</sub> C(O)NH <sub>2</sub>				
CO	HCO <sup>+</sup>	HCCN	HC <sub>3</sub> N	HC <sub>3</sub> NH <sup>+</sup>	H <sub>2</sub> CCHOH	CH <sub>2</sub> CHCHO (?)	C <sub>8</sub> H <sup>-</sup>				
CO <sup>+</sup>	HCS <sup>+</sup>	HCNH <sup>+</sup>	HC <sub>2</sub> NC	HC <sub>2</sub> CHO	C <sub>6</sub> H <sup>-</sup>	CH <sub>2</sub> CCHCN	C <sub>3</sub> H <sub>6</sub>				
CP	HOC <sup>+</sup>	HNCO	HCOOH	NH <sub>2</sub> CHO	CH <sub>3</sub> NCO 2015	H <sub>2</sub> NCH <sub>2</sub> CN	CH <sub>3</sub> CH <sub>2</sub> SH (?)				
SiC	H <sub>2</sub> O	HNCS	H <sub>2</sub> CNH	C <sub>5</sub> N		CH <sub>3</sub> CHNH					
HCl	H <sub>2</sub> S	HOCO <sup>+</sup>	H <sub>2</sub> C <sub>2</sub> O	<i>i</i> -HC <sub>4</sub> H <sup>+</sup>							
KCl	HNC	H <sub>2</sub> CO	H <sub>2</sub> NCN	<i>i</i> -HC <sub>4</sub> N							
NH	HNO	H <sub>2</sub> CN	HNC <sub>3</sub>	<i>c</i> -H <sub>2</sub> C <sub>3</sub> O							
NO	MgCN	H <sub>2</sub> CS	SiH <sub>4</sub> <sup>+</sup>	H <sub>2</sub> CCNH (?)							
NS	MgNC	H <sub>3</sub> O <sup>+</sup>	H <sub>2</sub> COH <sup>+</sup>	C <sub>5</sub> N <sup>-</sup>							
NaCl	N <sub>2</sub> H <sup>+</sup>	<i>c</i> -SiC <sub>3</sub>	C <sub>4</sub> H <sup>-</sup>	HNCHCN							
OH	N <sub>2</sub> O	CH <sub>3</sub> <sup>+</sup>	HC(O)CN								
PN	NaCN	C <sub>3</sub> N <sup>-</sup>	HNCNH								
SO	OCS	PH <sub>3</sub>	CH <sub>3</sub> O								

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

# List of molecules that have been detected in the ISM:

KCl	HNC	H <sub>2</sub> CO	H <sub>2</sub> NCN	<i>l</i> -HC <sub>4</sub> N
NH	HNO	H <sub>2</sub> CN	HNC <sub>3</sub>	<i>c</i> -H <sub>2</sub> C <sub>3</sub> O
NO	MgCN	H <sub>2</sub> CS	SiH <sub>4</sub> <sup>+</sup>	H <sub>2</sub> CCNH (?)
NS	MgNC	H <sub>3</sub> O <sup>+</sup>	H <sub>2</sub> COH <sup>+</sup>	C <sub>5</sub> N <sup>-</sup>
NaCl	N <sub>2</sub> H <sup>+</sup>	<i>c</i> -SiC <sub>3</sub>	C <sub>4</sub> H <sup>-</sup>	HNCHCN
OH	N <sub>2</sub> O	CH <sub>3</sub> <sup>+</sup>	HC(O)CN	
PN	NaCN	C <sub>3</sub> N <sup>-</sup>	HNCNH	
SO	OCS	CH <sub>3</sub>	CH <sub>3</sub> O	
SO <sup>+</sup>	SO <sub>2</sub>	HCNO	NH <sub>4</sub> <sup>+</sup>	
SiN	<i>c</i> -SiC <sub>2</sub>	HOCN	H <sub>2</sub> NCO <sup>+</sup> (?)	
SiO	CO <sub>2</sub> <sup>+</sup>	HSCN	NCCNH <sup>+</sup> 2015	
SiS	NH <sub>2</sub>	H <sub>2</sub> O <sub>2</sub>		
CS	H <sub>3</sub> <sup>+</sup> (•)	C <sub>3</sub> H <sup>+</sup>		
HF	SiCN	HMgNC		
HD	AlNC	HCCO 2015		
FeO ?	SiNC			
O <sub>2</sub>	HCP			
CF <sup>+</sup>	CCP			
SiH ?	AlOH			
PO	H <sub>2</sub> O <sup>+</sup>			
AlO	H <sub>2</sub> Cl <sup>+</sup>			
OH <sup>+</sup>	KCN			
CN <sup>-</sup>	FeCN			
SH <sup>+</sup>	HO <sub>2</sub>			
SH	TiO <sub>2</sub>			
HCl <sup>+</sup>	C <sub>2</sub> N			
TiO	Si <sub>2</sub> C 2015			
ArH <sup>+</sup>				
NO <sup>+</sup> ?				

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

# Chemistry in Molecular Gas

Abundance of molecules is set by rates of formation & destruction.

## Formation

- gas-phase reactions
  - neutral-neutral
  - ion-neutral
  - radiative association
- grain surface reactions

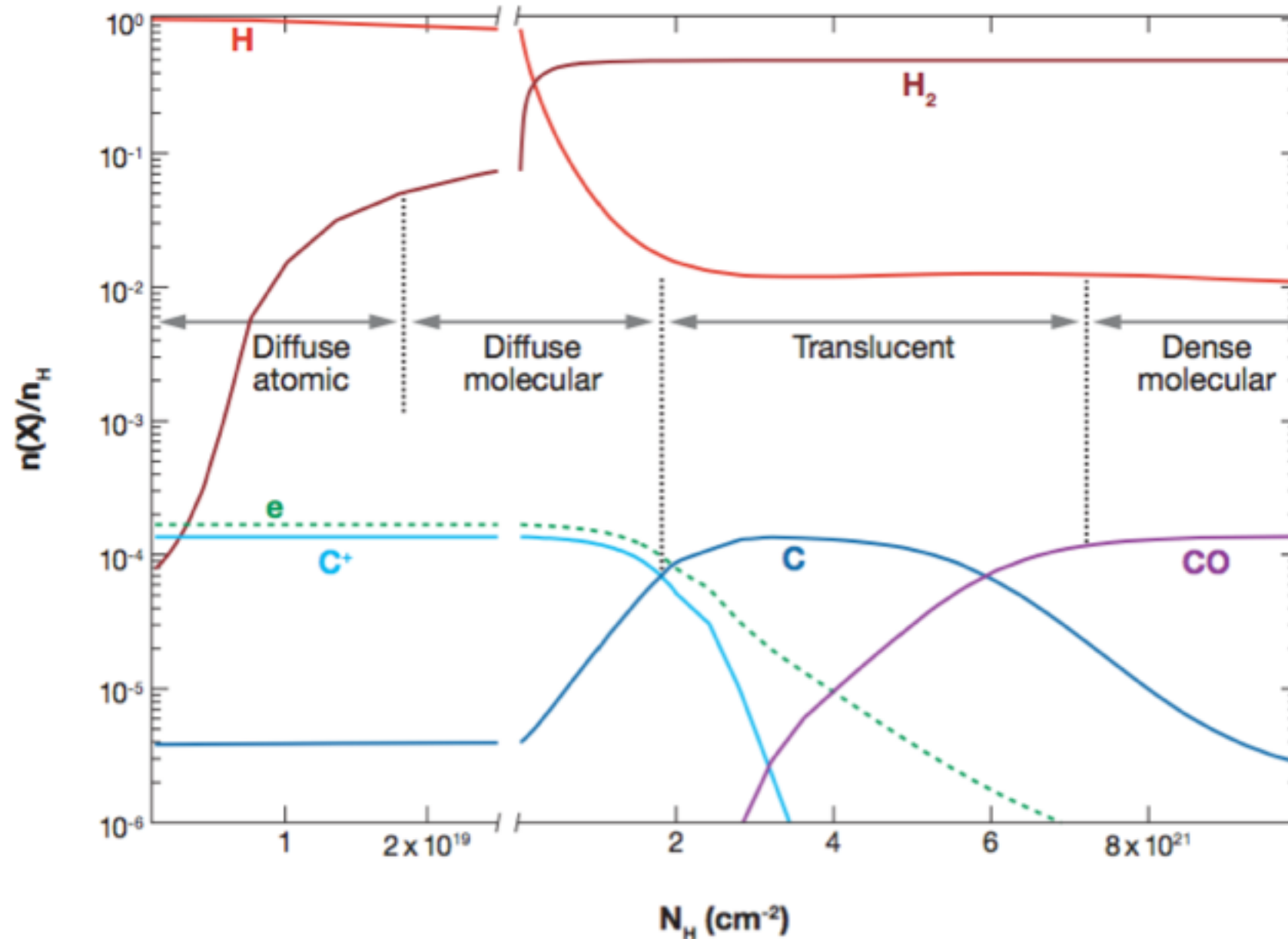
## Destruction

- photoionization
- photodissociation
- incorporation into other molecular species

Dense gas, shielded from UV, but still with ions & dust is ideal for chemistry.

# Chemistry in Molecular Gas

Snow & McCall 2006



**Figure 1**

Results from photodissociation region model [with  $n_H = 100 \text{ cm}^{-3}$  and  $\chi_{UV} = 1$ ] from Neufeld et al. (2005), illustrating the revised definitions of cloud types.

Chemistry happens in diffuse phases,

(& is very interesting - intermittent turbulent dissipation, shattering of dust grains, grain surface reactions, etc)

...but things really get going when  $H_2$  forms.

# Chemistry in Molecular Gas

Astrochemistry is really interesting!

The time scale to reach steady state in the interstellar medium is longer than the dynamical time scale of the physical condition evolution in most regions; as a consequence, the chemical composition depends on the initial conditions (initial chemical composition). For example, under dense cloud conditions (typical temperature of 10 K, density of a few  $10^4 \text{ cm}^{-3}$ , and a visual extinction  $A_V$  of 30 magnitudes<sup>104</sup>), the typical time to reach the steady state for a reservoir molecule such as CO is approximately  $10^9$  yr if both gas-phase chemistry and gas-grain interactions are considered, whereas the typical lifetime of such objects is  $10^7$  yr or shorter.<sup>105,106</sup> Since most chemical models of dense clouds do not take into account the formation of the cloud itself, the computed chemical composition depends on the initial conditions.

Agundez & Wakelam 2013 - arXiv:1310.3651

Chemistry is not in thermochemical equilibrium -  
governed by “chemical kinetics”.



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# Chemistry in Molecular Gas

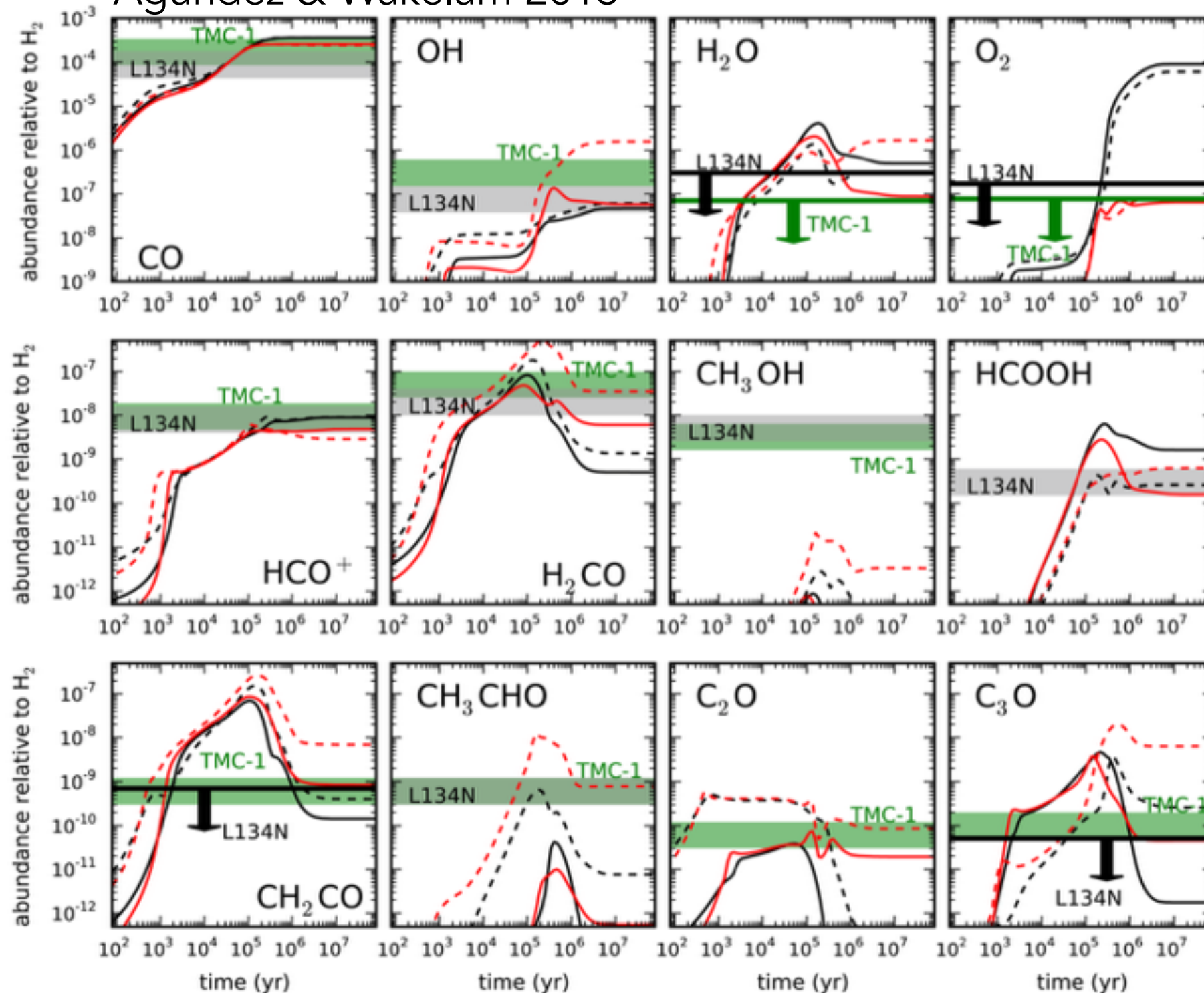
Evidence of non-equilibrium chemistry:

CO is the most abundant molecule after H<sub>2</sub>

Chemical equilibrium models at T=10 K would predict most carbon in CH<sub>4</sub> and most oxygen in H<sub>2</sub>O.

# Chemistry in Molecular Gas

Agundez & Wakelam 2013



# Chemistry in Molecular Gas

Key Elements of Gas Phase Chemistry in Dense Clouds:

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1. Hydrogen is dominantly **molecular** ( $\text{H}_2$  formation on grain surfaces).

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$$\text{H}_3^+ + \text{X} \rightarrow \text{XH}^+ + \text{H}_2.$$

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$$\text{H}_3^+ + \text{X} \rightarrow \text{XH}^+ + \text{H}_2.$$
4. Exothermic reactions with no activation barrier are strongly preferred due to low temperatures. **Ion-neutral reactions** are the most efficient path in these conditions - drive chemical networks.

# Chemistry in Molecular Gas

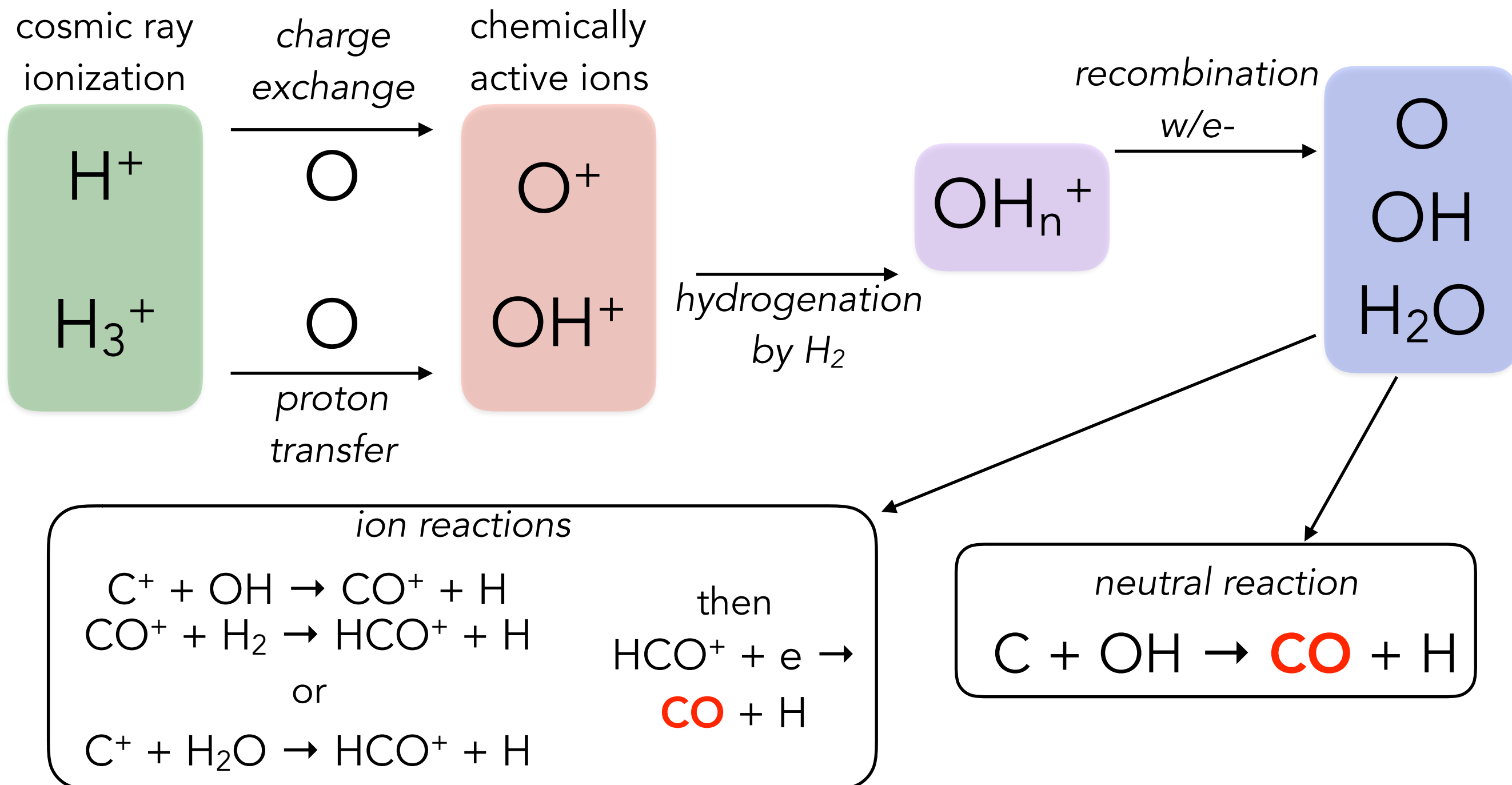
Some key gas phase reaction types:

Type	Example	Notes	typical rate coefficient (k)
Neutral-Radical	$O + H_2 \rightarrow OH + H$	some have thermal activation barriers	$\sim 10^{-10} \text{ cm}^3 \text{ s}^{-1}$
Ion-Molecule	$H^+ + O \rightarrow O^+ + H$ $O^+ + H_2 \rightarrow OH^+ + H$ $H_3^+ + O \rightarrow OH^+ + H_2$	<- charge exchange <- H abstraction <- proton transfer	$\sim 10^{-9} \text{ cm}^3 \text{ s}^{-1}$
Radiative Association	$H + H^+ \rightarrow H_2^+ + h\nu$	only important if other pathways lacking	very low
Photodissociation	$h\nu + OH \rightarrow O + H$	always important	$\sim 10^{-10} \text{ cm}^3 \text{ s}^{-1}$
Dissociative Recombination	$e + H_3^+ \rightarrow 3H, H_2 + H$ (branching 3:1)	always important	$\sim 10^{-7} \text{ cm}^3 \text{ s}^{-1}$

info from A. Glassgold Ay216 at Berkeley

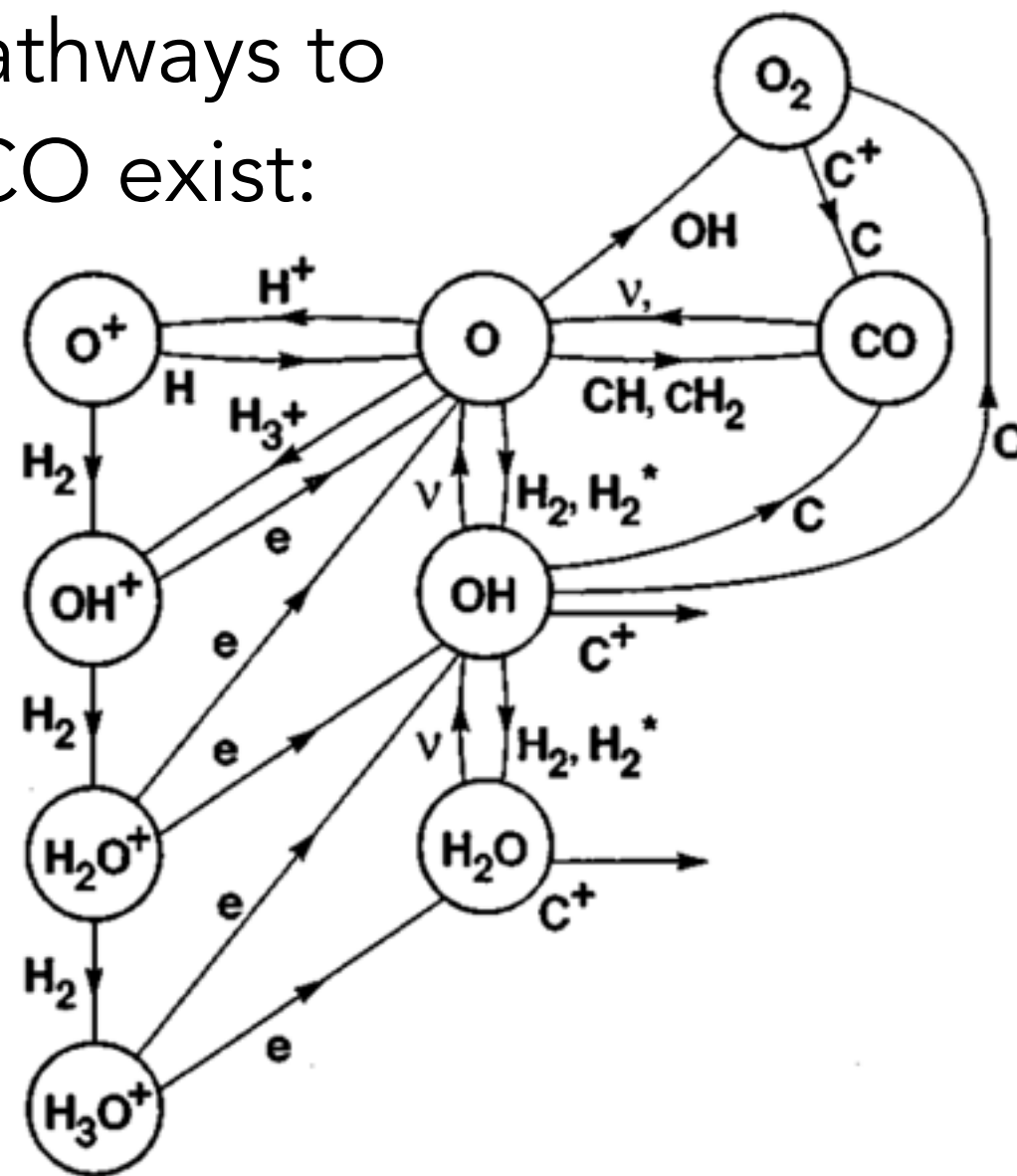
# Chemistry in Molecular Gas

Carbon Monoxide - most abundant molecule after  $H_2$

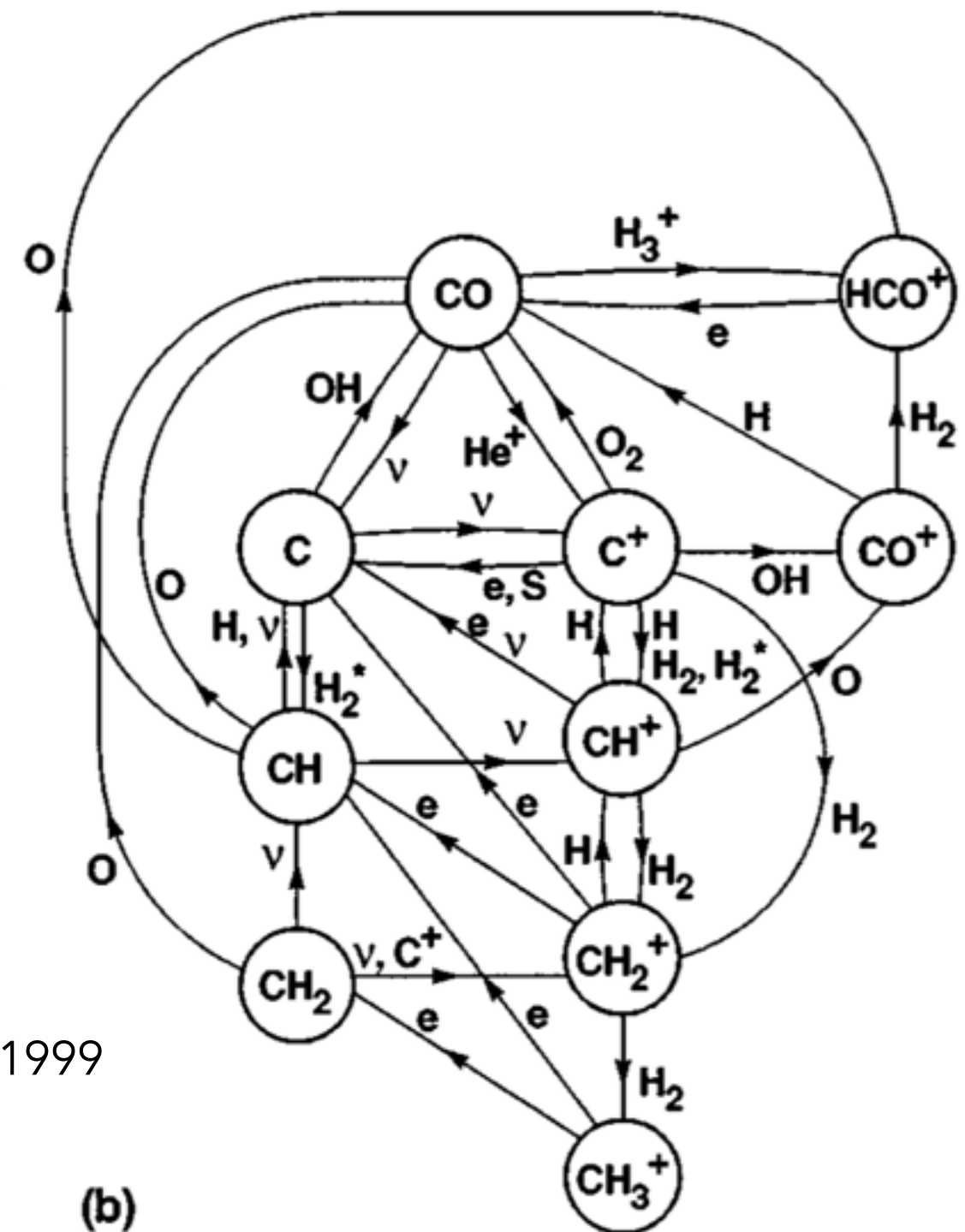


# Chemistry in Molecular Gas

Many pathways to form CO exist:



(a)



(b)

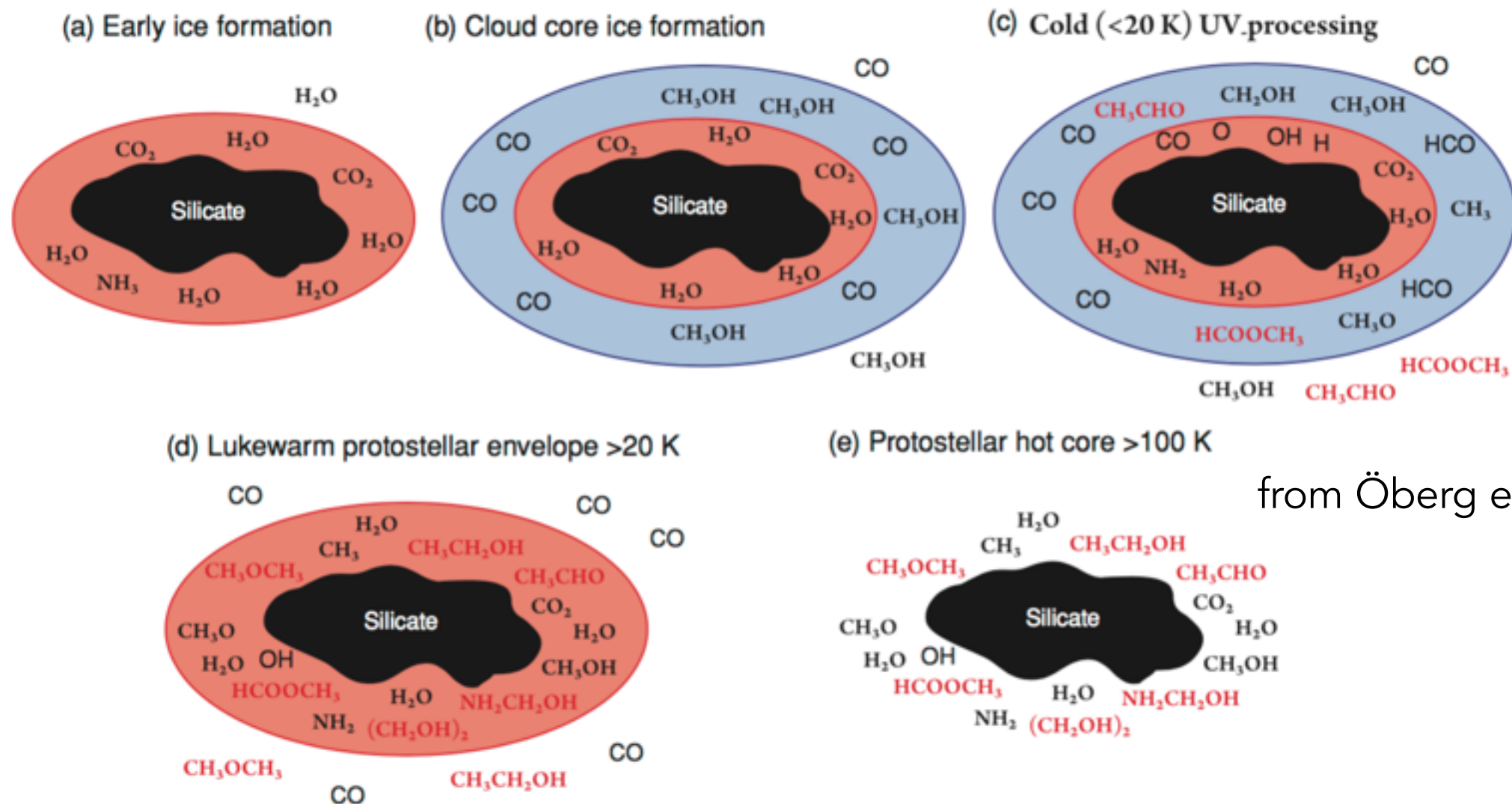
from Hollenbach & Tielens 1999



# Chemistry in Molecular Gas

In dense parts of clouds

CO can "freeze out" to form ice on grains.

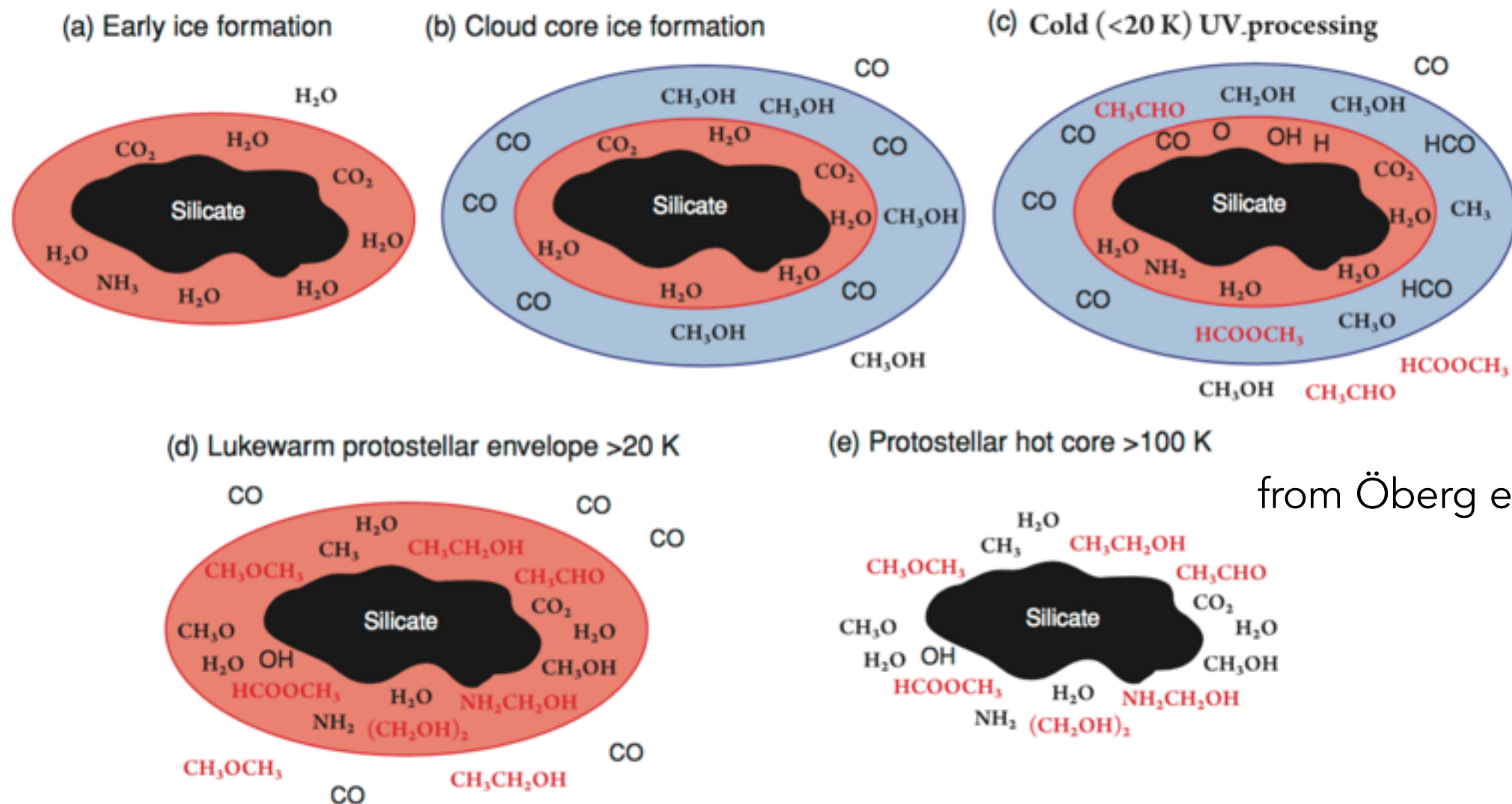


from Öberg et al. 2010

**Figure 7.** Suggested evolution of ices during star formation. Pink indicates an H<sub>2</sub>O-dominated ice and blue a CO-dominated ice. At each cold stage a small amount of the ice is released non-thermally. Early during cloud formation (a) an H<sub>2</sub>O-rich ice forms. Once a critical density and temperature is reached CO freezes out catastrophically (b), providing reactants for CH<sub>3</sub>OH ice formation. Far away from the protostar (c), photoprocessing of the CO-rich ice results in the production of, e.g., HCOOCH<sub>3</sub>. Closer to the protostar (d), following sublimation of CO, other complex molecules become abundant. Finally, all ice desorb thermally close to the protostar >100 K (e).

# Chemistry in Molecular Gas

Grain surface chemistry + Ice mantle chemistry  
can lead to complex molecules!



from Öberg et al. 2010

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# Tracing Molecular Gas

$\text{H}_2$  is difficult to detect in cold, dense gas.  
First rotational level requires  $T > 100 \text{ K}$  to excite.

Need “tracers” for molecular gas:

- CO rotational emission
- dust extinction or emission
- other molecules rotational lines
- $\gamma$ -rays

CO is the easiest -  
bright & can be observed from the ground

# Tracing Molecular Gas

## The CO-to-H<sub>2</sub> Conversion Factor

column  
density of H<sub>2</sub>

integrated  
intensity of CO line

$$N_{\text{H}_2} = X_{\text{CO}} I_{\text{CO}}$$

$$X_{\text{CO}}: [\text{cm}^{-2} (\text{K km s}^{-1})^{-1}]$$

molecular gas  
mass surface  
density

integrated  
intensity of CO line

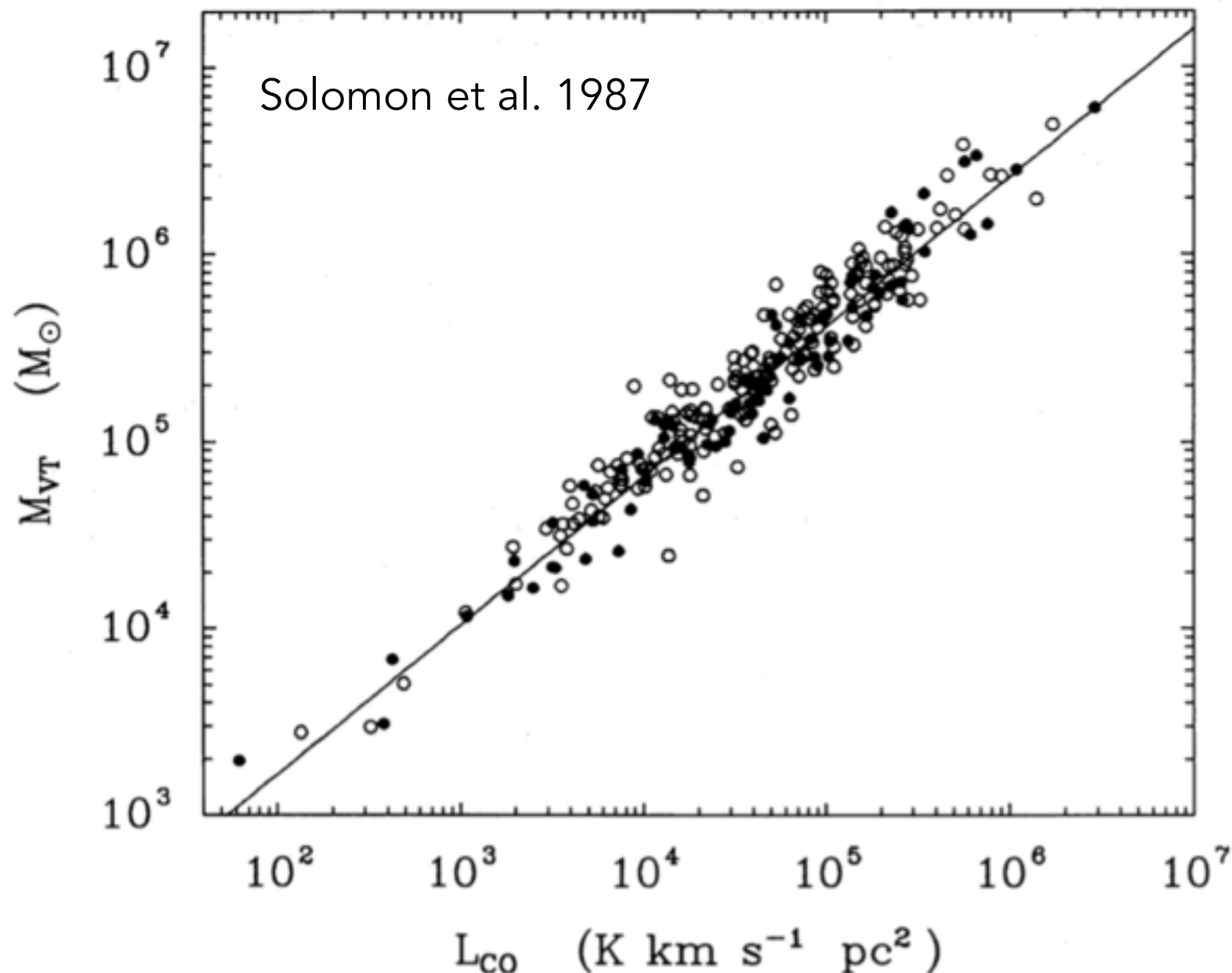
$$\Sigma_{\text{mol}} = \alpha_{\text{CO}} I_{\text{CO}}$$

$$\alpha_{\text{CO}}: [M_{\odot} \text{ pc}^{-2} (\text{K km s}^{-1})^{-1}]$$



# Tracing Molecular Gas

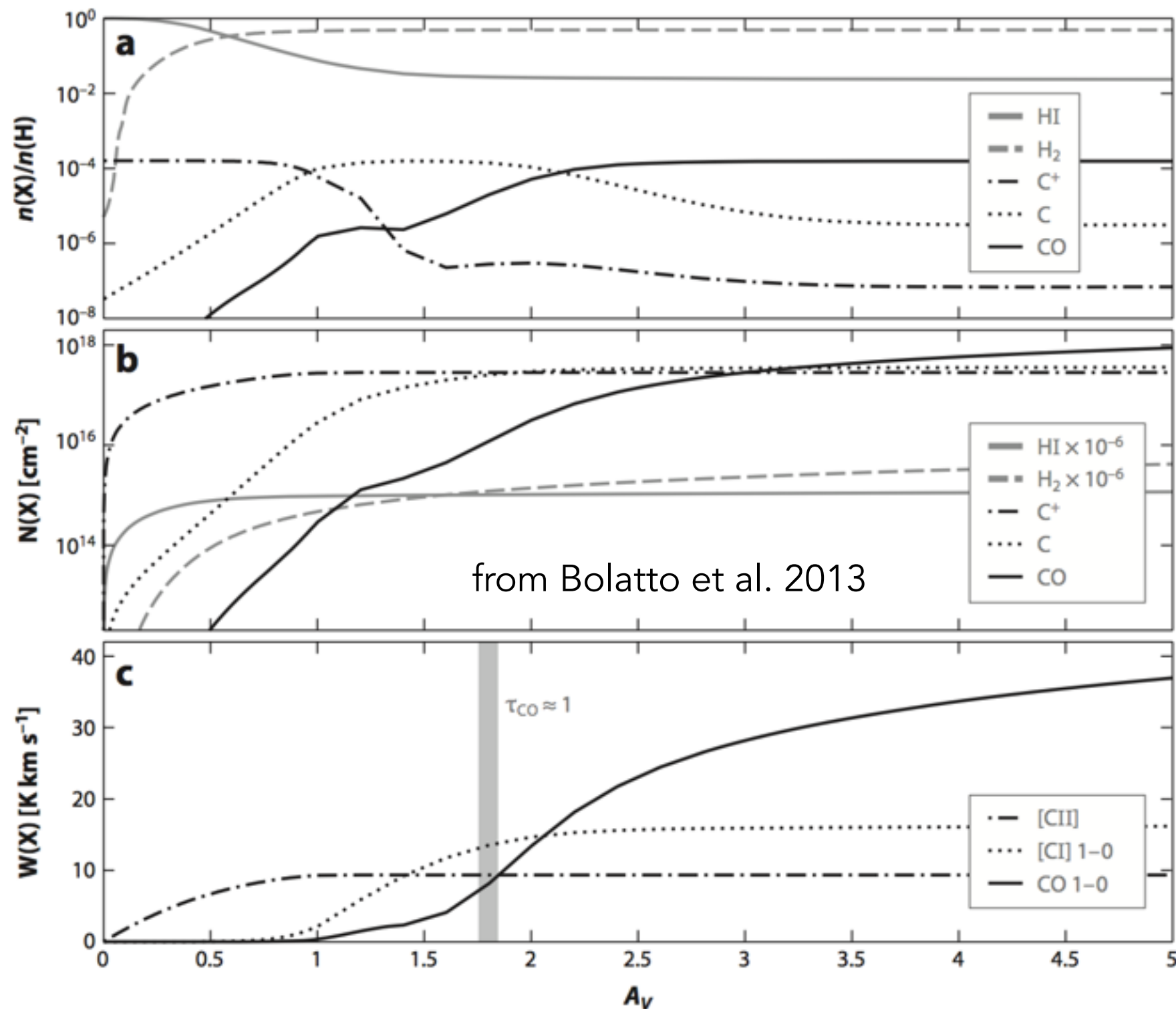
## The CO-to-H<sub>2</sub> Conversion Factor



assuming clouds  
are in virial equilibrium  
you can use their  
velocity dispersion &  
sizes to calculate  
their mass

Correlation between  
CO luminosity & inferred  
mass led to first  
 $X_{\text{CO}}$  calibrations

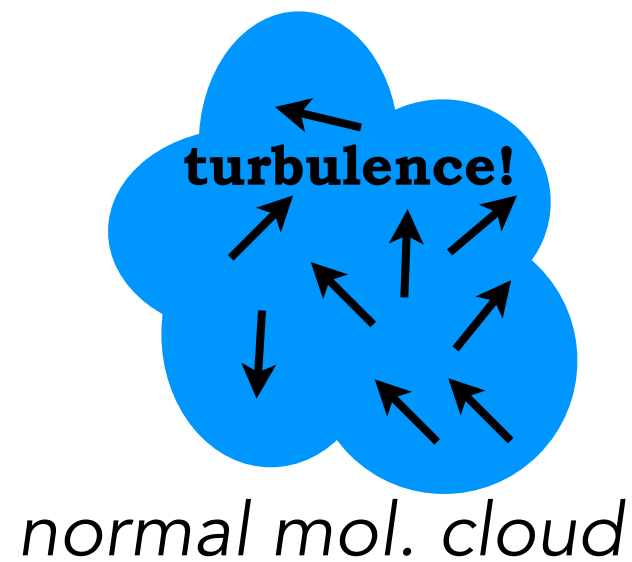
# Tracing Molecular Gas



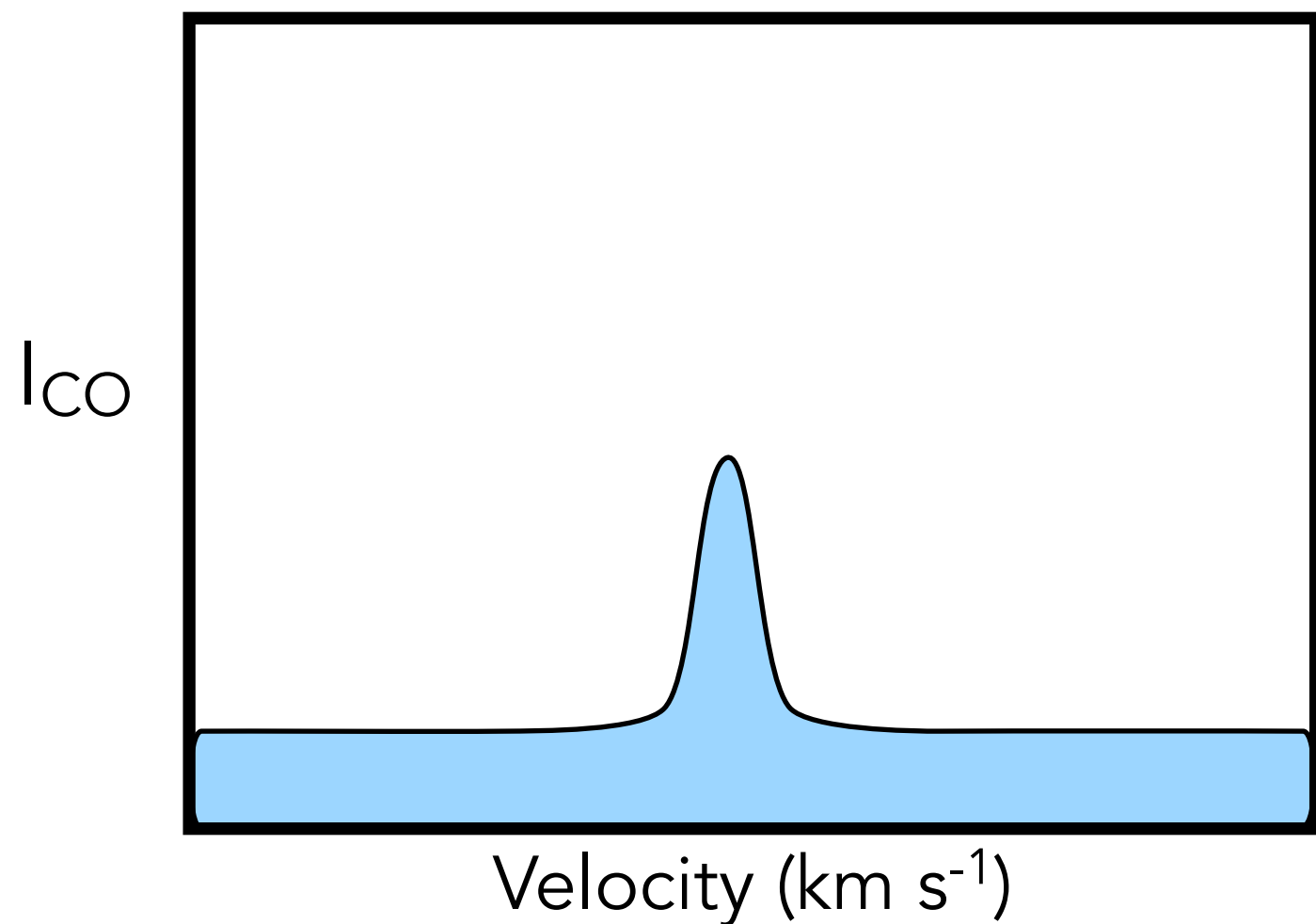
One key point:  
<sup>12</sup>CO low-J  
 rotational emission  
 is very optically  
 thick!

*How does an  
 optically thick line  
 tell you the mass?*

# What Sets $\alpha_{\text{CO}}$ ?



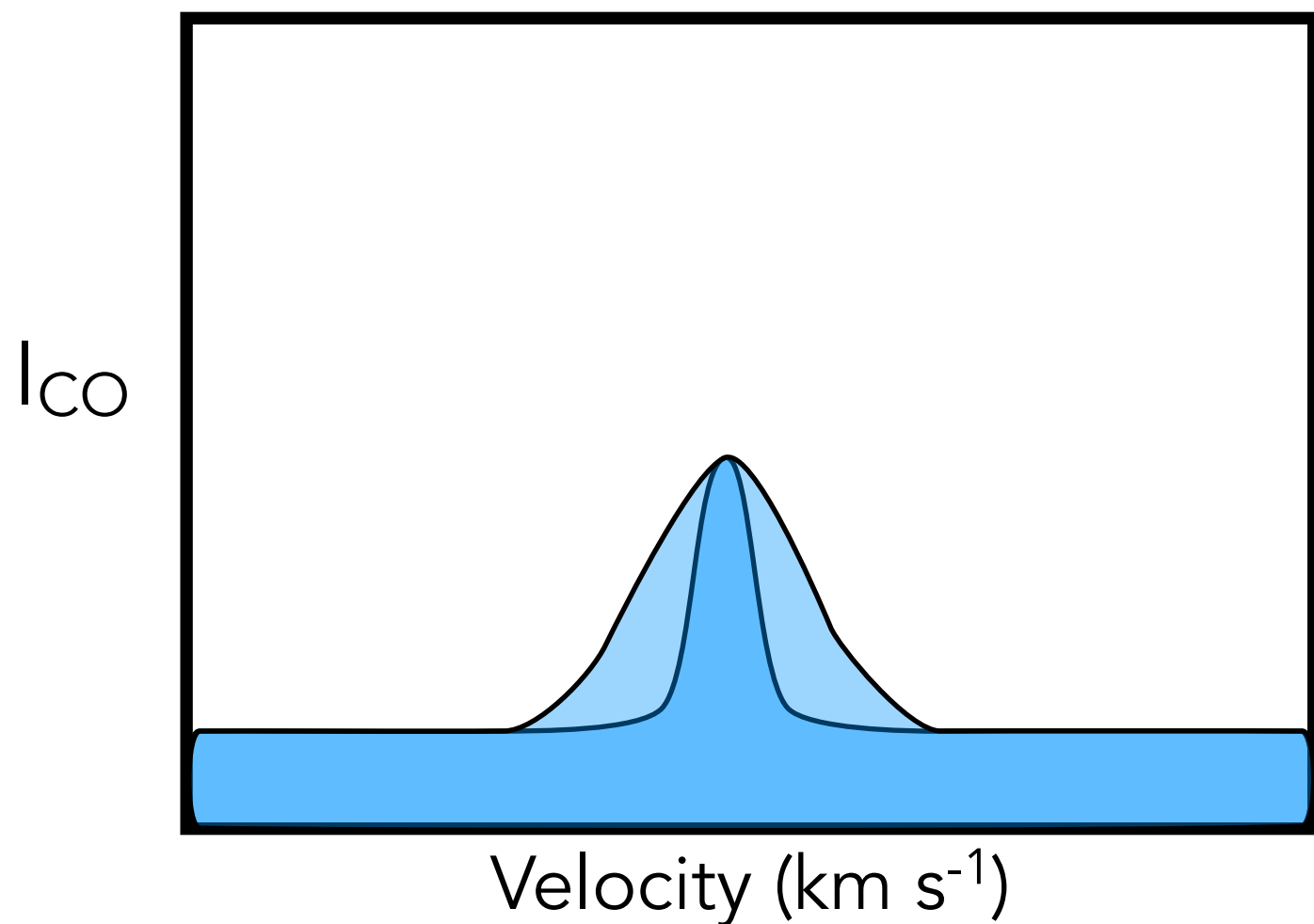
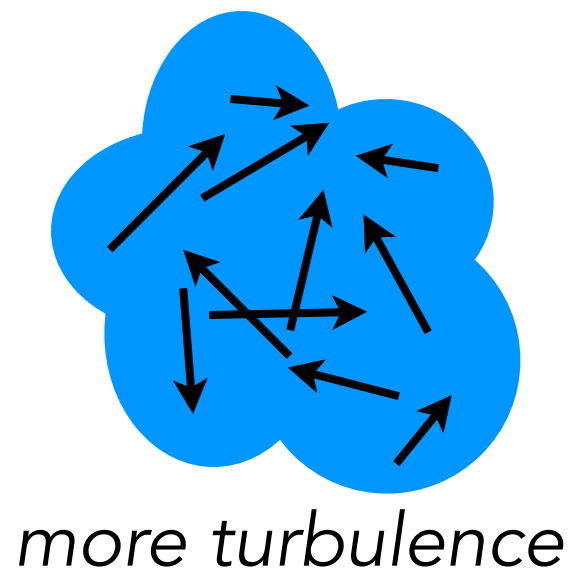
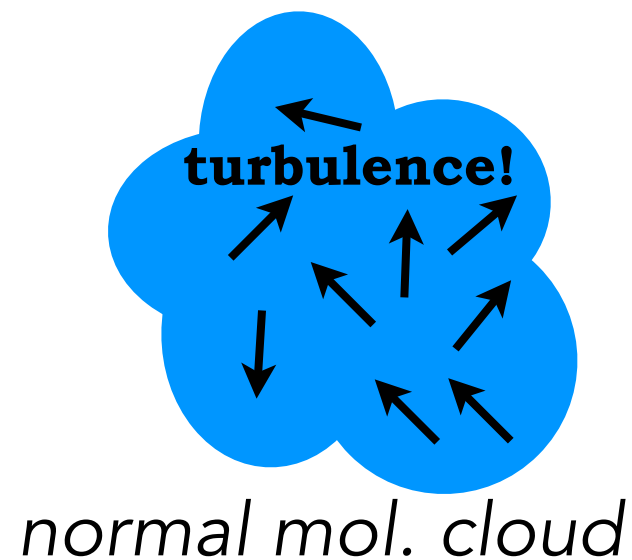
Effects of molecular cloud properties  
on  $\alpha_{\text{CO}}$ .



Peak brightness = excitation temperature of CO  
line width = turbulent velocity dispersion

# What Sets $\alpha_{\text{CO}}$ ?

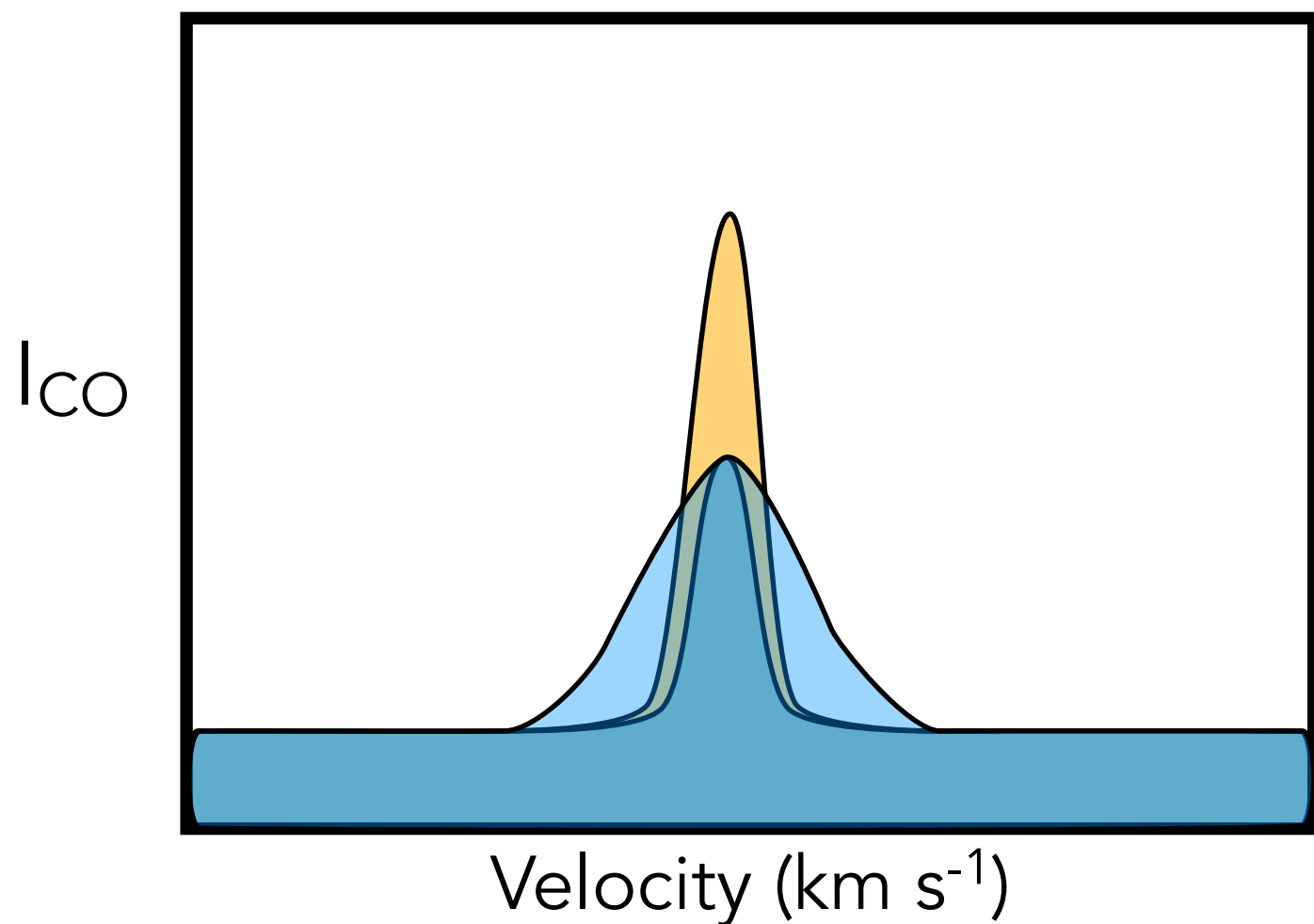
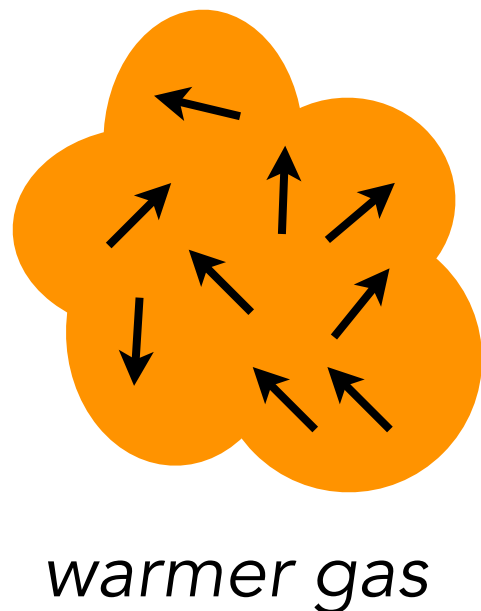
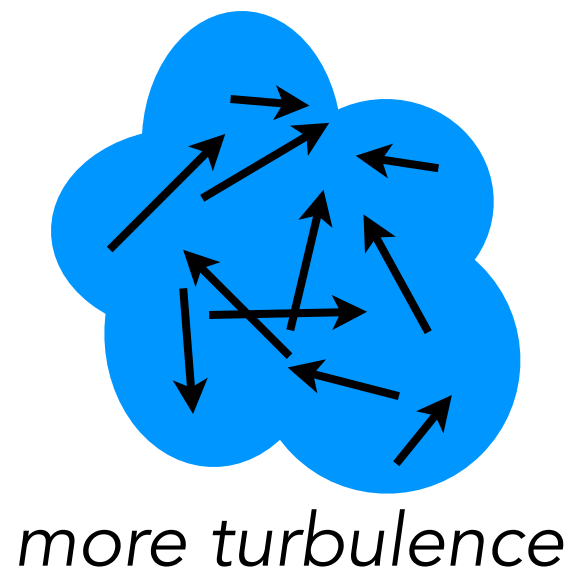
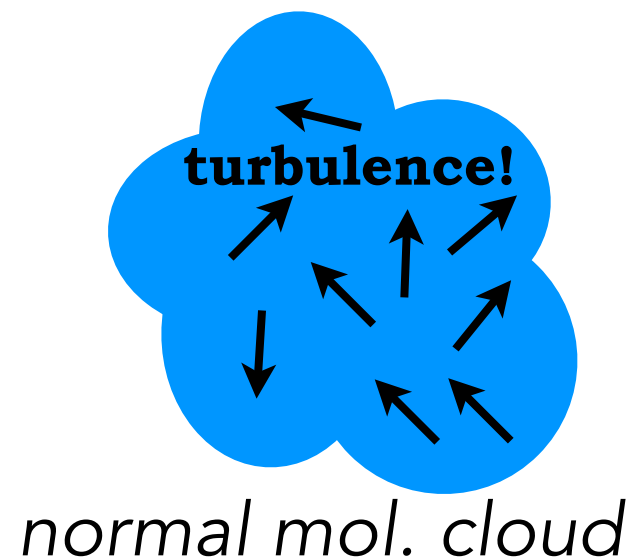
Effects of molecular cloud properties  
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Effects of molecular cloud properties  
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Peak brightness = excitation temperature of CO  
line width = turbulent velocity dispersion



# Tracing Molecular Gas

The CO-to-H<sub>2</sub> Conversion Factor

X<sub>CO</sub> works to first order because:

- 1) turbulent velocity dispersion is correlated with the mass (& size) of cloud - *Larson's Laws*
- 2) clouds we see around us in the MW have pretty limited ranges of n,T

# Tracing Molecular Gas

## The CO-to-H<sub>2</sub> Conversion Factor

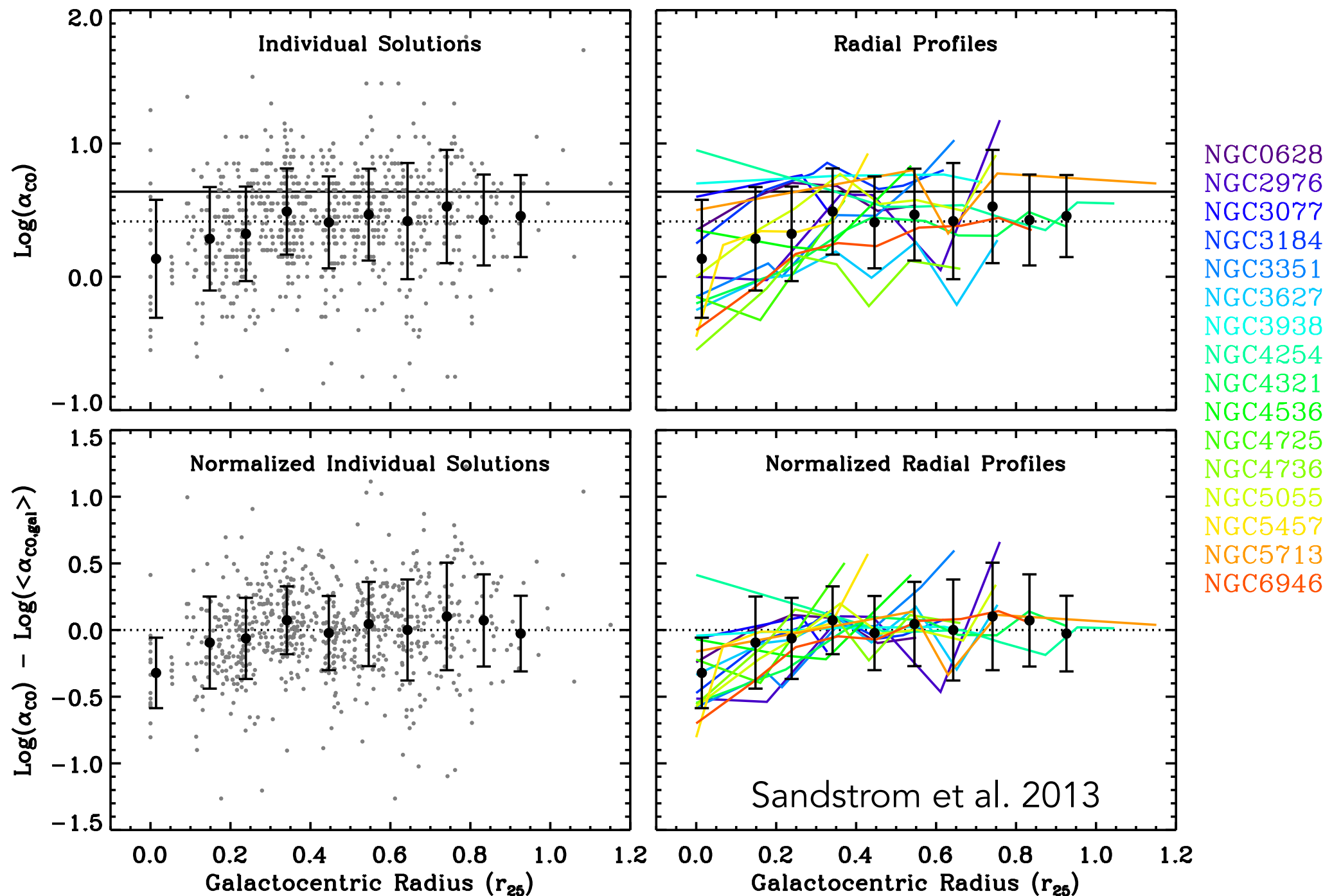
**Table 1** Representative  $X_{\text{CO}}$  values in the Milky Way disk

from Bolatto et al. 2013

Method	$X_{\text{CO}}/10^{20}\text{cm}^{-2}$ (K km s <sup>-1</sup> ) <sup>-1</sup>	References
Virial	2.1	Solomon et al. (1987)
	2.8	Scoville et al. (1987)
Isotopologues	1.8	Goldsmith et al. (2008)
Extinction	1.8	Frerking, Langer & Wilson (1982)
	2.9–4.2	Lombardi, Alves & Lada (2006)
	0.9–3.0	Pineda, Caselli & Goodman (2008)
	2.1	Pineda et al. (2010b)
	1.7–2.3	Paradis et al. (2012)
Dust emission	1.8	Dame, Hartmann & Thaddeus (2001)
	2.5	Planck Collaboration XIX et al. (2011)
$\gamma$ -rays	1.9	Strong & Mattox (1996)
	1.7	Grenier, Casandjian & Terrier (2005)
	0.9–1.9 <sup>a</sup>	Abdo et al. (2010c)
	1.9–2.1 <sup>a</sup>	Ackermann et al. (2011, 2012c)
	0.7–1.0 <sup>a</sup>	Ackermann et al. (2012a,b)

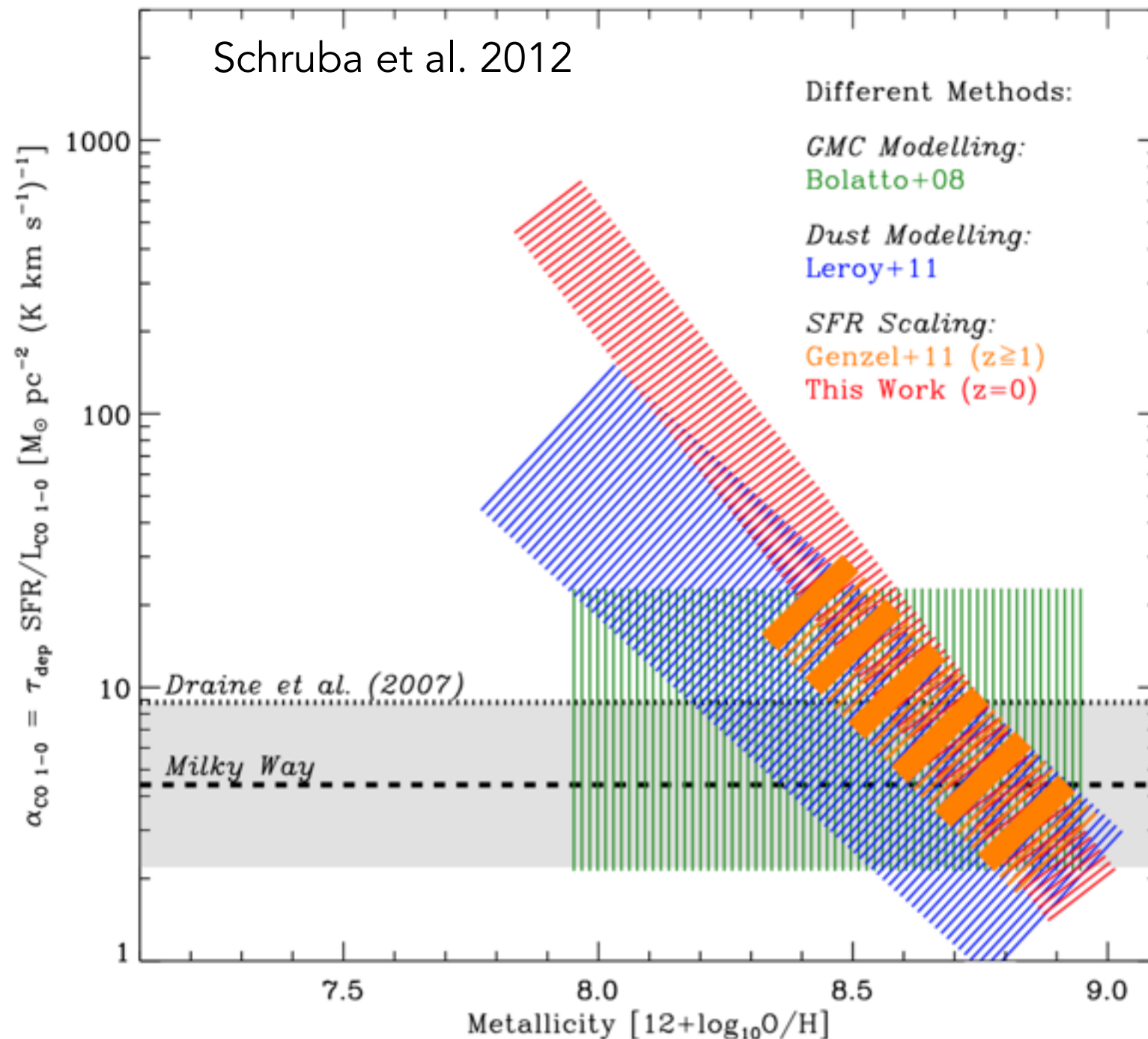
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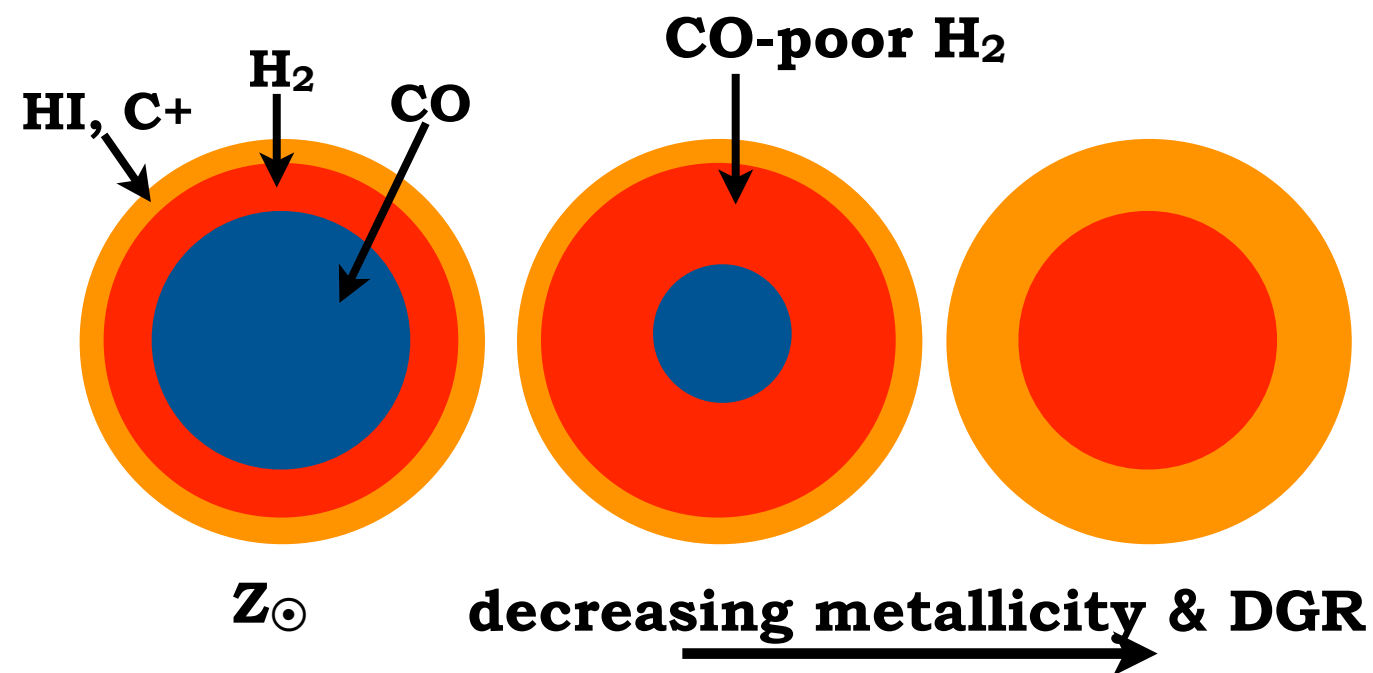
Things really fall apart  
at low metallicity!

$$X_{\text{CO}} \gg X_{\text{CO}, \text{MW}}$$

# Tracing Molecular Gas

## The CO-to-H<sub>2</sub> Conversion Factor

H<sub>2</sub> self-shields, but CO relies on dust,  
when there is little dust, CO is photodissociated.

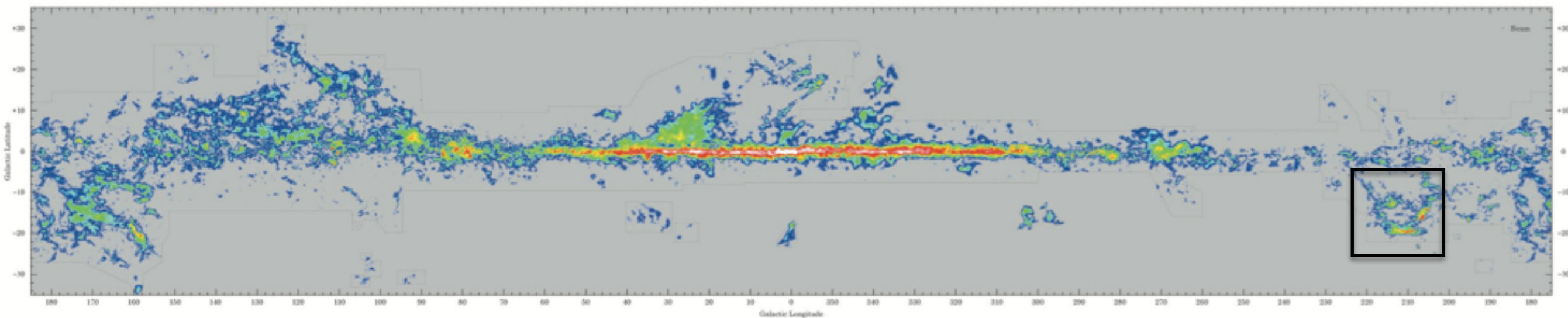


e.g. Maloney & Black 1988, Bolatto et al. 1999,  
Wolfire et al. 2010, Glover & Mac Low 2011

# Observations of Molecular Gas

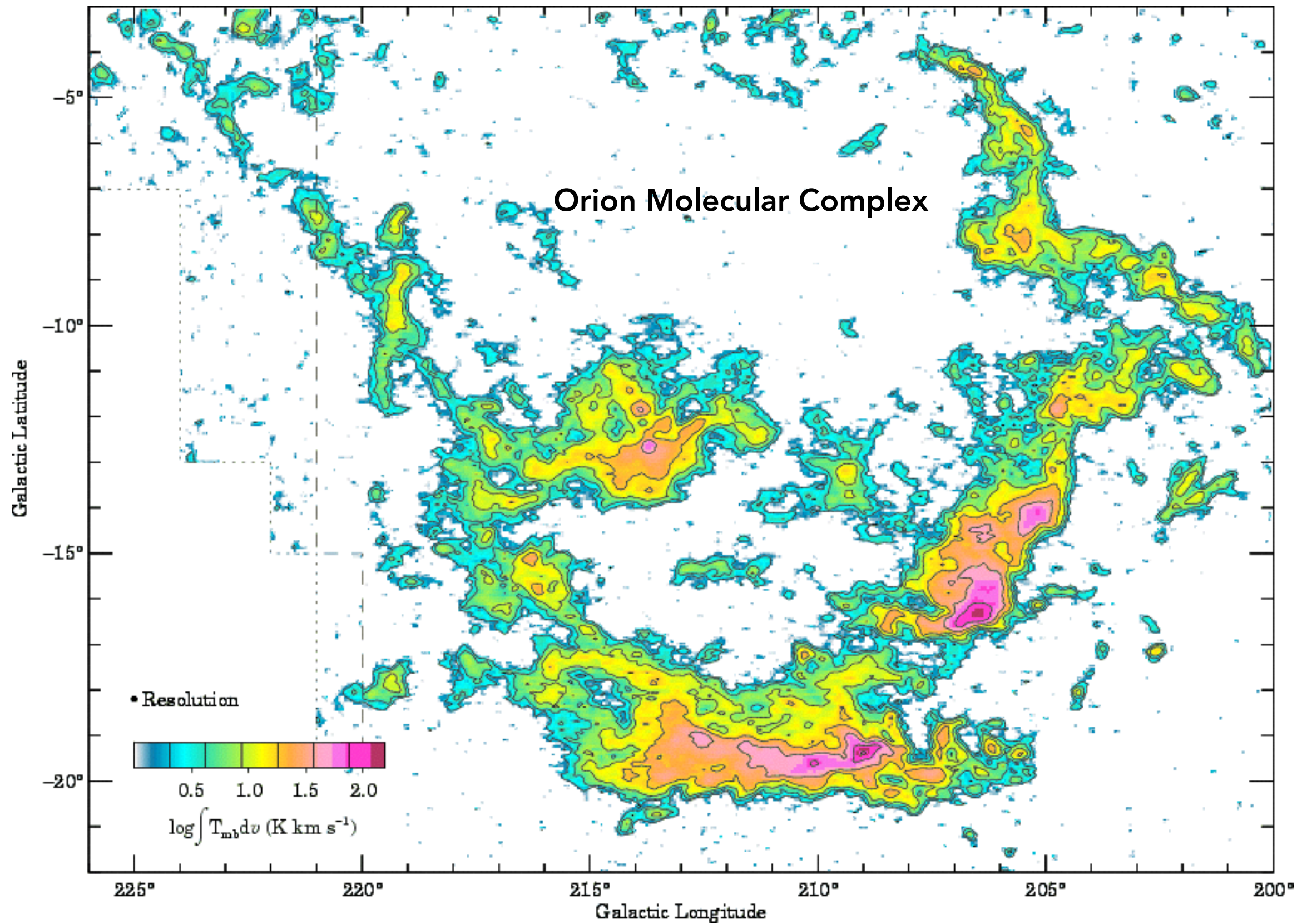
What are “clouds”?

Dame et al. 2001

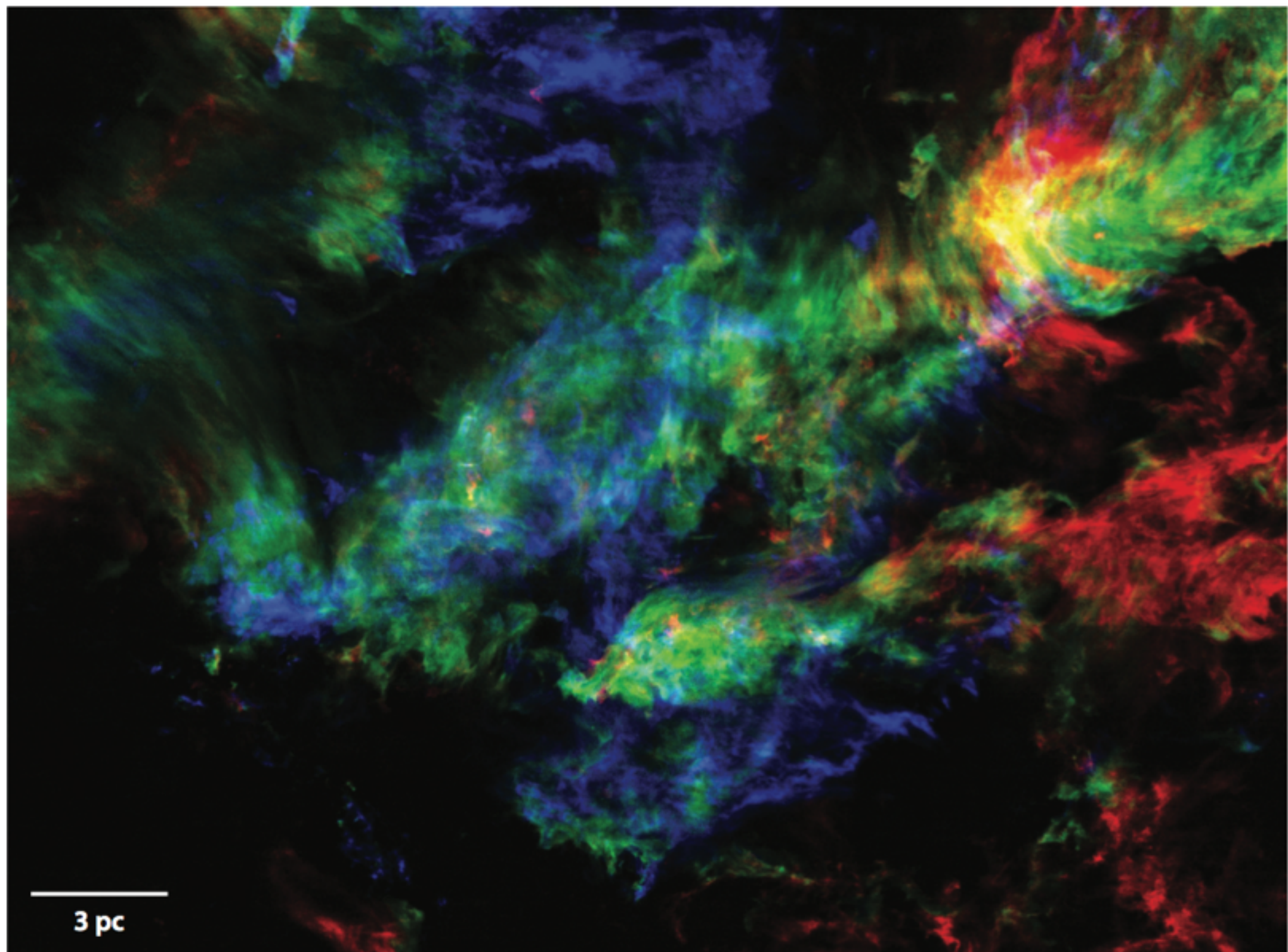




Wilson et al. 2005







**Taurus Molecular cloud**

Heyer & Dame 2015

**Figure 10**

An image of  $^{12}\text{CO } J = 1-0$  emission from the Taurus molecular cloud integrated over  $v_{\text{LSR}}$  intervals  $0-5 \text{ km s}^{-1}$  (*blue*),  $5-7.5 \text{ km s}^{-1}$  (*green*), and  $7.5-12 \text{ km s}^{-1}$  (*red*), illustrating the intricate surface brightness distribution and complex velocity field of the Taurus cloud. The data are from Narayanan et al. (2008). Adapted from figure 12 of Goldsmith et al. (2008) and reproduced with permission from AAS.