Physics 224
The Interstellar Medium

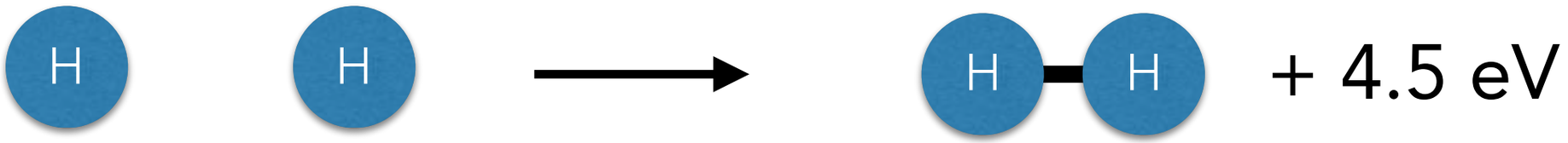
Lecture #14: Molecular Gas, Photodissociation Regions & the HI to H_2 transition

Outline

- Part I: HI to H_2 Transition
- Part II: Photodissociation Regions
- Part III: Molecular Gas Chemistry
- Part IV: Tracing Molecular Gas
- Part V: Observations of Molecular Gas

Forming H_2

Formation of H_2 by gas-phase reactions is slow



no effective way to carry away 4.5 eV worth of binding energy when two H bond, no dipole moment

negligible rate for this reaction

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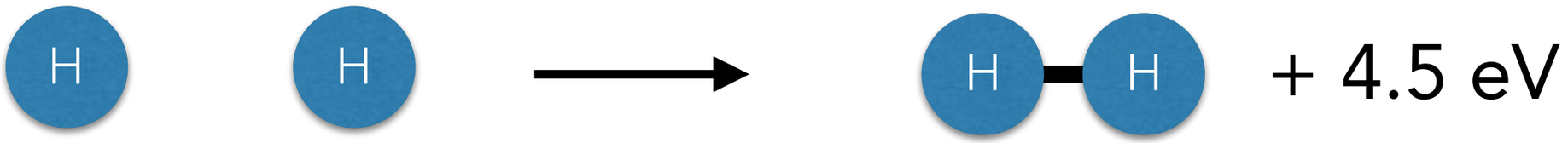

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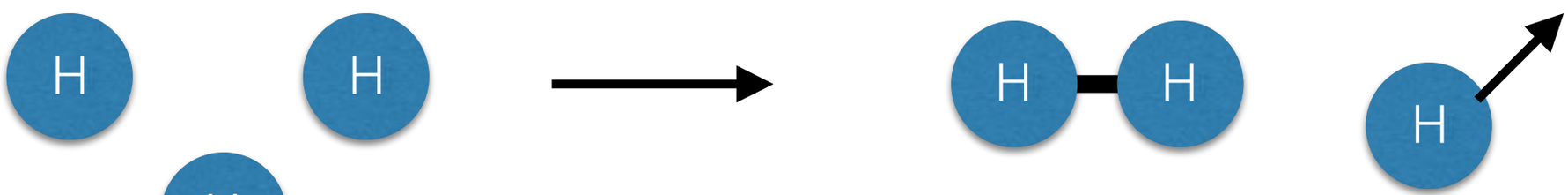


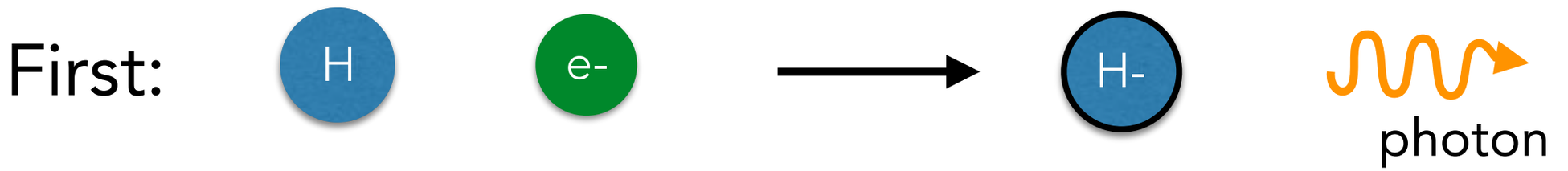
3-body reaction can occur quicker

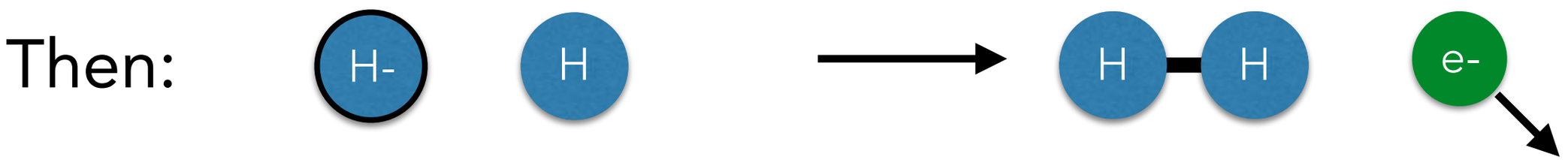
but this is still very slow

Forming H_2

Formation of H_2 by gas-phase reactions is slow

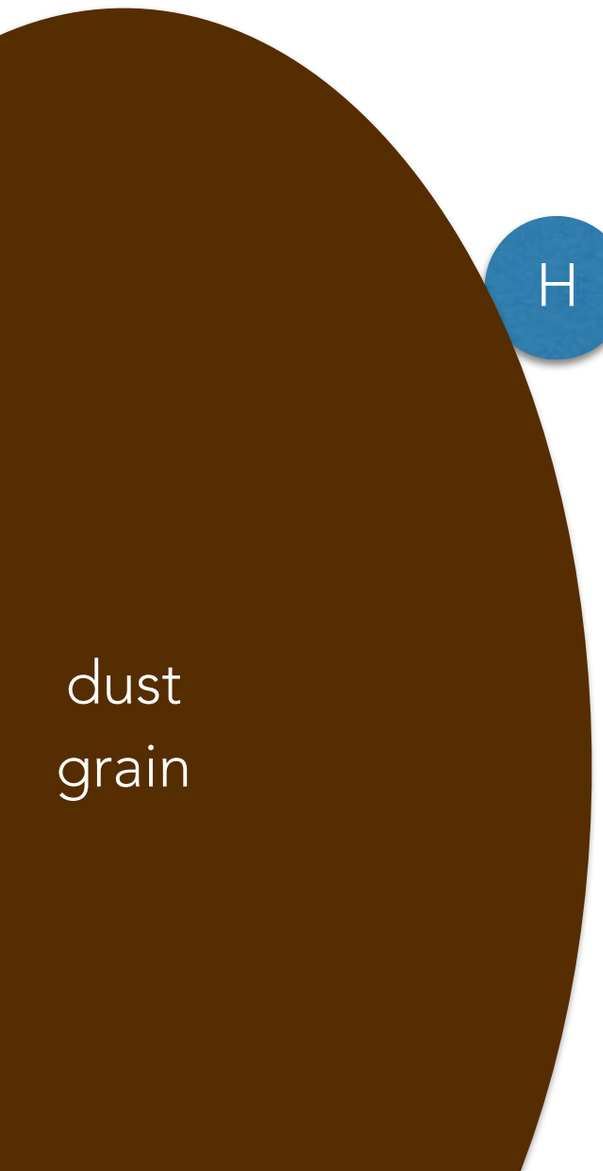
Fastest gas-phase route is “associative attachment”





Forming H_2

Grain Surface H_2 formation is much faster if there is dust.



Depends on:
collision rate of H with grain (n,T)
available grain surface area
"sticking" probability

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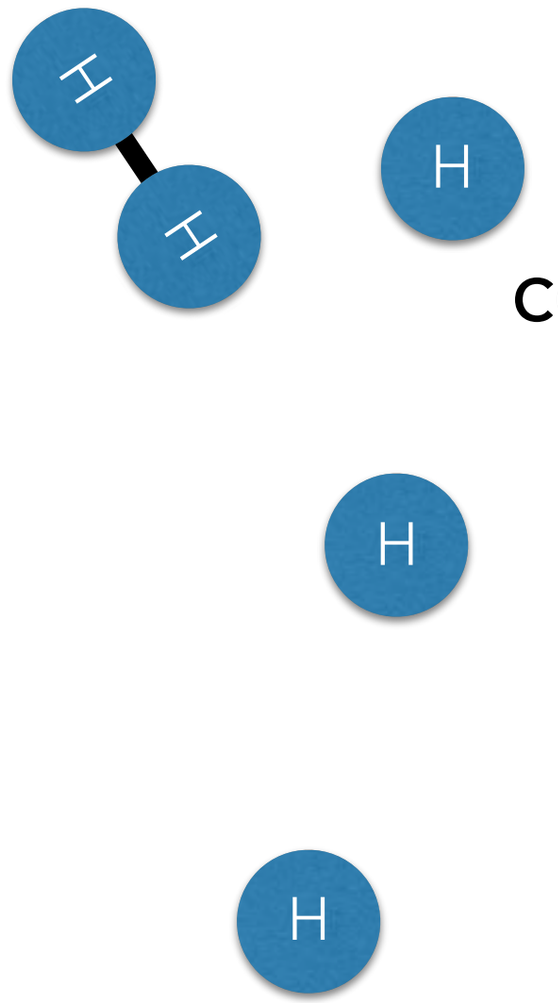

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$$\left(\frac{dn(\mathrm{H_2})}{dt}\right)_{\mathrm{gr}} = R_{\mathrm{gr}}\ n_H\ n(H)$$

n_H: total density of hydrogen in any form

$n(H)$: density of H atoms

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density of H atoms

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$$R_{\mathrm{gr}} = \frac{1}{2}\left(\frac{8kT}{\pi m_H}\right)^{1/2} \langle \epsilon_{\mathrm{gr}} \rangle\, \Sigma_{\mathrm{gr}}$$

v_{thermal}

average "sticking" coeff for grain pop

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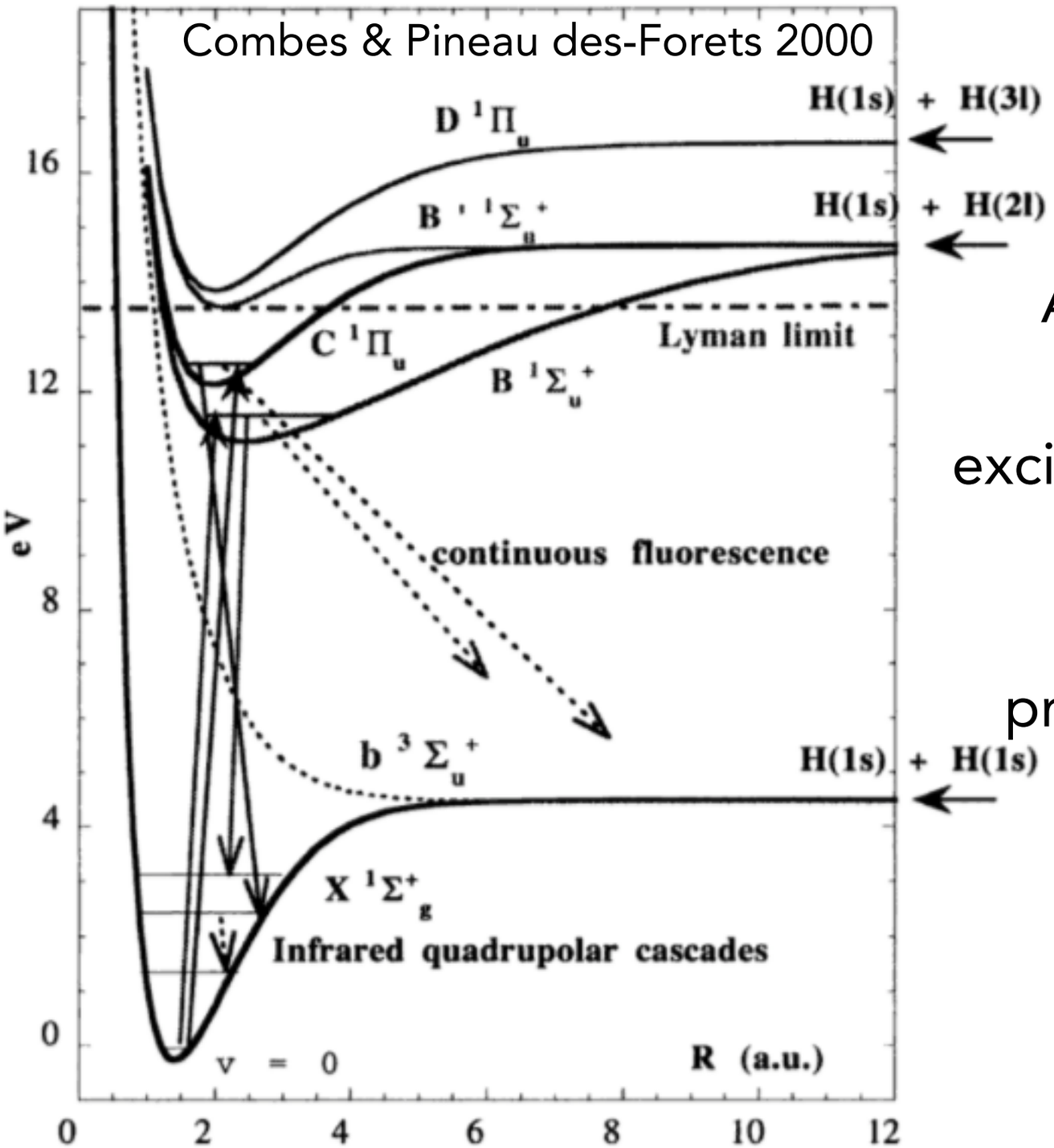
$v_{thermal}$

average "sticking" coeff for grain pop

Grain surface area

$$\Sigma_{\mathrm{gr}} \equiv \frac{1}{n_H} \int \pi a^2 \frac{dn_{\mathrm{gr}}}{da} da$$

Photodissociation of H_2



After H_2 absorbs a UV photon from ground to one of the excited levels (Lyman-Werner bands) has ~85% probability of radiative decay, ~15% probability of photo-dissociating

Lyman band = ground -> B
Werner band = ground -> C

Photodissociation of H_2

$$\varsigma_{\rm diss} = \sum_u \varsigma_{l \rightarrow u} \, p_{{\rm diss},u}$$

dissociation rate

sum of rates for transitions from ground state to excited states

probability of photo-dissociation from upper state

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probability of photo-dissociation from upper state

depends on quantum mechanics and radiation field intensity at relevant wavelengths

H_2 Abundance

In steady state:

photo-dissociation

$$\varsigma_{\rm diss} n(H_2) = R_{\rm gr} n_H n(H)$$

formation on dust grains

For CNM conditions this is pretty small:

$$\frac{n(H_2)}{n_{/\!/}} \approx 1.8 \times 10^{-5} \left(\frac{n(H)}{30{\rm cm}^{-3}}\right) \left(\frac{R_{\rm gr}}{3 \times 10^{-17}{\rm cm}^3{\rm s}^{-1}}\right) \left(\frac{\varsigma_{\rm diss}}{5 \times 10^{-11}{\rm s}^{-1}}\right)^{-1}$$

But we have left out an important component: shielding

H_2 Abundance

Sternberg et al. 2014

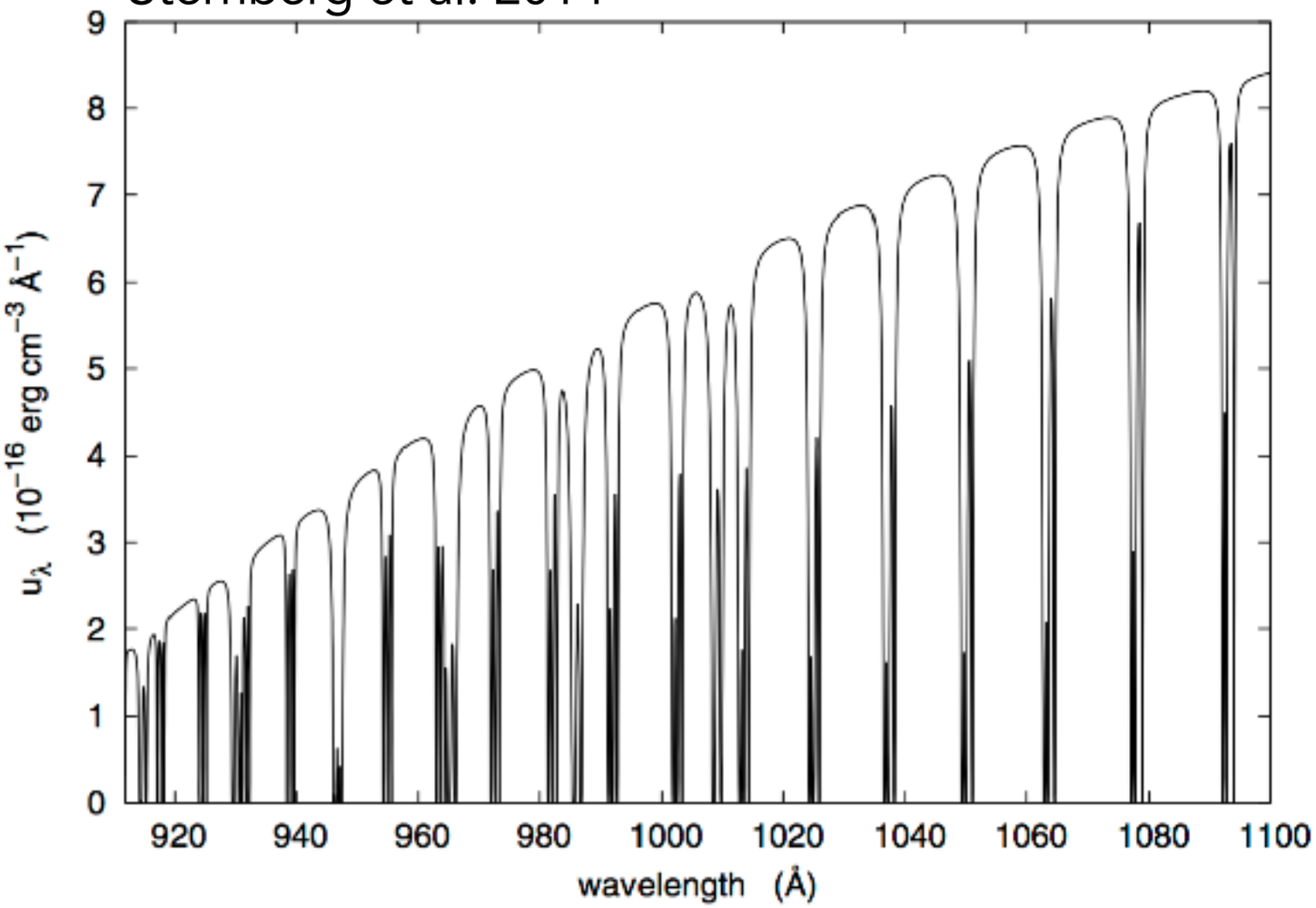
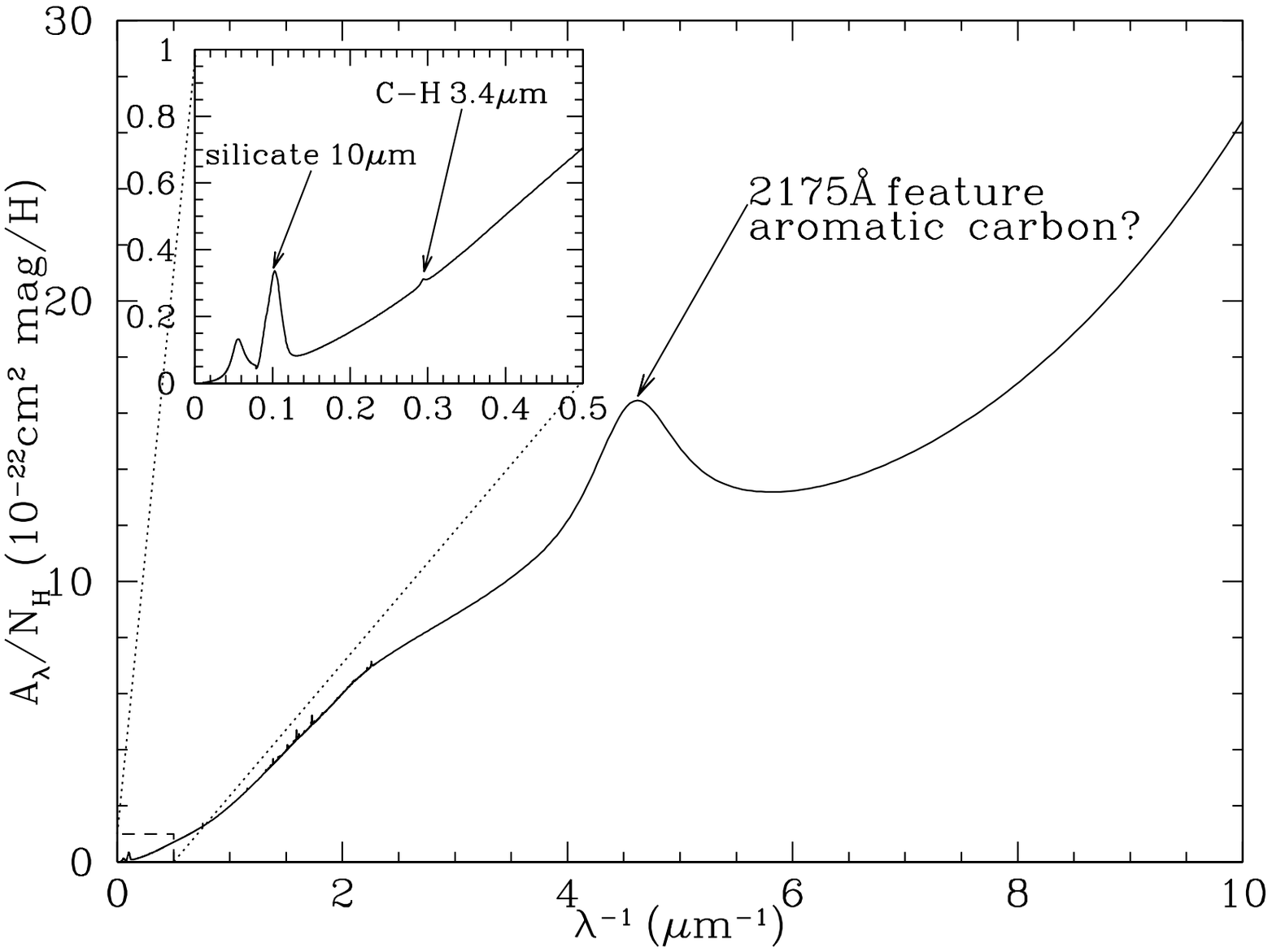


Figure 2. Absorbed far-UV spectrum showing partially overlapping Lyman–Werner band absorption lines, for beamed radiation into a cloud, at a total hydrogen gas column density of 3.74×10^{20} cm^{-2}, for a free-space radiation intensity $I_{\rm UV} = 35.5$, gas density $n = 10^3$ cm^{-3}, and metallicity $Z' = 1$ ($\alpha G/2 = 1$).

H_2 Lyman-Werner bands can become optically thick and shield interior H_2 from being dissociated.

H_2 Abundance



At UV wavelengths even small A_V corresponds to substantial amounts of UV extinction.

H_2 Abundance

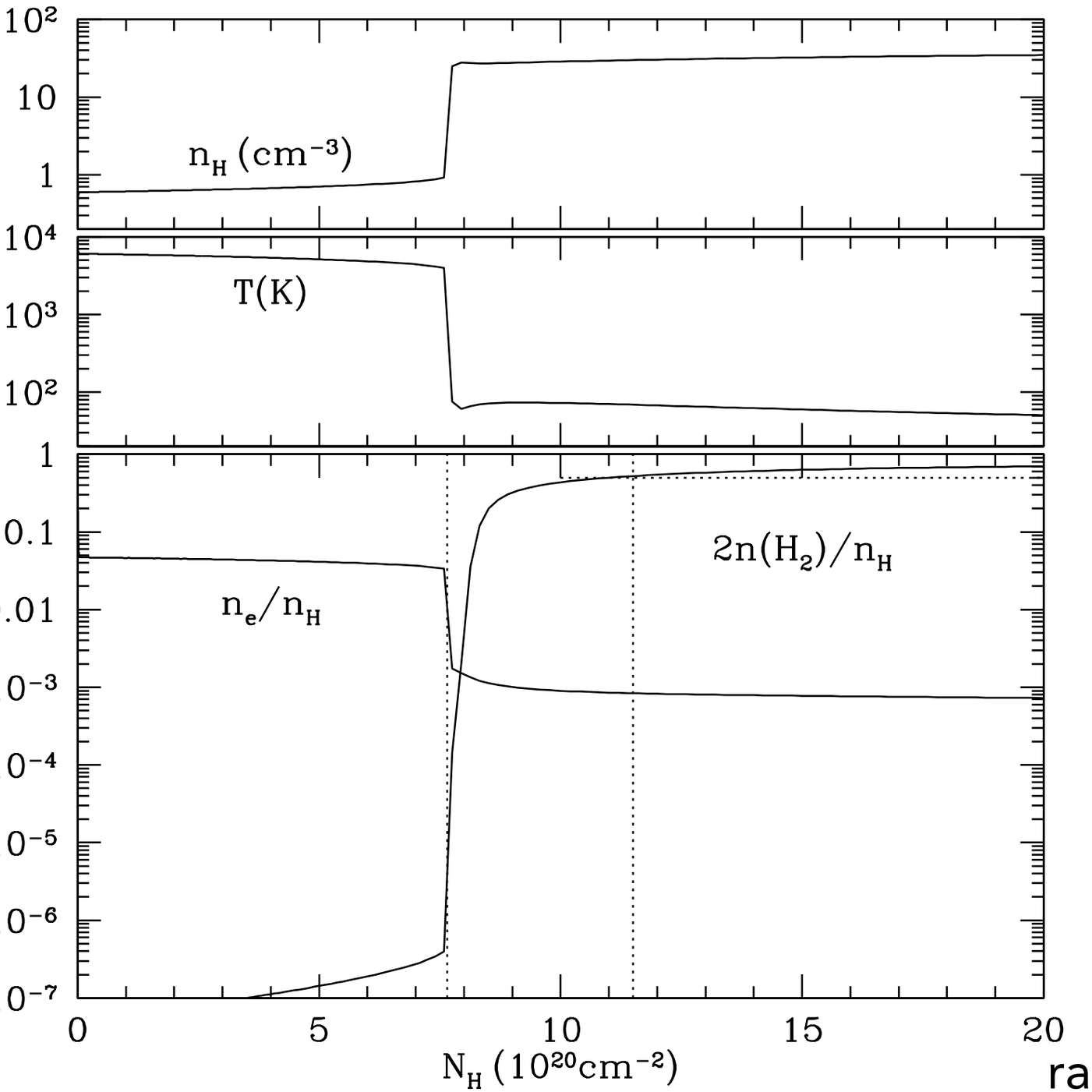
$$\varsigma_{\rm diss} \approx \varsigma_{\rm diss,0}\ f_{\rm shield}\ e^{-\tau_{d,1000}}$$

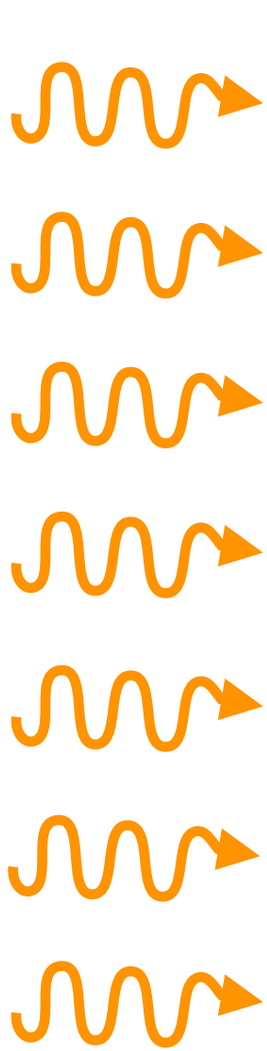
dissociation rate with no shielding

self-shielding factor

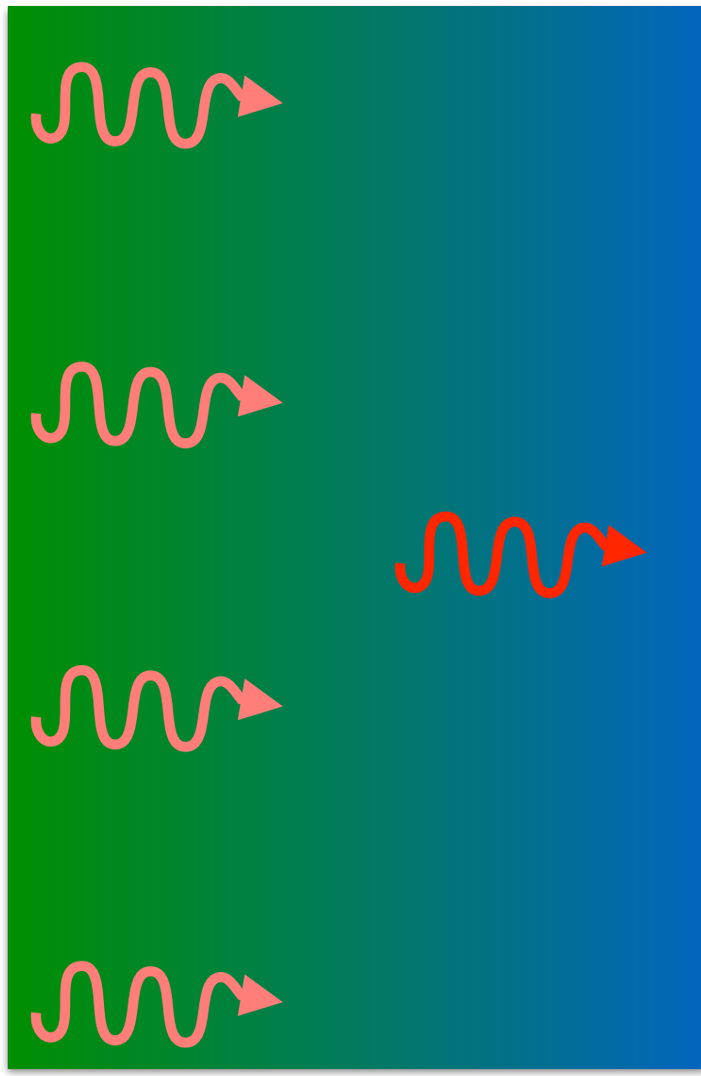
dust extinction at 1000 Å

H_2 Abundance





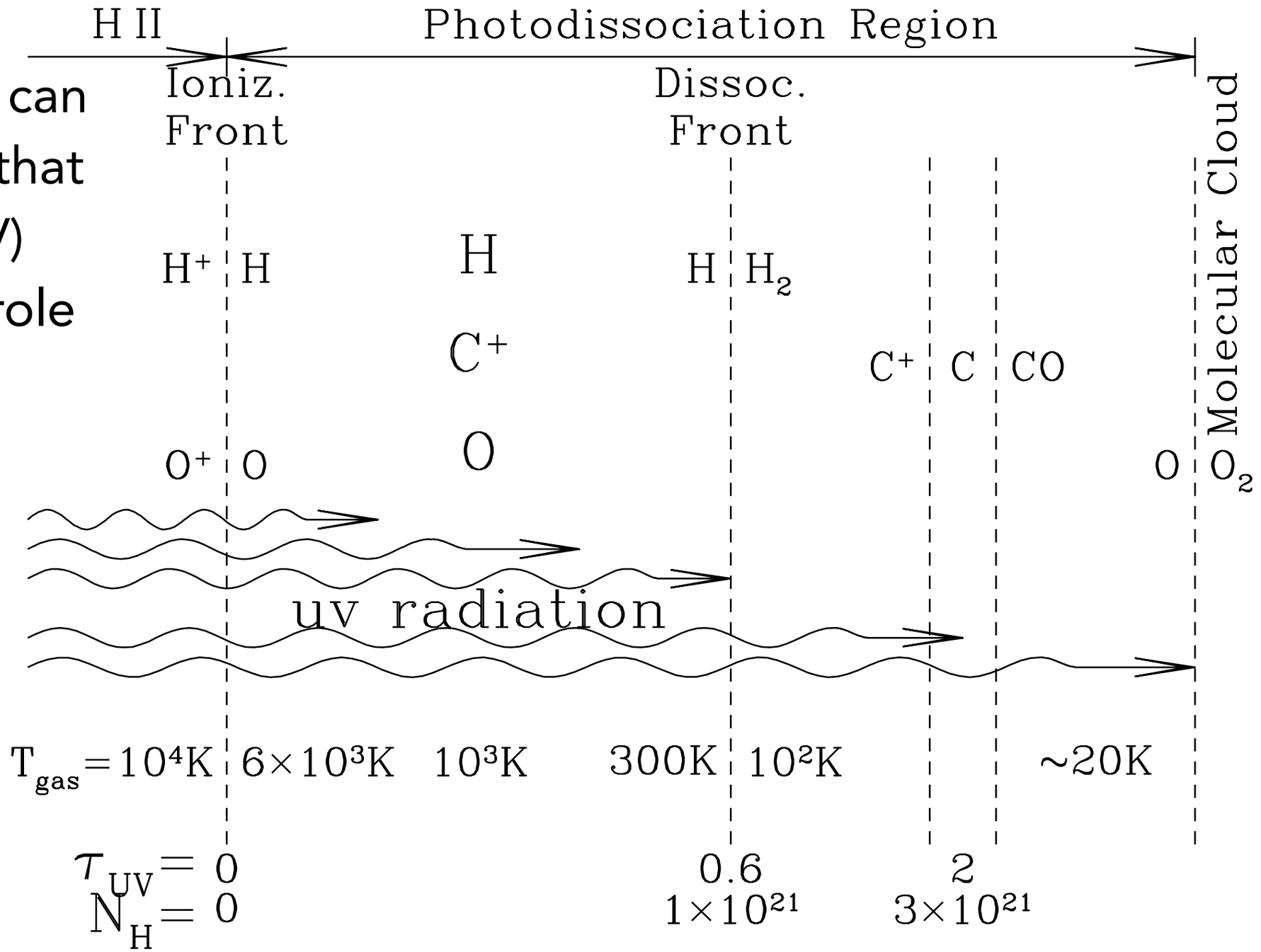
external radiation field



plane-parallel distribution of gas

Photodissociation Regions

Very general term, can refer to anywhere that far-UV (<13.6 eV) photons play key role in chemistry, ionization, etc.



Photodissociation Regions

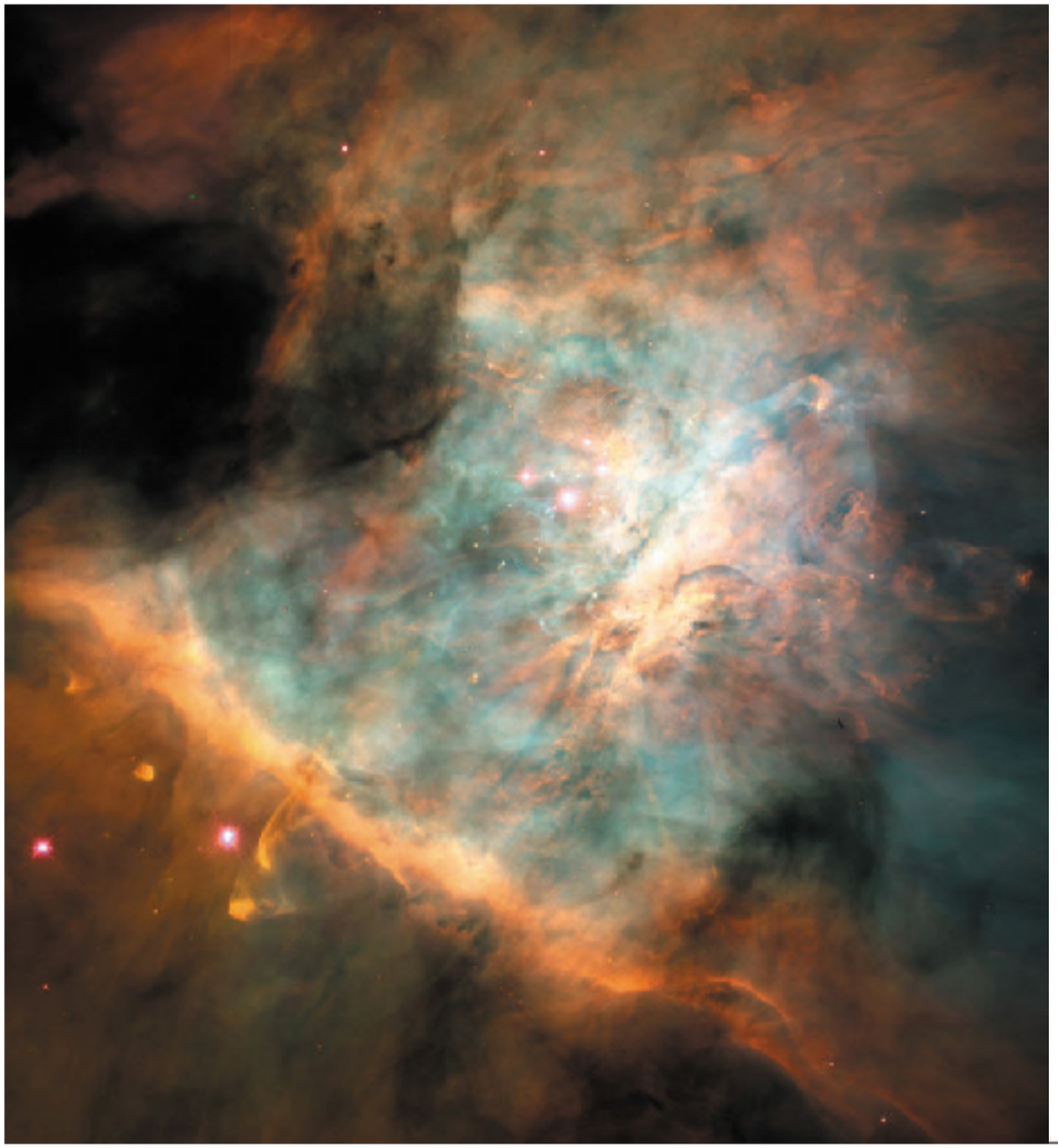


Image: NASA/C. R. O'Dell & S. K. Wong (Rice Univ.)

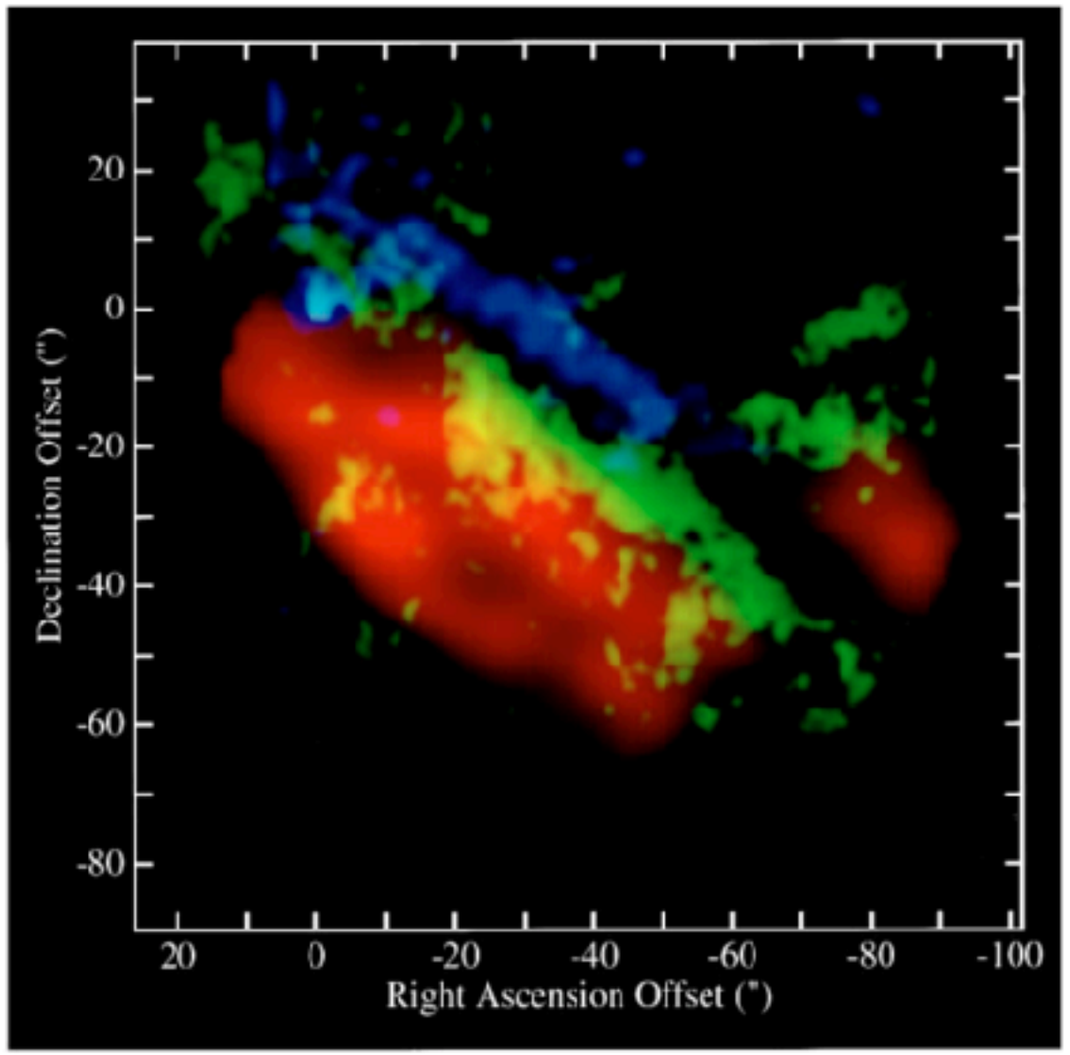
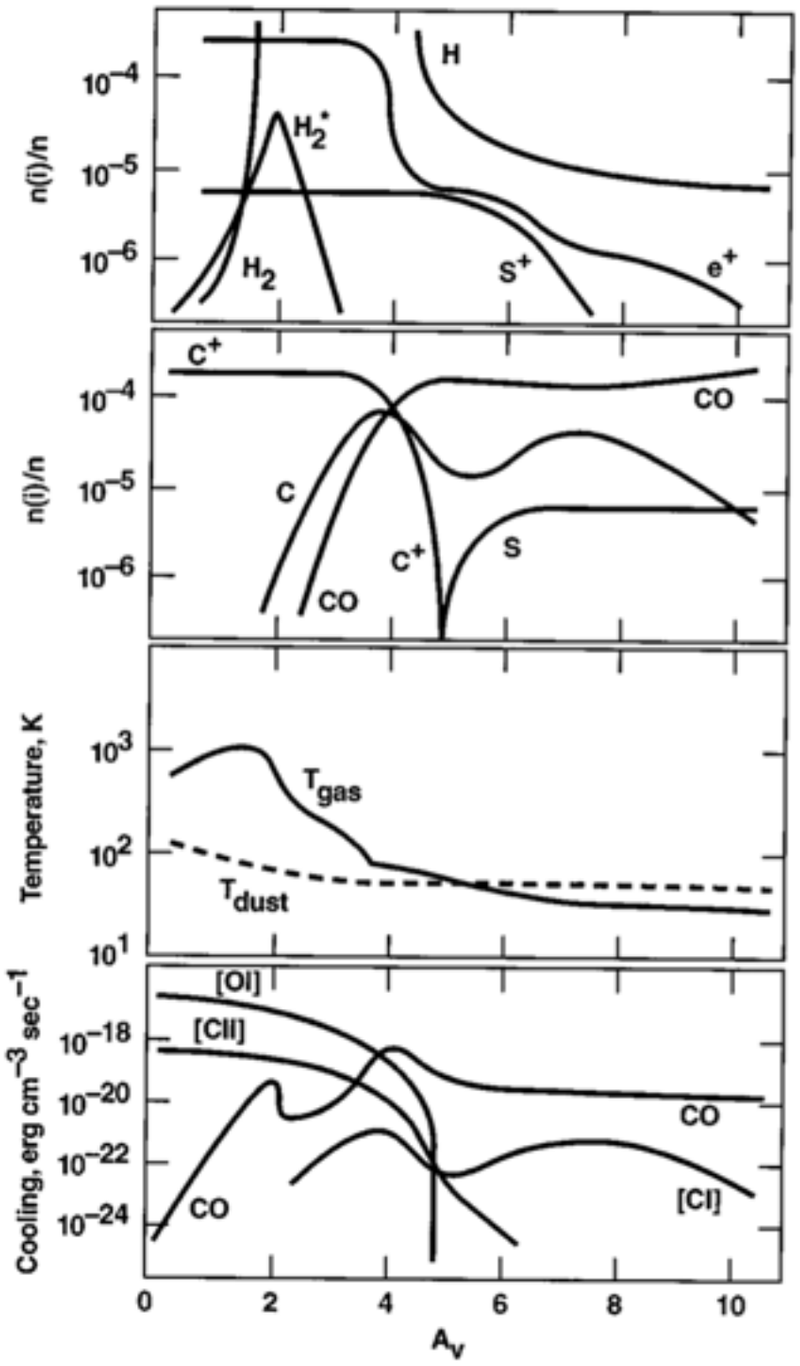
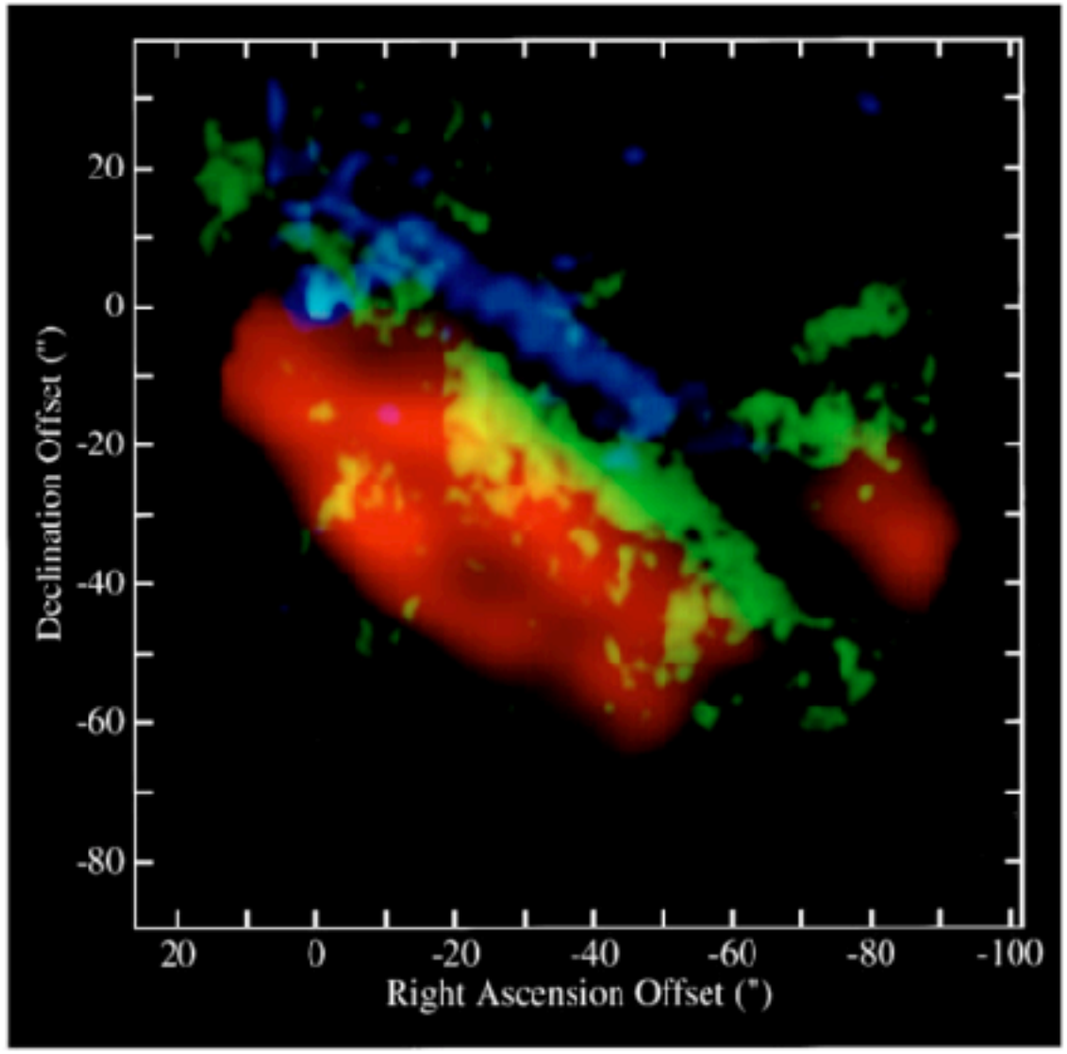


FIG. 2. (Color) The Orion Bar region mapped in the 3.3-μm PAH feature (blue), H_2 1-0 S(1) emission (yellow), and CO $J = 1-0$ emission (red; Tielens *et al.*, 1993). The (0,0) position corresponds to the (unrelated) star θ^2 A Ori. The illuminating source, θ^1 C Ori, and the ionized gas are located to the northwest (upper right). For all three tracers, the emission is concentrated in a bar parallel to but displaced to the southeast from the ionization front. The PDR is seen edge on; a separation of $\simeq 10''$ is seen between the PAH emission and the H_2 emission, and between the H_2 emission and the CO emission, as predicted by PDR models (see text).

Hollenbach & Tielens 1999 Review

Photodissociation Regions





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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_2	C_3 *	*c*-C_3H	C_5 *	C_5H	C_6H	CH_3C_3N	CH_3C_4H	CH_3C_5N	HC_9N	*c*-C_6H_6 *	$HC_{11}N$
AlF	C_2H	*l*-C_3H	C_4H	*l*-H_2C_4	CH_2CHCN	$HC(O)OCH_3$	CH_3CH_2CN	$(CH_3)_2CO$	CH_3C_6H	*n*-C_3H_7CN	C_{60} *
AlCl	C_2O	C_3N	C_4Si	C_2H_4 *	CH_3C_2H	CH_3COOH	$(CH_3)_2O$	$(CH_2OH)_2$	C_2H_5OCHO	*i*-C_3H_7CN	C_{70} *
C_2 **	C_2S	C_3O	*l*-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2OH	CH_3CH_2CHO	$CH_3OC(O)CH_3$	$C_2H_5OCH_3$?	C_{60}^+ *
CH	CH_2	C_3S	*c*-C_3H_2	CH_3NC	CH_3CHO	C_6H_2	HC_7N				
CH^+	HCN	C_2H_2 *	H_2CCN	CH_3OH	CH_3NH_2	CH_2OHCHO	C_8H				
CN	HCO	NH_3	CH_4 *	CH_3SH	*c*-C_2H_4O	*l*-HC_6H *	$CH_3C(O)NH_2$				
CO	HCO^+	HCCN	HC_3N	HC_3NH^+	H_2CCHOH	CH_2CHCHO (?)	C_8H^-				
CO^+	HCS^+	$HCNH^+$	HC_2NC	HC_2CHO	C_6H^-	CH_2CCHCN	C_3H_6				
CP	HOC^+	HNCO	HCOOH	NH_2CHO	CH_3NCO 2015	H_2NCH_2CN	CH_3CH_2SH (?)				
SiC	H_2O	HNCS	H_2CNH	C_5N		CH_3CHNH					
HCl	H_2S	$HOCO^+$	H_2C_2O	*l*-HC_4H *							
KCl	HNC	H_2CO	H_2NCN	*l*-HC_4N							
NH	HNO	H_2CN	HNC_3	*c*-H_2C_3O							
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 *	HC(O)CN								
PN	NaCN	C_3N^-	HNCNH								
SO	OCS	PH_3	CH_3O								

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

List of molecules that have been detected in the ISM:

KCl	HNC	H_2CO	H_2NCN	*l*-HC_4N
NH	HNO	H_2CN	HNC_3	*c*-H_2C_3O
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 *	HC(O)CN	
PN	NaCN	C_3N^-	HNCNH	
SO	OCS	PH_3	CH_3O	
SO^+	SO_2	HCNO	NH_4^+	
SiN	*c*-SiC_2	HOCN	H_2NCO^+ (?)	
SiO	CO_2 *	HSCN	$NCCNH^+$ 2015	
SiS	NH_2	H_2O_2		
CS	H_3^+ (•)	C_3H^+		
HF	SiCN	HMgNC		
HD	AlNC	HCCO 2015		
FeO ?	SiNC			
O_2	HCP			
CF^+	CCP			
SiH ?	AlOH			
PO	H_2O^+			
AlO	H_2Cl^+			
OH^+	KCN			
CN^-	FeCN			
SH^+	HO_2			
SH	TiO_2			
HCl^+	C_2N			
TiO	Si_2C 2015			
ArH^+				
NO^+ ?				

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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

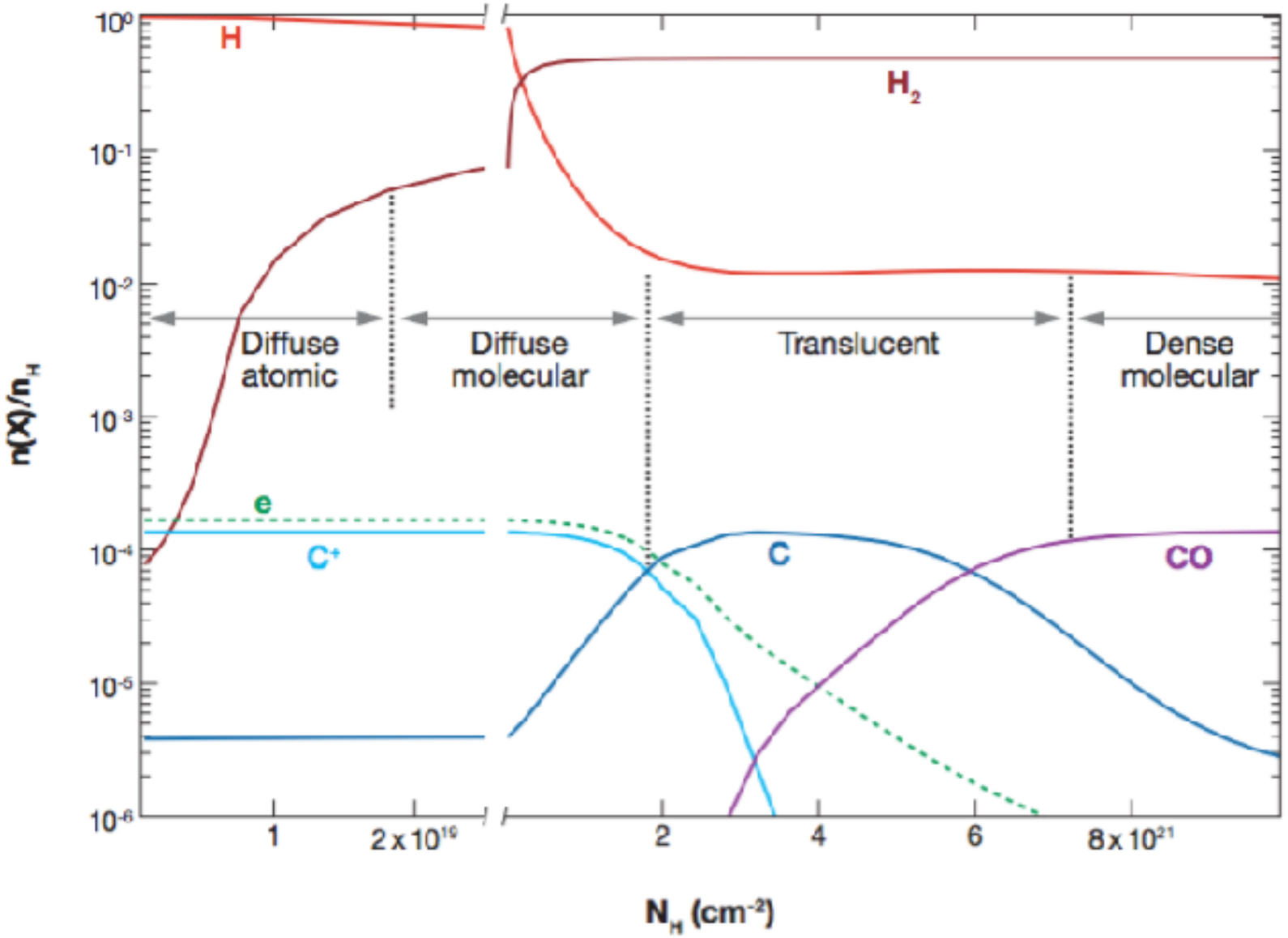

Figure 1

Results from photodissociation region model [with $n_H = 100$ 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 $10^4\,cm^{-3}$, and a visual extinction A_V of 30 magnitudes[104]), 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.[105,106] 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

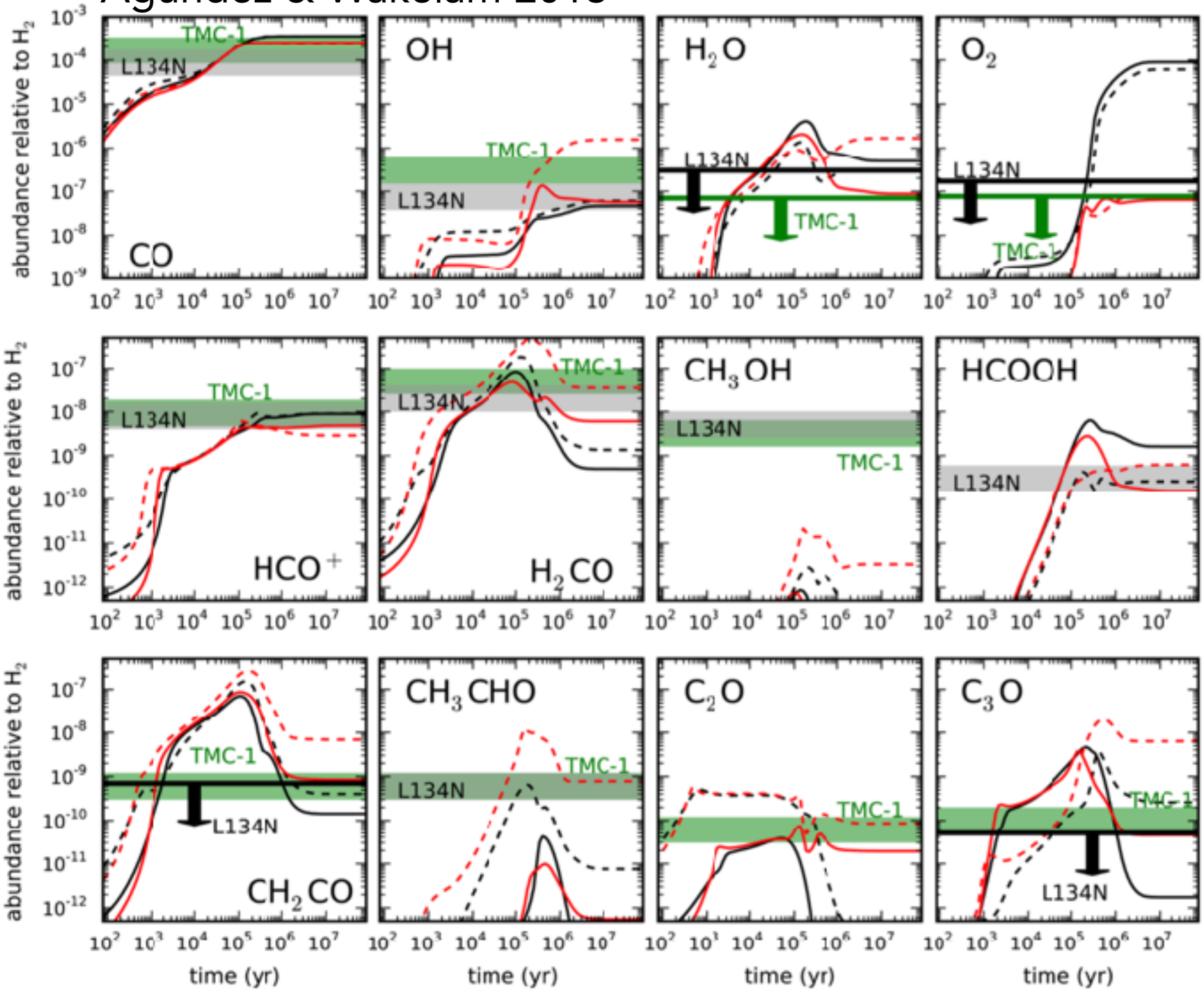
<u>Evidence of non-equlibrium chemistry:</u>

CO is the most abundant molecule after H_2

Chemical equilibrium models at T=10 K would predict most carbon in CH_4 and most oxygen in H_2O.

Chemistry in Molecular Gas

Agundez & Wakelam 2013



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2. **Cosmic rays** provide ionization even in very dense clouds, UV absorbed in outer layers of cloud. H_2^+ quickly reacts with H to form H_3^+, a key reactant.

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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.