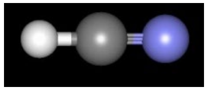

Astrochemistry Lecture 4

Diffuse and translucent clouds, PDRs

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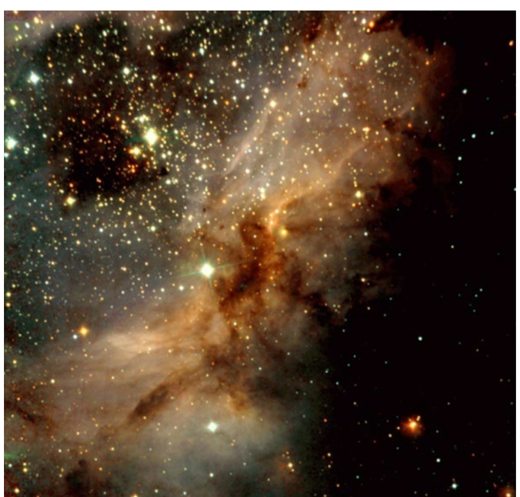
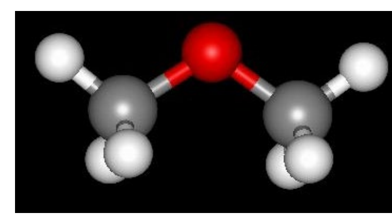
Leiden Observatory

May-June 2022



Van Dishoeck 1998, in MA II
Snow & McCall 2006, Gerin et al. 2016 ARA&A
Tielens Chap. 9



Summary lectures 1+2

- Large variety of molecules observed in ISM
- Basic processes for formation and destruction identified
- Networks built for explaining abundances (lectures 3 and 4)
- Results depend on thousands of input rates
  - Many not known under astrophysical conditions (but for many accurate rates not needed)
  - Key: identify those reactions which are important to study well
- Many experiments and theory on basic processes over last 30 years
  - New chemical physics insight
  - Significant progress in neutral-neutral reactions, surface reactions
- Some processes now well understood, others take decades of hard work to make just a little progress
  - Funding of lab astrophysics groups issue
  - Note: photoionization codes got atomic input data thanks to a century of efforts in atomic and plasma physics

Summary Lecture 3

- Chemistry starts at era of recombination $z \sim 1000$
  - Only H, D He, Li, no dust
  - First molecules He_2^+ and HeH^+
- Small fraction of H_2 forms through H^+ and H^- routes
  - HD from reactions of D^+ with H_2
- H_2 and HD important coolants of primordial clouds and thus their fragmentation
  - Determines mass of the first stars
- Observations of molecules now up to $z \sim 7$

Outline

A. Diffuse and translucent clouds

- Introduction
- Physical structure
- Gas-phase chemistry networks
- Steady-state models: $H \rightarrow H_2$, $C^+ \rightarrow CO$

B. Photon-dominated regions (PDRs)

- Introduction
- Chemical structure
- Examples: from Orion to galaxies at low metallicity to protoplanetary disks

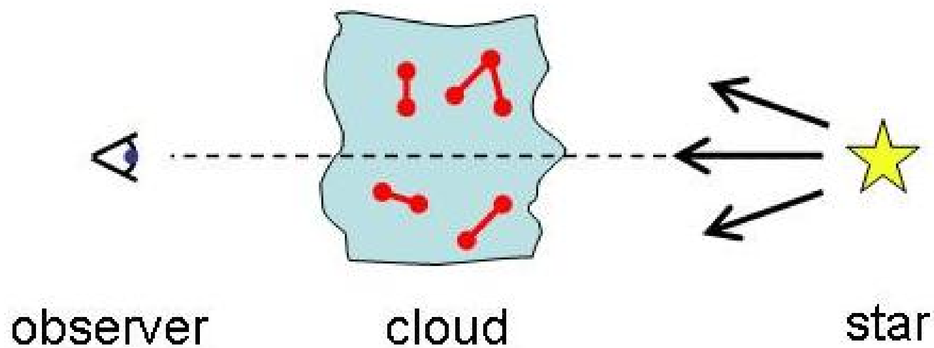
A. Diffuse and translucent clouds
4.1 Introduction

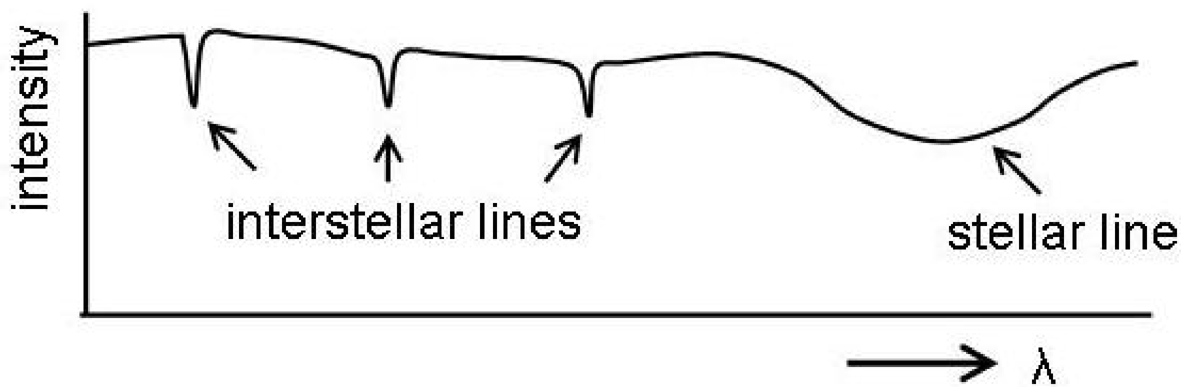
- Diffuse clouds with $A_V \approx 1$ mag are the best testing ground for basic interstellar chemistry because

  Mostly
  - ~~Only~~ simplest diatomic molecules found
  - Gas-phase elemental abundances directly measured
  - H and H_2 directly measured
  - UV penetrates $\Rightarrow$ short timescales $\Rightarrow$ chemical equilibrium
  - No embedded / hidden energy sources
- Models first considered by Kramers & ter Haar (1946) and Bates & Spitzer (1951). Subsequent models include ion-molecule network developed by Herbst & Klemperer (1973)

Recall relation A_V and total column density N_H

Observations of diffuse clouds





Questions

- To what extent can ion-molecule gas-phase chemistry reproduce observed abundances?
- What is role of shocks and turbulence?
- What is role of grains in formation molecules other than H_2?
- What is relation diffuse – dense clouds?

$\Rightarrow$ study also ***translucent**** clouds with A_V=1-5 mag

* Term coined by van Dishoeck & Black (1989)

Observations diffuse clouds

VIS + UV absorption lines

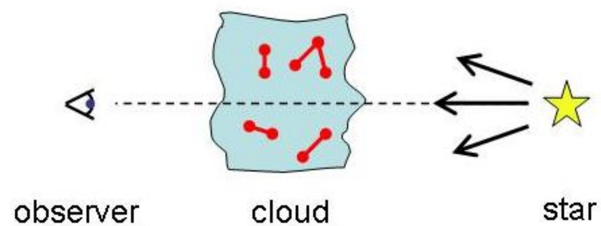
- Many atomic lines $\Rightarrow$ depletion of elements C, O, N, ..
  - Chemistry sensitive to C/O ratio
- Few molecular lines detected
  - H_2, HD
  - CH, CH^+, C_2, C_3
  - OH, OH^+, CO
  - NH, CN, HCl
- Not detected at optical wavelengths:
  - H_2O, H_2O^+, C_4, …
  - MgH, NaH, SH^+, …

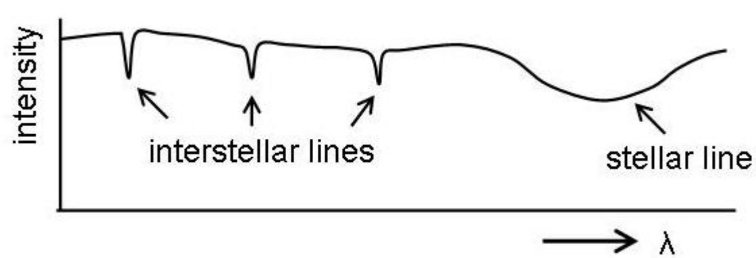
Millimeter/far-IR absorption and emission lines

- Weak emission, many absorption lines

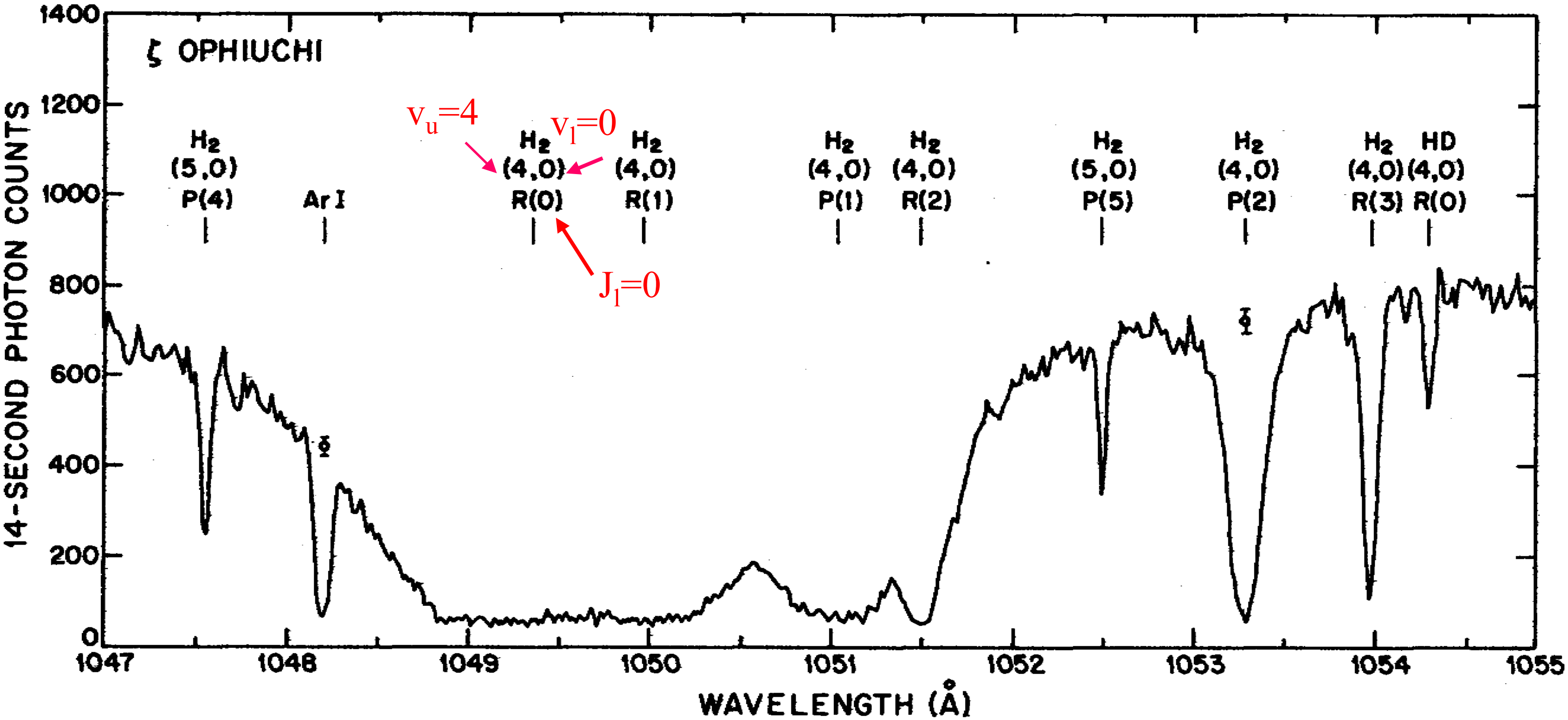
Observations of diffuse clouds

- Observed primarily by absorption lines at visible (since 1900's) and UV wavelengths (since 1970's: *Copernicus, FUSE, HST*)
- Classical example: line-of-sight toward ζ Oph
- Spectra show sharp interstellar lines super-imposed on broad stellar lines





Interstellar H_2 lines towards ζ Ophiuchi



Jenkins et al., Copernicus satellite

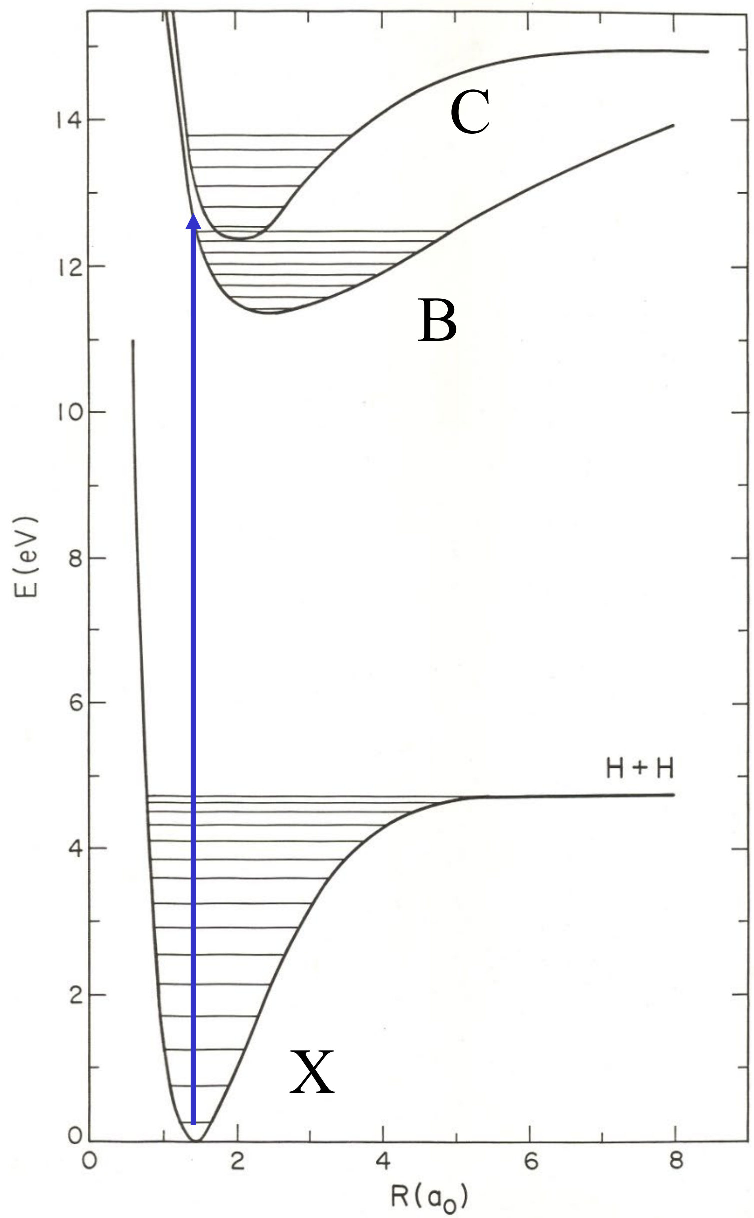
- $\Delta J = J_u - J_l = +1$: R-branch
- $\Delta J =$ -1: P branch

R(0): $J_u=1 - J_l=0$

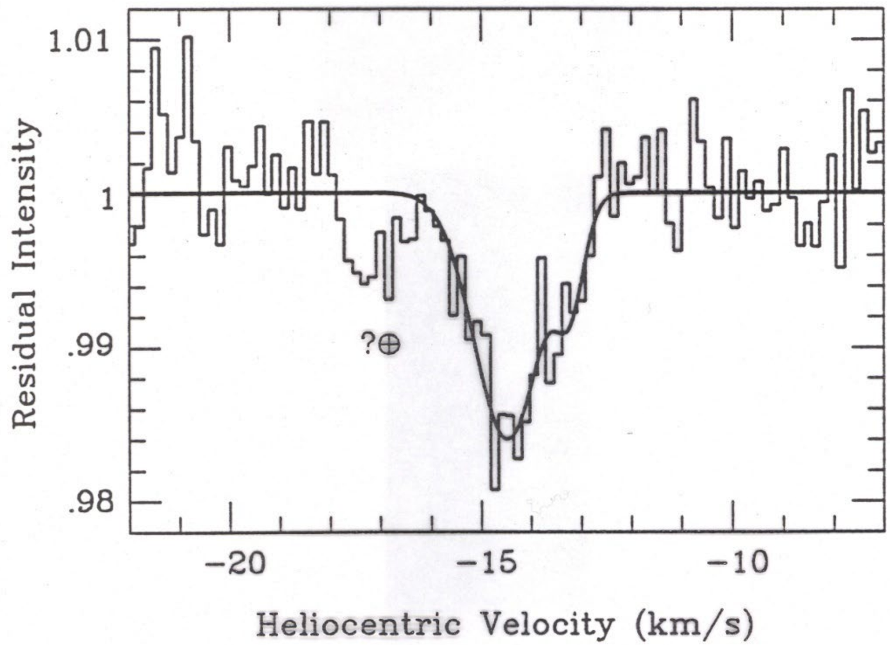
H_2 absorption

B-X: Lyman system
C-X: Werner system

P-lines: J_u-J_l=-1
R-lines: J_u-J_l=1



Example: NH toward ζ Oph



Crawford & Williams 1997

- Ultra high resolution observations R=800000
- Two component fit:
  - v=-14.5 km s^{-1}, b=0.91±0.15⇒ T<750 K
  - v=-13.2 km s^{-1}, b=0.33±0.13⇒ T<100 K
- Upper limits on T from line width exclude N + H_2 → NH + H reaction

Lines are narrow (except CH^+)→ excludes strong shocks!

Typical abundances (ζ Oph, ζ Per)

- CH $\approx 2\times10^{13}$ cm^{-2} $\Rightarrow$ $x(CH)=N(CH)/N(H_2) \approx 4\times10^{-8}$
- OH $\approx 4\times10^{13}$ $\Rightarrow$ $x(OH) \approx 8\times10^{-8}$
- NH $\approx 9\times10^{11}$ $\Rightarrow$ $x(NH) \approx 2\times10^{-9}$
- CO $\approx 10^{14}$-10^{15} $\Rightarrow$ $x(CO) \approx 2\times10^{-7}$ - 2×10^{-6}
- $CH^+ \approx 10^{12}$-10^{13} $\Rightarrow$ $x(CH^+) \approx 2\times10^{-9}$ - 2×10^{-8}

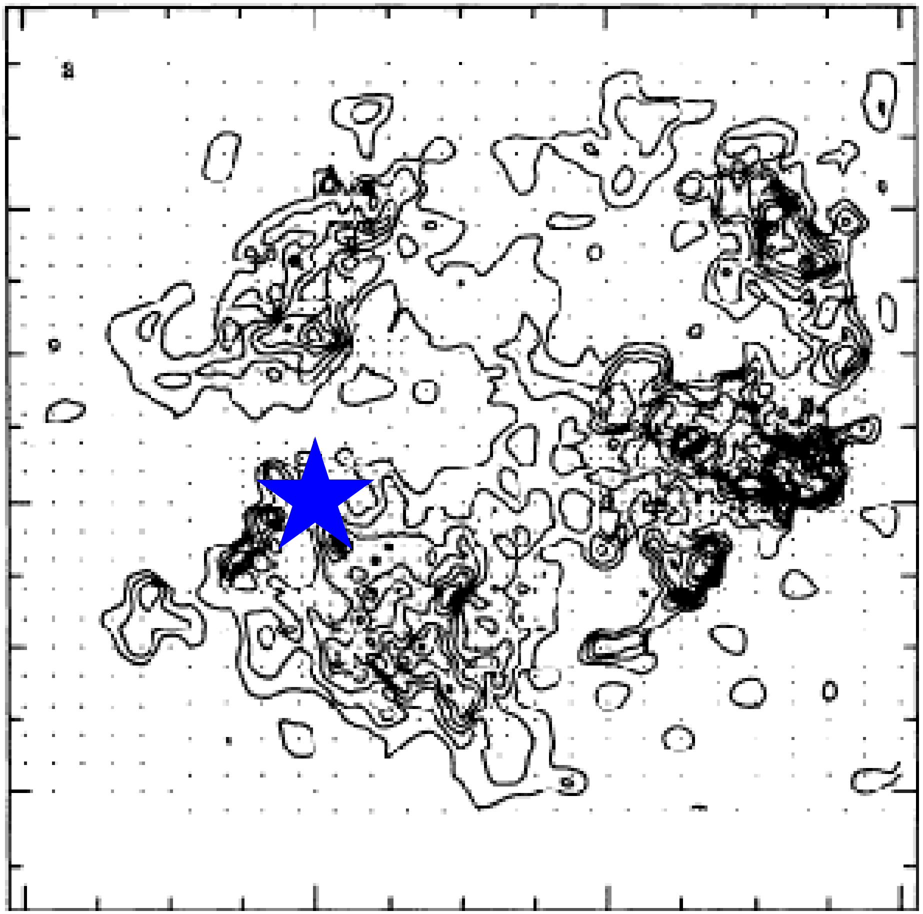
- The fact that the observed column densities of CH, OH >> NH indicates that grain surface chemistry not dominant for carbon- and oxygen chemistry in diffuse clouds

See Appendix on how to derive N from observed equivalent width

Translucent clouds

- Can be isolated clouds, edges of dark clouds or GMCs, high-latitude clouds
- Visible absorption lines of CH^+, CH, CN, C_2, ….
- UV absorption lines with FUSE $\Rightarrow$ H_2, HD, CO
  - Only for some clouds
- Clouds thick enough for mm emission $\Rightarrow$ CO and very weak [C I], CS, CN, HCO^+, …. ***'CO dark gas'***
- Mm absorption lines against background quasars $\Rightarrow$ ***surprisingly*** large column densities of HCO^+, HCN, …
- Infrared absorption $\Rightarrow$ threshold for ice mantle formation at $A_V \geq 3$ mag

High latitude cloud toward HD 210121

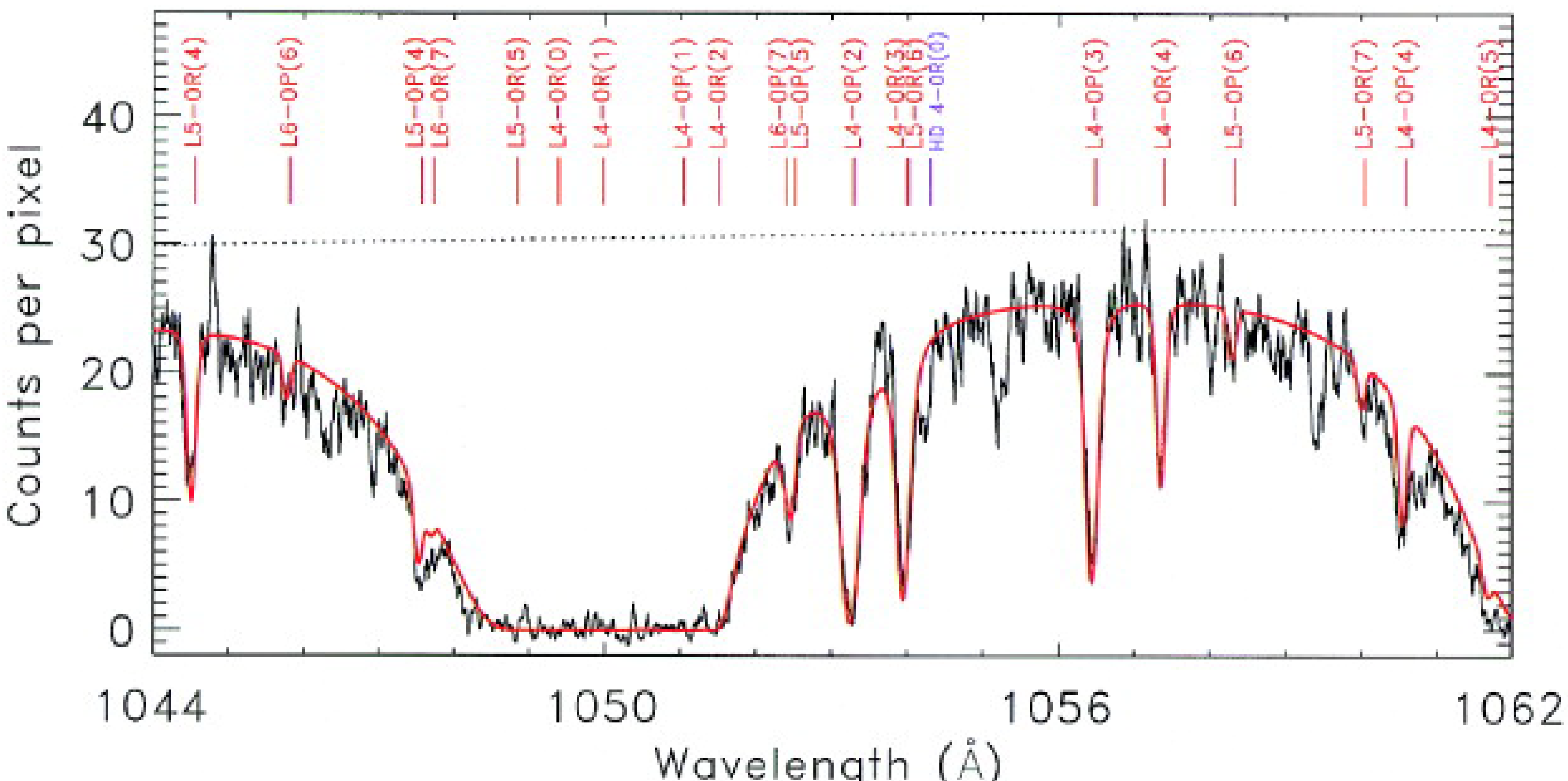


CO *J*=1-0 map

Gredel et al. 1992

UV spectroscopy: FUSE

HD 73882

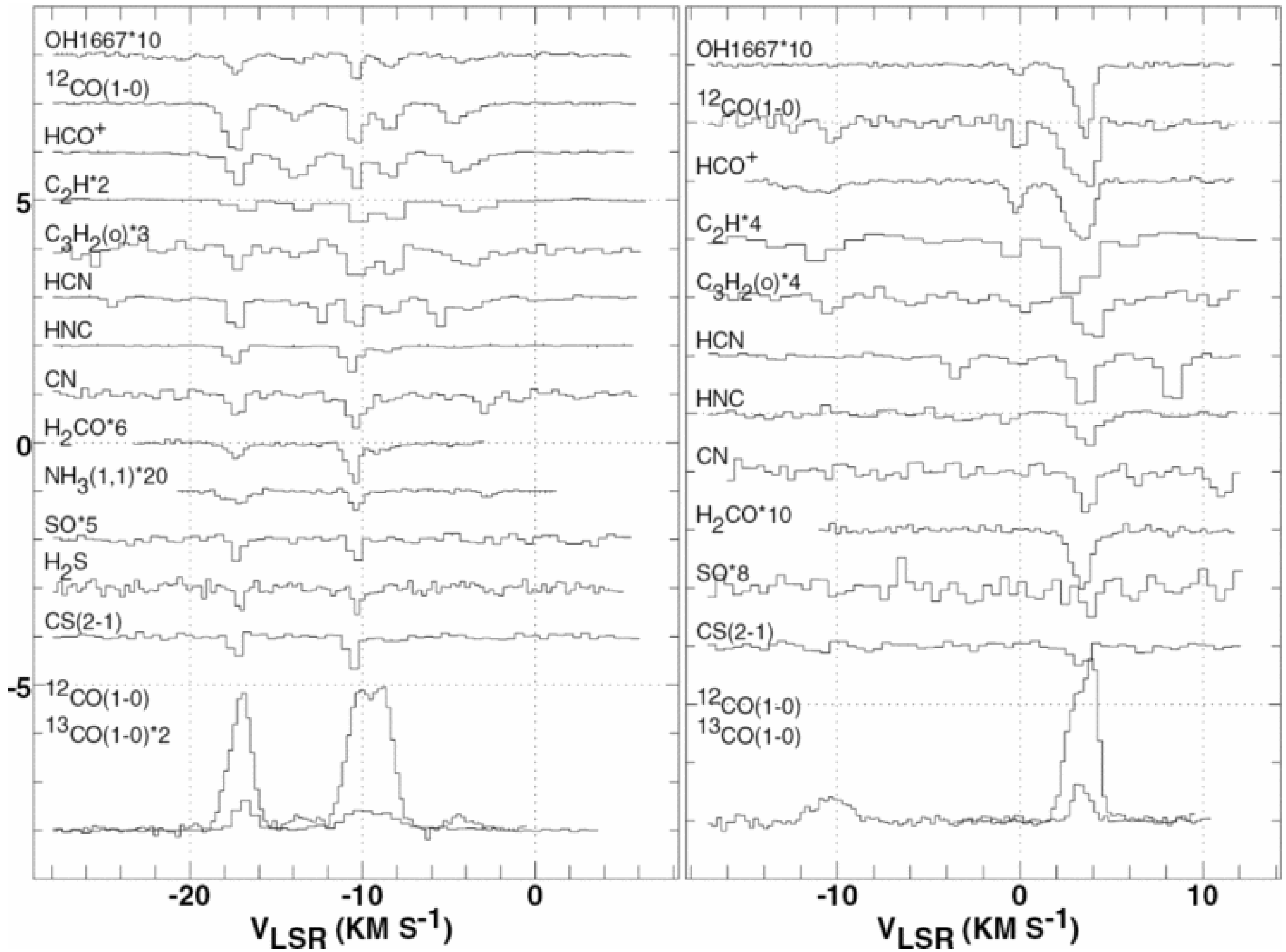


Snow et al. 2000

FUSE spectrum toward HD 73882 translucent cloud showing H_2 and HD lines

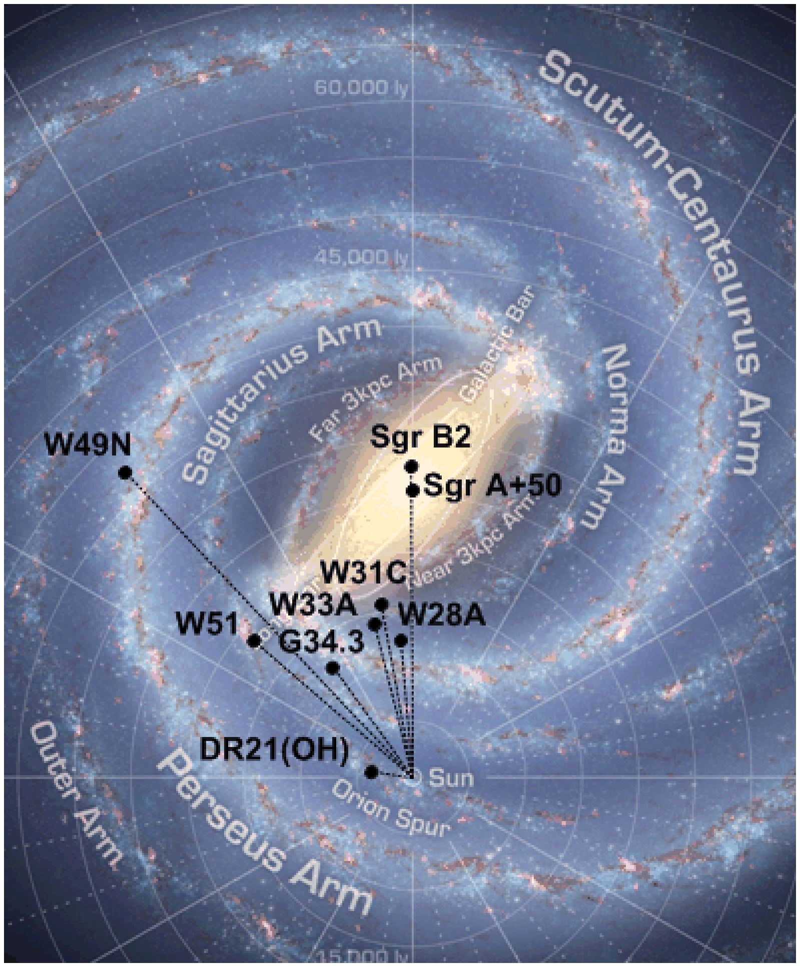
Mm absorption lines: quasars

B0355+508 B0212+735



Lucas & Liszt 94-05
Hogerheijde et al. 1995
Liszt 2005, IAU 231

Far-infrared absorption

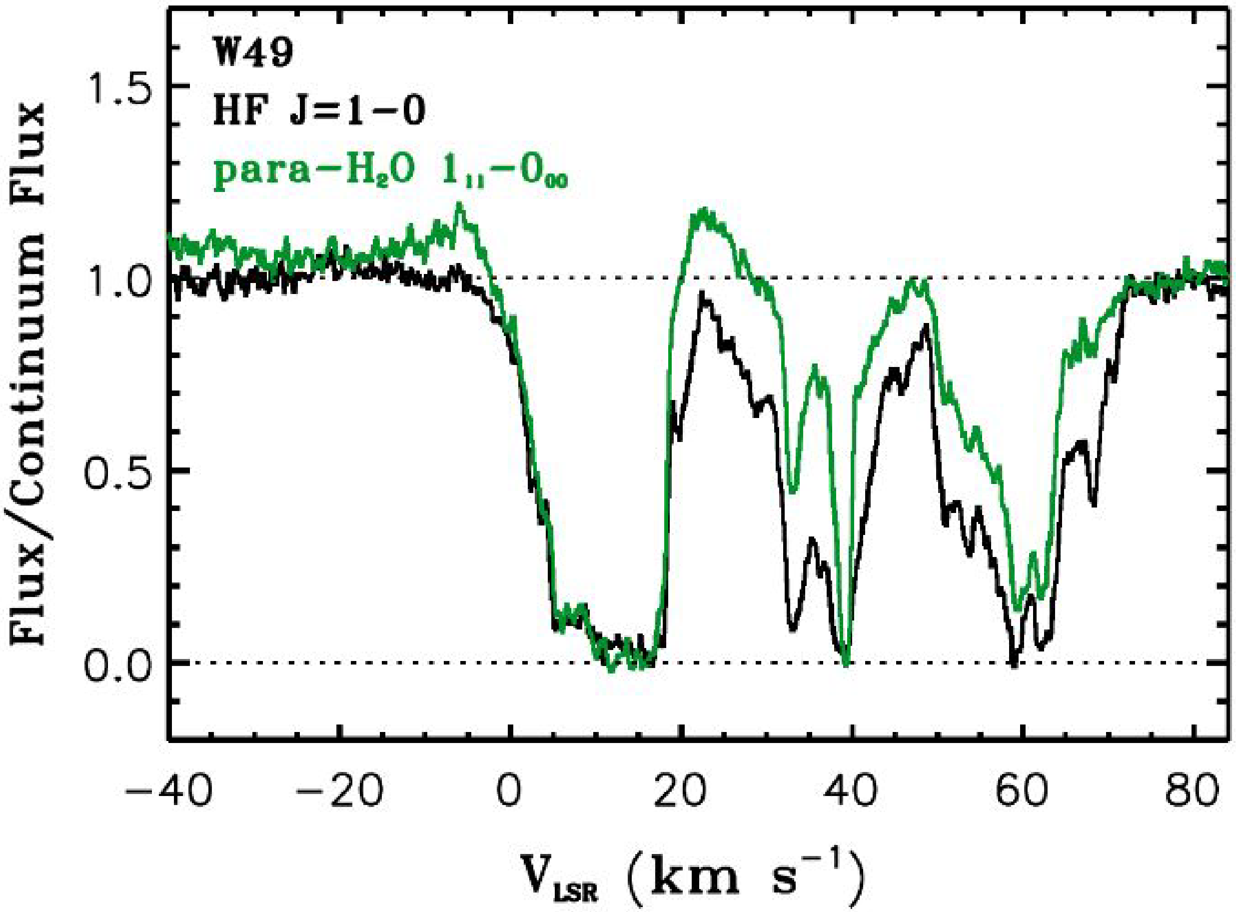


Gerin et al. 2016, ARA&A

PRISMAS survey

- Absorption against bright far-IR continuum
- Clouds A_V ~few mag
- Hydrides have their lowest transitions at higher frequencies (submm/far-IR wavelengths) because of lower mass than CO
- All molecules in ground level→simple analysis

Far-IR absorption lines: HF and H_2O



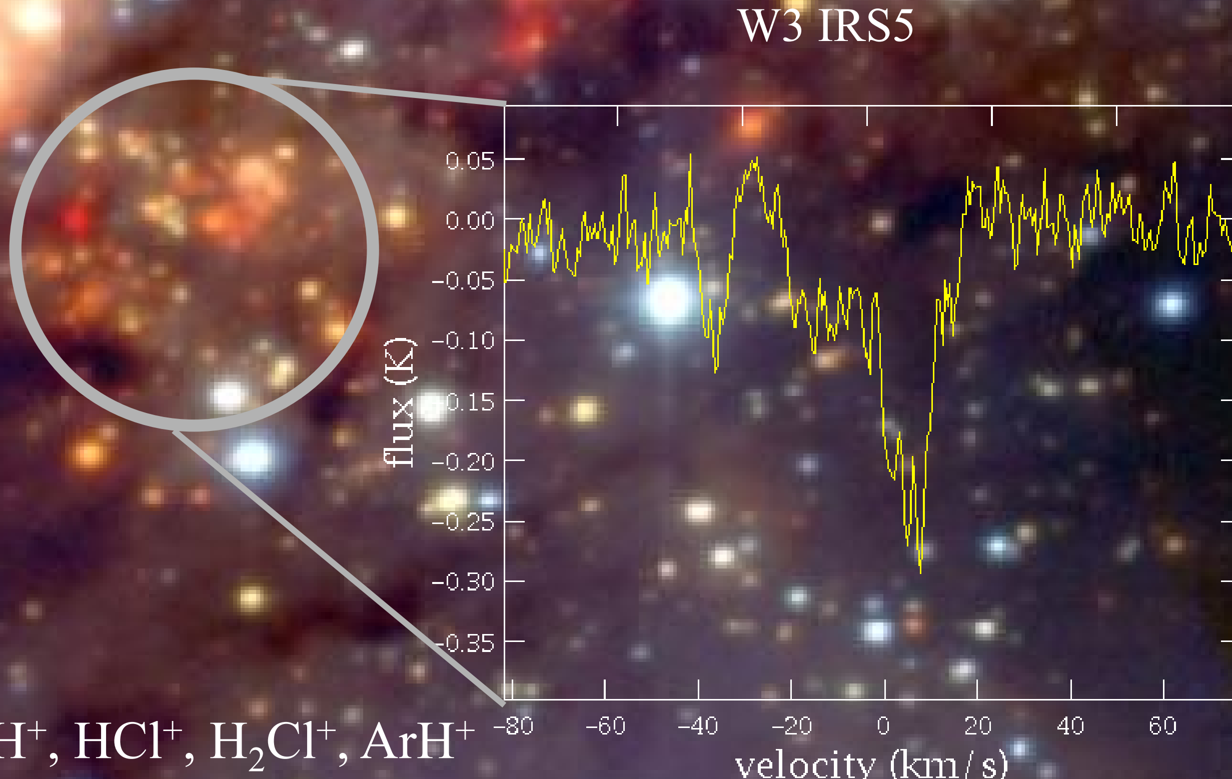
Herschel-HIFI

Gerin et al 2016

- Every feature is a diffuse or translucent cloud along the line of sight
- HF as tracer of H_2 column density because of simple chemistry
- Constant H_2O/H_2 abundance of $5x10^{-8}$

Herschel Surprise: H_2O^+ widespread

Points to an ISM phase with high H/H_2 (see Exercise on ArH^+)



Benz, Bruderer et al. 2010
Gerin et al. 2010, Ossenkopf et al. 2010

Also observed: OH^+, CH^+, SH^+, HCl^+, H_2Cl^+, ArH^+
OH, H_2O, CH, NH, HF, SH, HCl

4.2 Physical structure: diagnostics

Species	Probes	Diffuse clouds	Transl. clouds
H_2 low J	T	+	-
H_2 high J, v>0	I_{UV}, formation	+	-
C_2 low J	T	+	+
C_2 high J	I_R/n_H	+	+
C, C^+, O(J)	n_H, T	+	-
CO low J	n_H, T	+	+
CN J	n(e)	+	+
HCO^+, ….	n(e), n_H	-	+

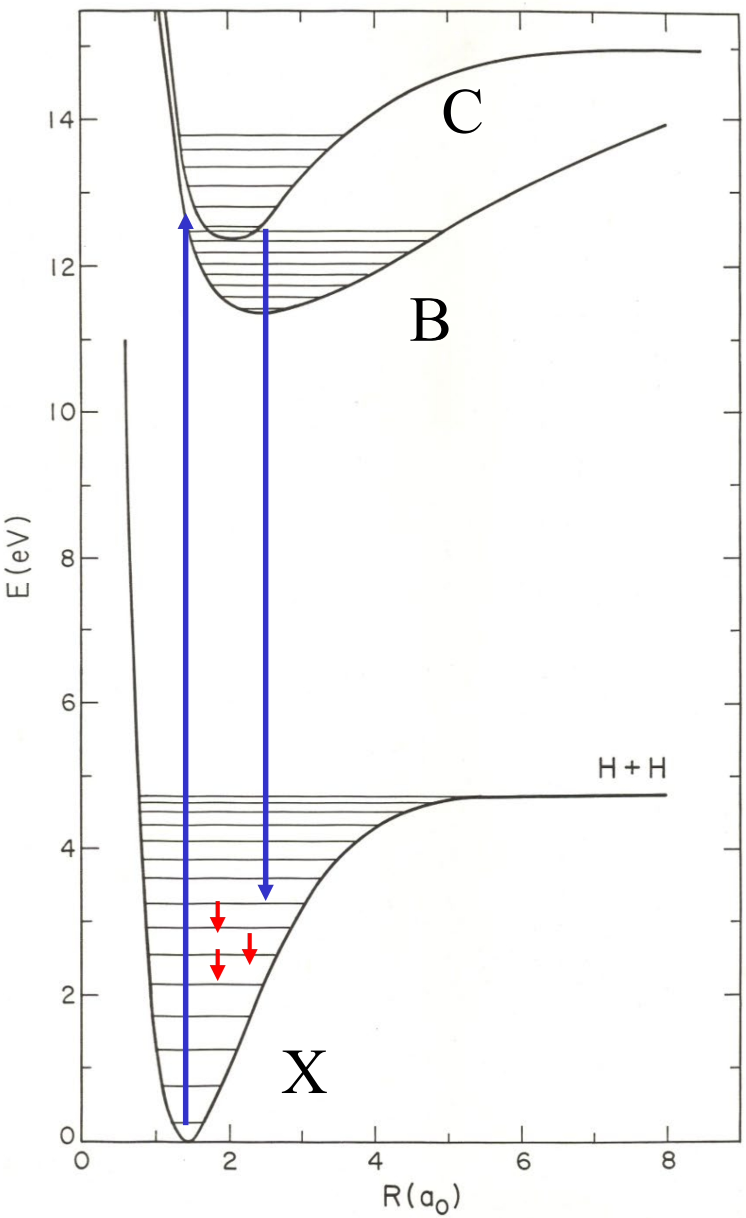
a. Rotational excitation of H_2

- H_2 lines out of $J = 0\text{-}7$ detected with Copernicus + FUSE
- Population distribution non-thermal
  - Low J: excitation dominated by collisions
    $\Rightarrow$ ***sensitive to T and n_H***
    - Abundance H^+ large enough that ortho/para exchange rapid and J=1/J=0 gives T_{kin}
  - High J: energy levels lie very high (> 1000 K) $\Rightarrow$ not populated by collisions at $T = 40 - 80$ K $\Rightarrow$ populated by optical pumping process through B $\rightarrow$ X and C $\rightarrow$ X systems
    $\Rightarrow$ ***proportional to interstellar radiation field I_{UV}***
    - Formation process may play a small role as well

I_{UV} is scaling factor w.r.t. general interstellar radiation field (ISRF) in 6-13.6 eV range (also called G_0)

H_2 excitation

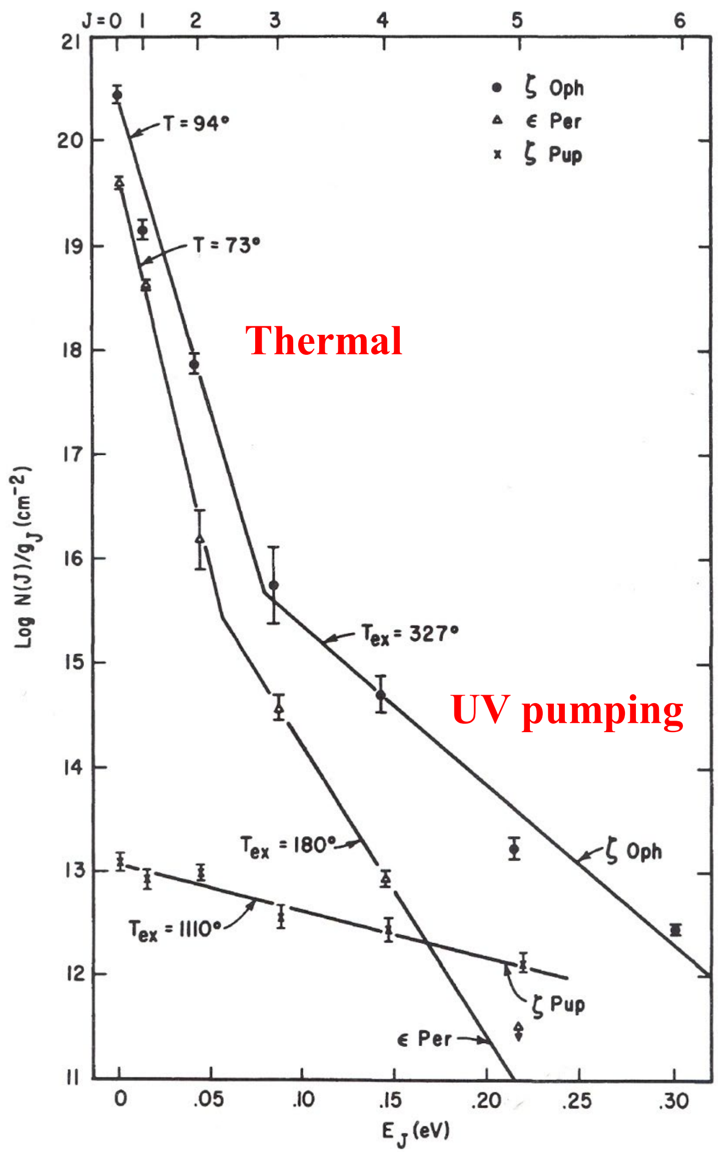
B-X: Lyman system
C-X: Werner system



Observed H_2 rotational excitation

Diffuse clouds

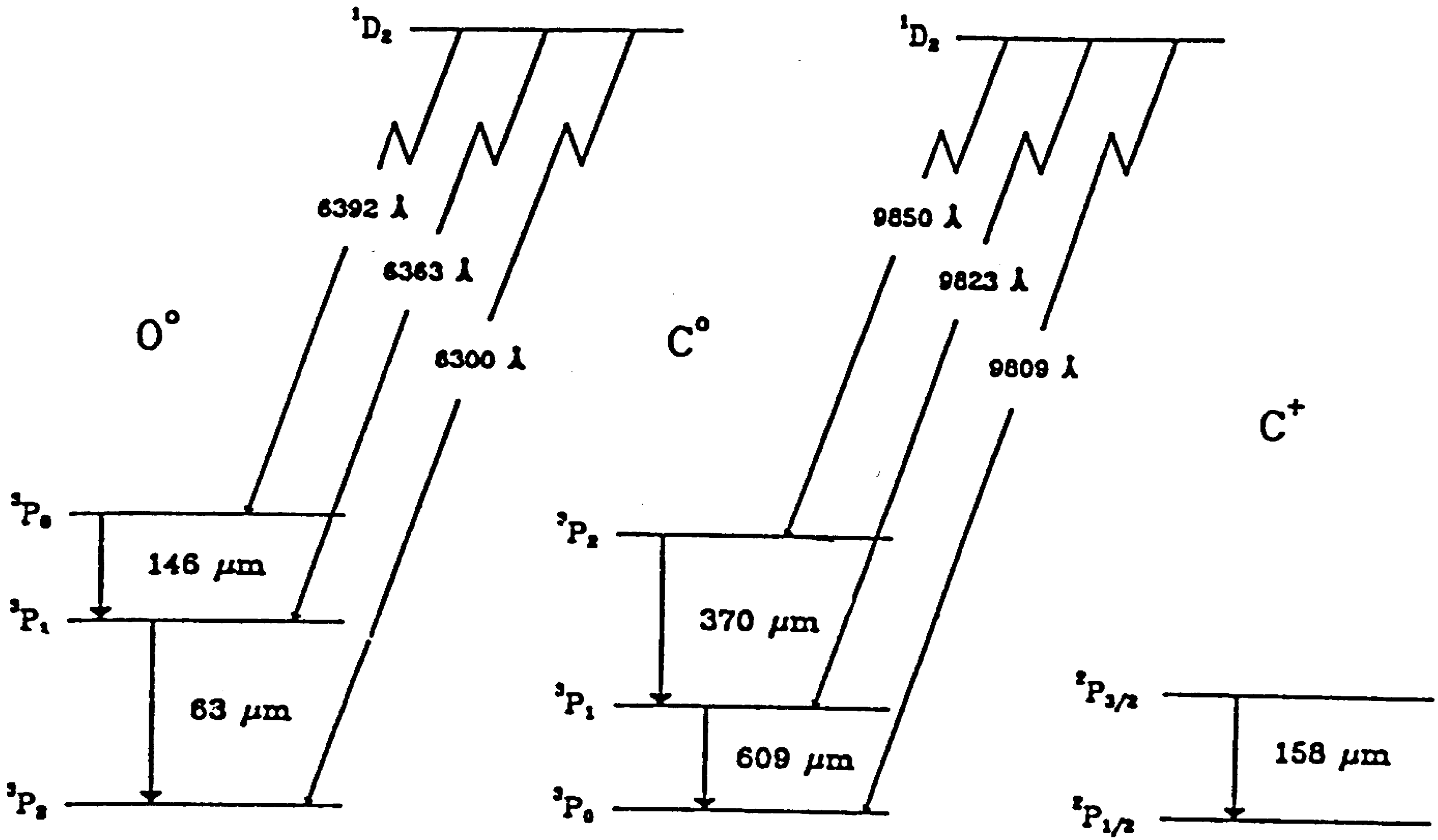
ln N_J/g_J



b. Other diagnostics

- C_2: similar to H_2, but pumping by radiation around 1 μm => ***sensitive to I_R, T and n_H***
- CO rotational excitation
  - Small dipole moment => lowest levels can be populated by collisions even at low densities => ***sensitive to T and n_H***
- C, C^+, O fine-structure excitation
  - Fine-structure populations determined by collisions => ***sensitive to T and n_H***

O I , C I and C II fine structure lines



Results physical parameters

- Diffuse clouds

  Edge **Center**

  - n_H: 100 → 500 cm^{-3} gradient $n_H = n(H) + 2n(H_2)$
  - T: 100-200 → 25-40 K
  - I_{UV}: 1-2×ISRF→ decrease depending on λ

- Translucent clouds
  - Similar, but with temperatures down to 15 K and densities up to a few thousand cm^{-3}

Bottom line: diffuse cloud densities a few hundred cm^{-3}, translucent cloud densities a few thousand cm^{-3}

4.3 Chemistry networks

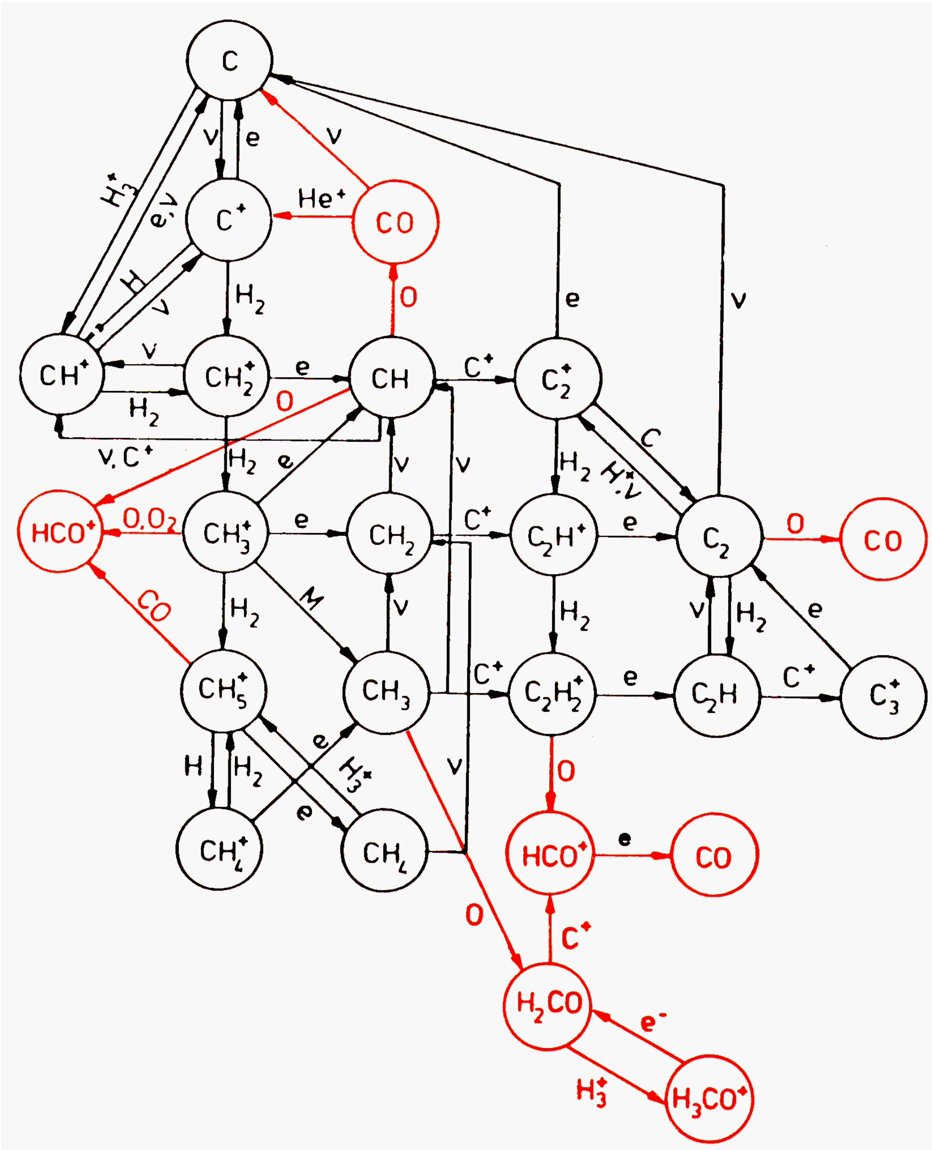
	k (cm^3 s^{-1})
▪ <u>Formation</u> of bonds	
▪ Radiative association:	$\sim 10^{-17} - 10^{-14}$
▪ Grain surface:	$\sim 10^{-17}$
▪ <u>Destruction</u> of bonds	
▪ Photo-dissociation:	$\sim 10^{-10} - 10^{-8}$ s^{-1}
▪ Dissociative recombination:	$\sim 10^{-7} - 10^{-6}$
▪ <u>Rearrangement</u> of bonds	
▪ Ion-molecule reactions:	$\sim 10^{-9} - 10^{-8}$
▪ Neutral-neutral reactions:	$\sim 10^{-10} - 10^{-9}$

Hydrogen is dominant element $\Rightarrow$ if species can react with H or H_2, it will be the dominant route

Carbon chemistry

- Need to have ions and molecules to start ion-molecule chemistry
- I.P. of C < 13.6 eV $\Rightarrow$ carbon mostly C^+
- $C^+ + H_2 \rightarrow CH_2^+ + h\nu$ possible at low T (initiating reaction)
- Once CH_2^+ formed, rapid ion-molecule reactions lead to CH, C_2, …
- $C^+ + H_2 \not\rightarrow CH^+ + H$: endothermic by 0.4 eV

Carbon chemistry and its coupling with oxygen



Vertical

Down: H_2

Up: photon ν

Horizontal

Ion: *e*

Neutral: C^+

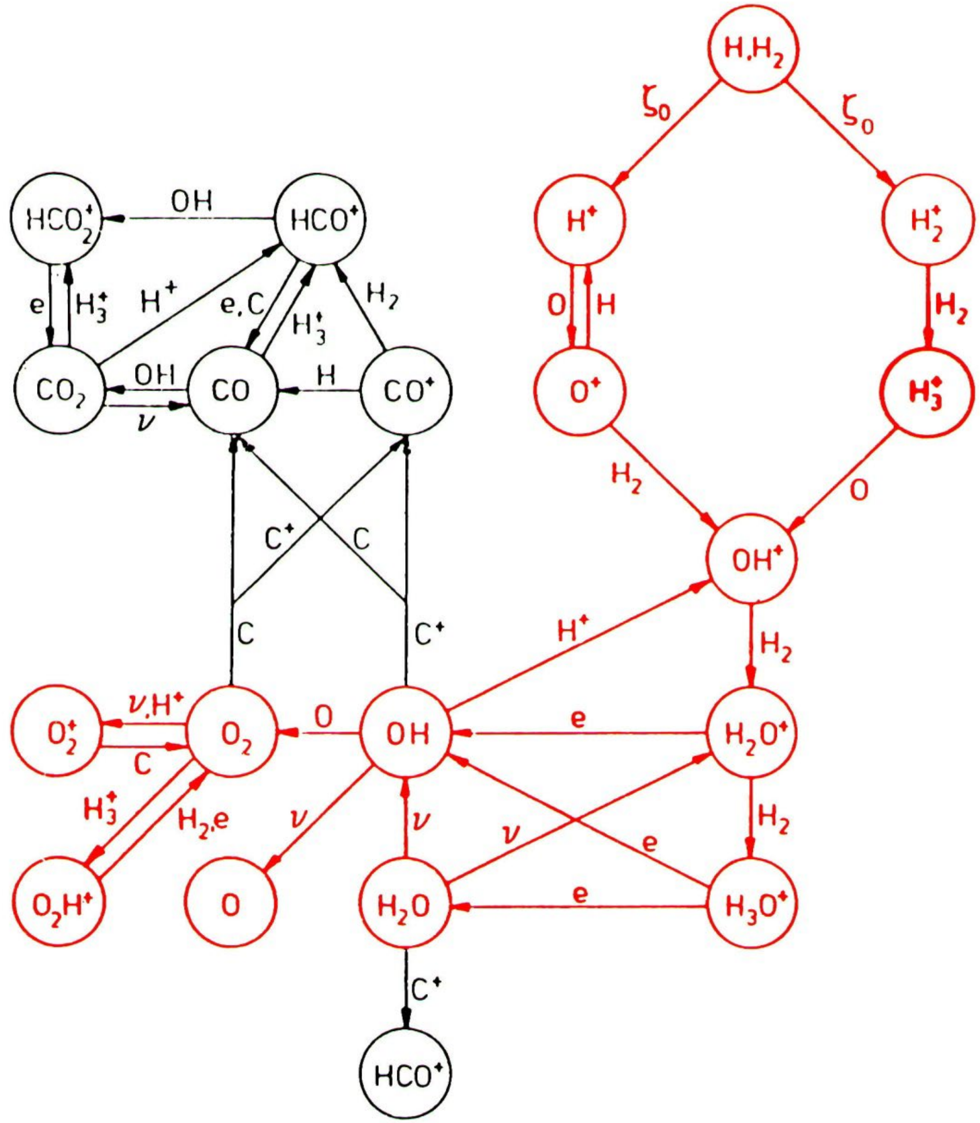
Oxygen chemistry

- I.P. of O > 13.6 eV $\Rightarrow$ oxygen mostly neutral O
- Ionization provided by cosmic rays
  - H_2 or H + C.R. $\rightarrow H_2^+$ or H^+ + C.R. + e
  - $H_2^+ + H_2 \rightarrow H_3^+ + H$ (very fast)
- H^+ or H_3^+ can react with oxygen
  - $H^+ + O \leftrightarrow H + O^+$ ΔE=227 K; $O^+ + H_2 \rightarrow OH^+ + H$
  - $H_3^+ + O \rightarrow OH^+ + H_2$

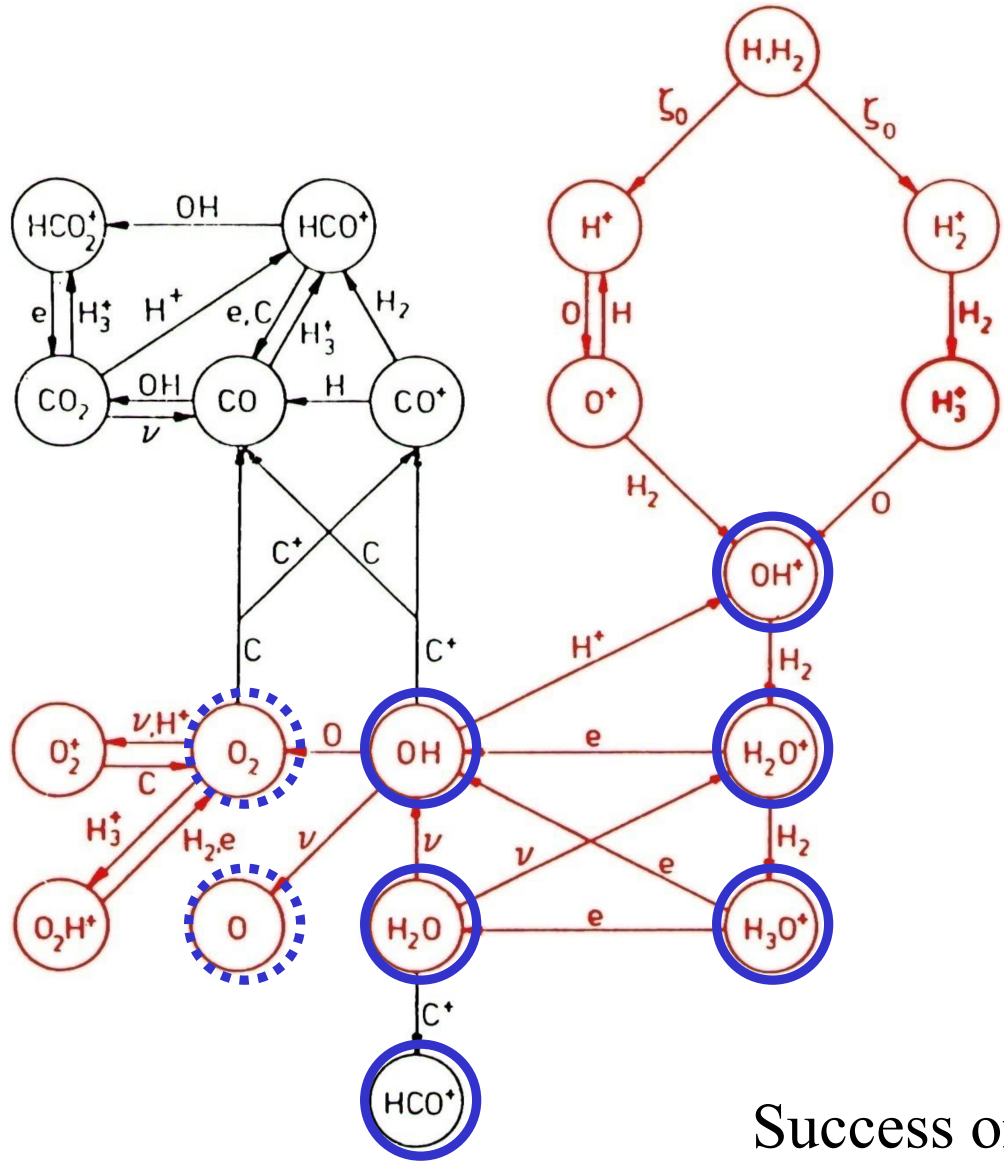
Oxygen chemistry

- Once OH^+ formed, rapid ion-molecule reactions lead to OH, H_2O and CO
- Note that OH abundance proportional to cosmic ray ionization rate ζ_{CR} => can use observed OH abundance to determine ζ_{CR}

Oxygen chemistry and its coupling with carbon



All key species in oxygen chemistry detected!

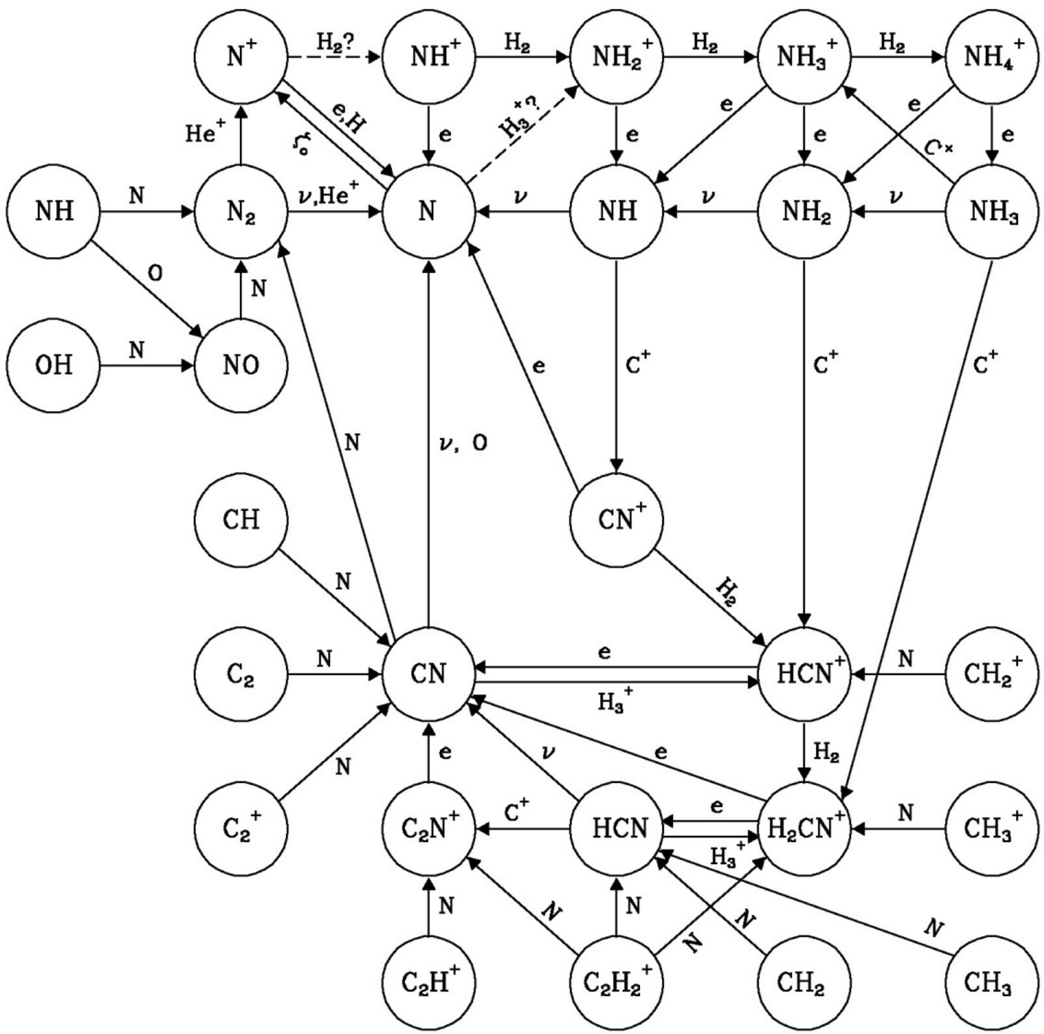


Success or ....???

Nitrogen chemistry

- I.P. N > 13.6 eV => nitrogen mostly neutral N
- Nitrogen chemistry initiated by
  - $N + H_3^+ \rightarrow NH_2^+ + H$? energy barrier?
  - $N^+ + H_2 \rightarrow NH^+ + H$? small barrier ~100 K
- Link with carbon chemistry
  - $CH, C_2 + N \rightarrow CN + H, C$
  - $CH_3^+ + N \rightarrow H_2CN^+ + H$
  - $H_2CN^+ + e \rightarrow HCN$ or $HNC + H$

Nitrogen chemistry

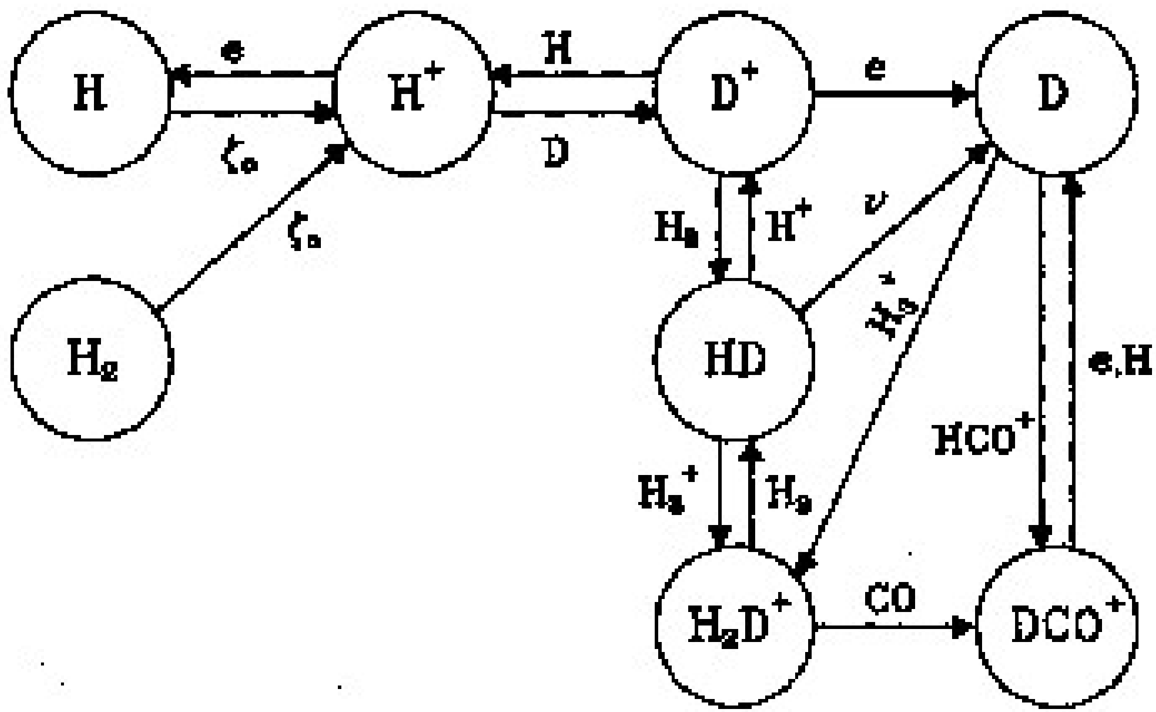


Deuterium chemistry

- HD formed mostly by rapid gas-phase reactions (*not on grains*), in contrast with H_2
  - $H^+ + D \leftrightarrow H + D^+$
  - $D^+ + H_2 \rightarrow HD + H^+$
- HD more rapidly destroyed by photodissociation than H_2, because column densities too small for self-shielding

$\Rightarrow$ Both formation and destruction up to 10^5-10^6 times faster;
Result: overall $HD/H_2 \sim 10^{-6}$-10^{-5} vs $[D]/[H]=1.5\times10^{-5}$

Deuterium network



4.4 Steady-state models

- Because photorates change with depth into cloud, models of diffuse clouds need to be depth-dependent
- Most reactions are fast (except H_2 formation) $\Rightarrow$ steady-state usually good assumption: $\mathrm{d}n_\mathrm{i}/\mathrm{d}t=0$

density $$n_i(z) = \frac{\text{formation rate}}{\text{destruction rate}} \quad \text{cm}^{-3}$$

column density $$N_i = \int n_i(z)\mathrm{d}z \quad \text{cm}^{-2}$$

Parameters

- Geometry: plane parallel
- Elemental abundances: C, O, N, S, Fe, Mg, …
  - Often constrained by observations
- Density structure: $n_H(z)$
  - Constrained by observations
- Temperature structure: $T(z)$
  - Constrained by observations or by solving thermal balance
- Incident radiation field: I_{UV} × standard field, plus grain absorption + scattering parameters
  - Constrained by observations
  - $I_V = I_0 10^{-0.4Av}$ (definition of A_V)
  - $I_{UV}(\lambda) = I_0 \exp(-\tau_d(\lambda))$ $\tau_d(\lambda) = n_d C_{ext}(\lambda) L$
- Cosmic ray ionization rate: ζ (s^{-1})

Rate equations

$$dn(i)/dt = \sum_l \sum_j K_{lj} n(l) n(j) - n(i) \sum_j K_{ij} n(j)$$

$$- R_{\rm acc}(i) + t_{\rm evap}(i)^{-1} n_s(i) \, ,$$

Gas

$$dn_s(i)/dt = \sum_l \sum_j k_{lj} n_s(l) n_s(j) - n_s(i) \sum_j k_{ij} n_s(j)$$

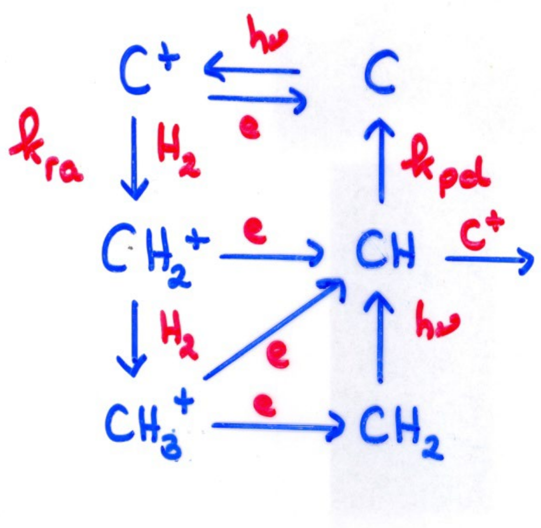
$$+ R_{\rm acc}(i) - t_{\rm evap}(i)^{-1} n_s(i) \, ,$$

Surface

Databases (KIDA, UMIST, …..) parametrize rate coefficients

$k=\alpha(T/300)^{\beta} \exp(-\gamma/T)$ $cm^3\ s^{-1}$ for bimolecular reaction
$k=\alpha$ s^{-1} for cosmic ray ionization
$k=\alpha \exp(-\gamma A_V)$ s^{-1} for photodissociation or photoionization

Example: CH



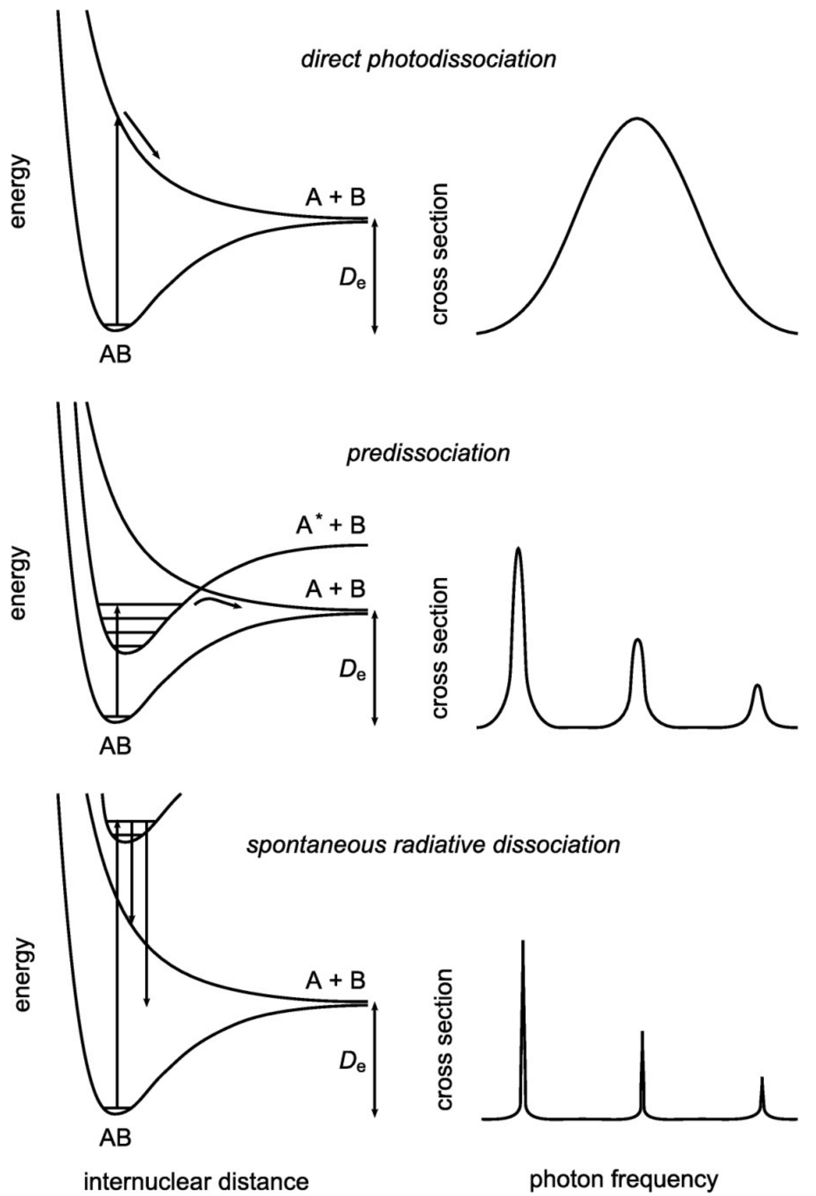
$$n(\mathrm{CH}) \propto \frac{n(\mathrm{C}^+)n(\mathrm{H}_2)k_{ra}}{k_{pd}}$$

- All rates well known (within factor 2) ⇒ it is possible to fit observed CH column densities
  - cannot claim that *all* CH is formed by this scheme; up to 50% could result from other processes
- Test: can consistent model be made that reproduces all observational data with same set of physical conditions and molecular parameters?

Comprehensive models

- Comprehensive models attempted by several groups, e.g., Black & Dalgarno (1977), van Dishoeck & Black (1986), Meudon group, UMIST, ….
- Chemistry governed by $H \rightarrow H_2$ and $C^+ \rightarrow C \rightarrow CO$ transitions
- Because of self-shielding, these transitions are ***sharp*** as functions of depth into cloud

Recall photodissociation Lecture 1



Direct p.d.

Ex: H_2^+, OH, H_2O

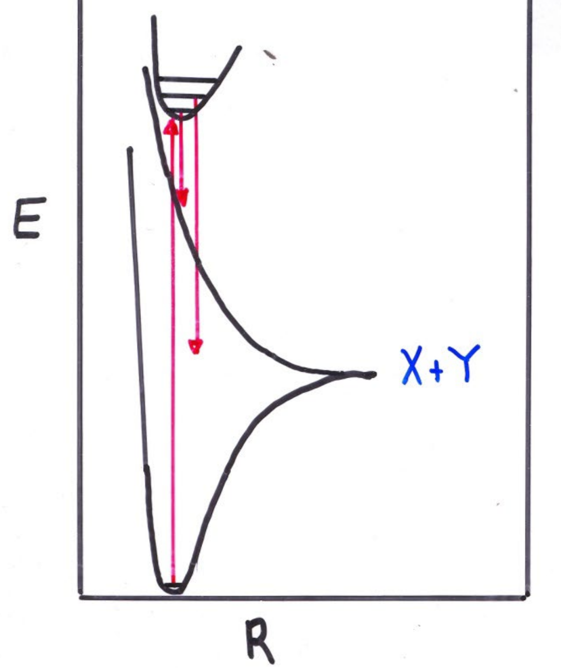
Predissociation

Ex: CO

Spontaneous radiative dissociation

Ex: H_2

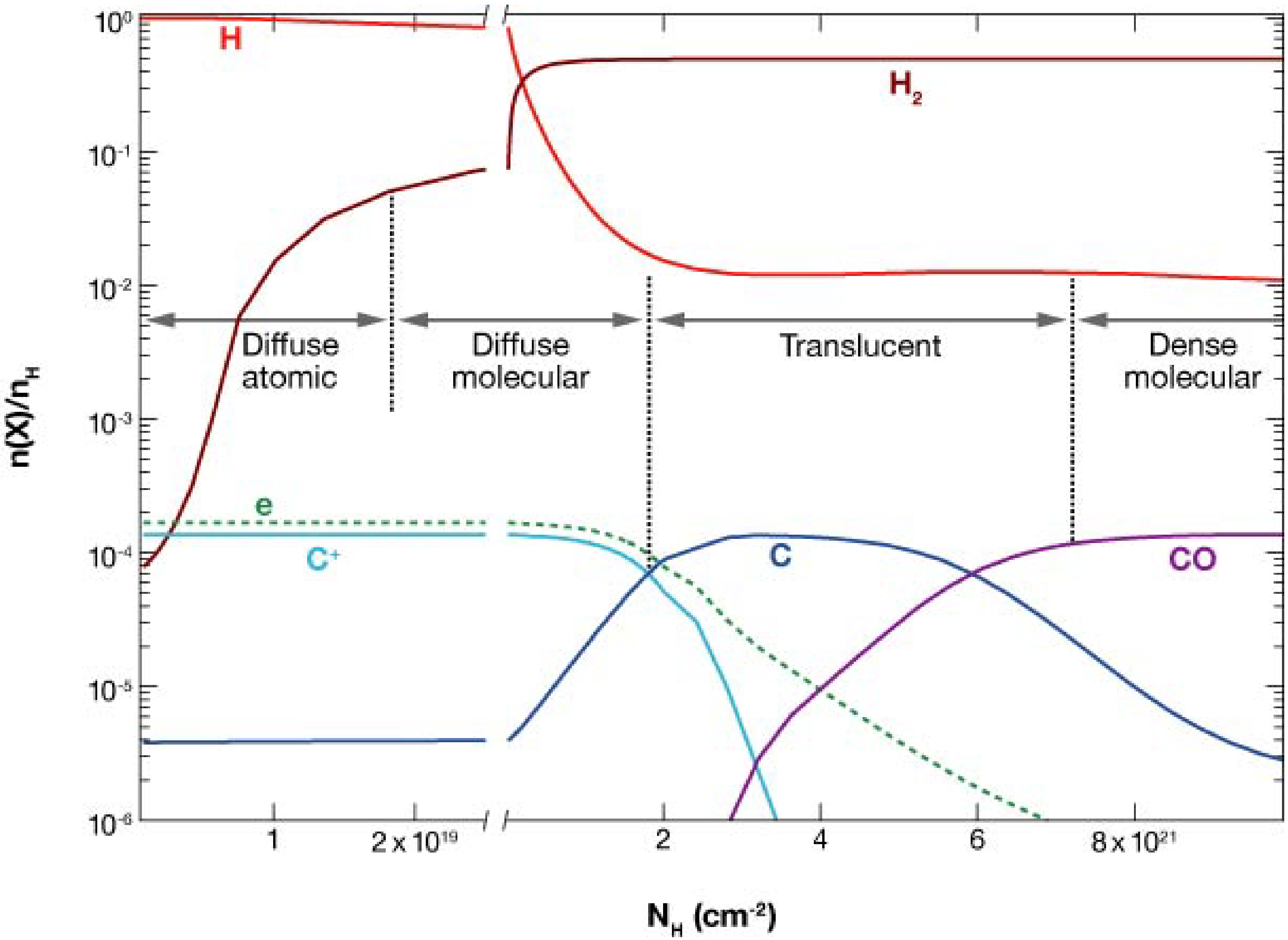
Photodissociation: self-shielding



Spontaneous radiation dissociation
Ex: H_2

- Photodissociation of both H_2 and CO occurs by line absorption → lines can become optically thick → **self-shielding** inside clouds
  - Molecules lying at the edge of the cloud absorb all available photons at that wavelength, so that molecules lying deeper in the cloud are protected***: sharp*** transition!

Types of molecular clouds



Snow TP, McCall BJ. 2006.
Annu. Rev. Astron. Astrophys. 44:367–414

CO formation and destruction

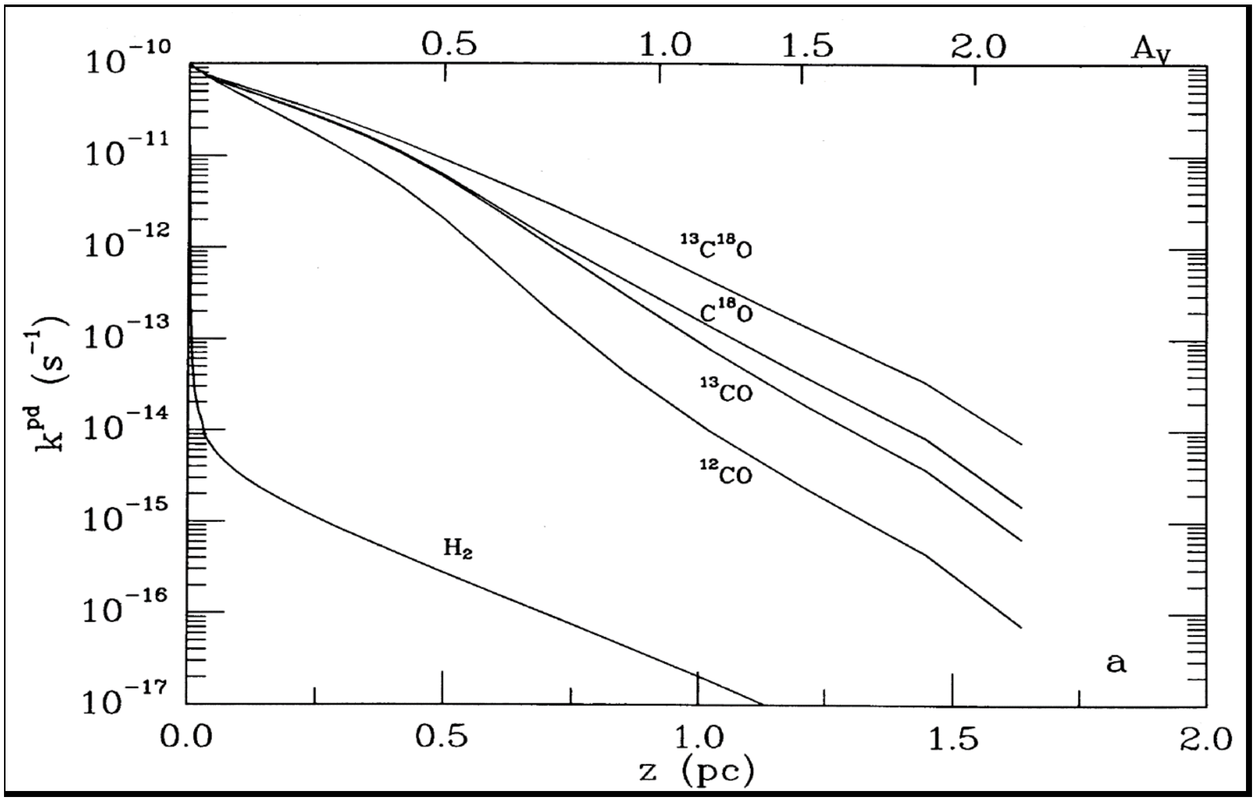
- CO is most abundant molecule after H_2 and is easily observed through (sub-) mm lines $\Rightarrow$
  - Good tracer of H_2
- At edge of cloud, most of carbon is C^+
- Transition $C^+ \rightarrow C \rightarrow CO$ with increasing depth
- CO is very stable ($D_e = 11.09$ eV $\Leftrightarrow$ 1118 Å) $\Rightarrow$ can only be dissociated at 912 Å $< \lambda <$ 1118 Å

CO photodissociation

- Like H_2, CO has no direct dissociation channels $\Rightarrow$ dissociation through line absorption (predissociation) $\Rightarrow$
  - Self-shielding, but at greater depth than H_2 because of lower abundance
  - Mutual shielding of CO by H_2
  - Mutual shielding of ^{13}CO by ^{12}CO
  - Attenuation by dust

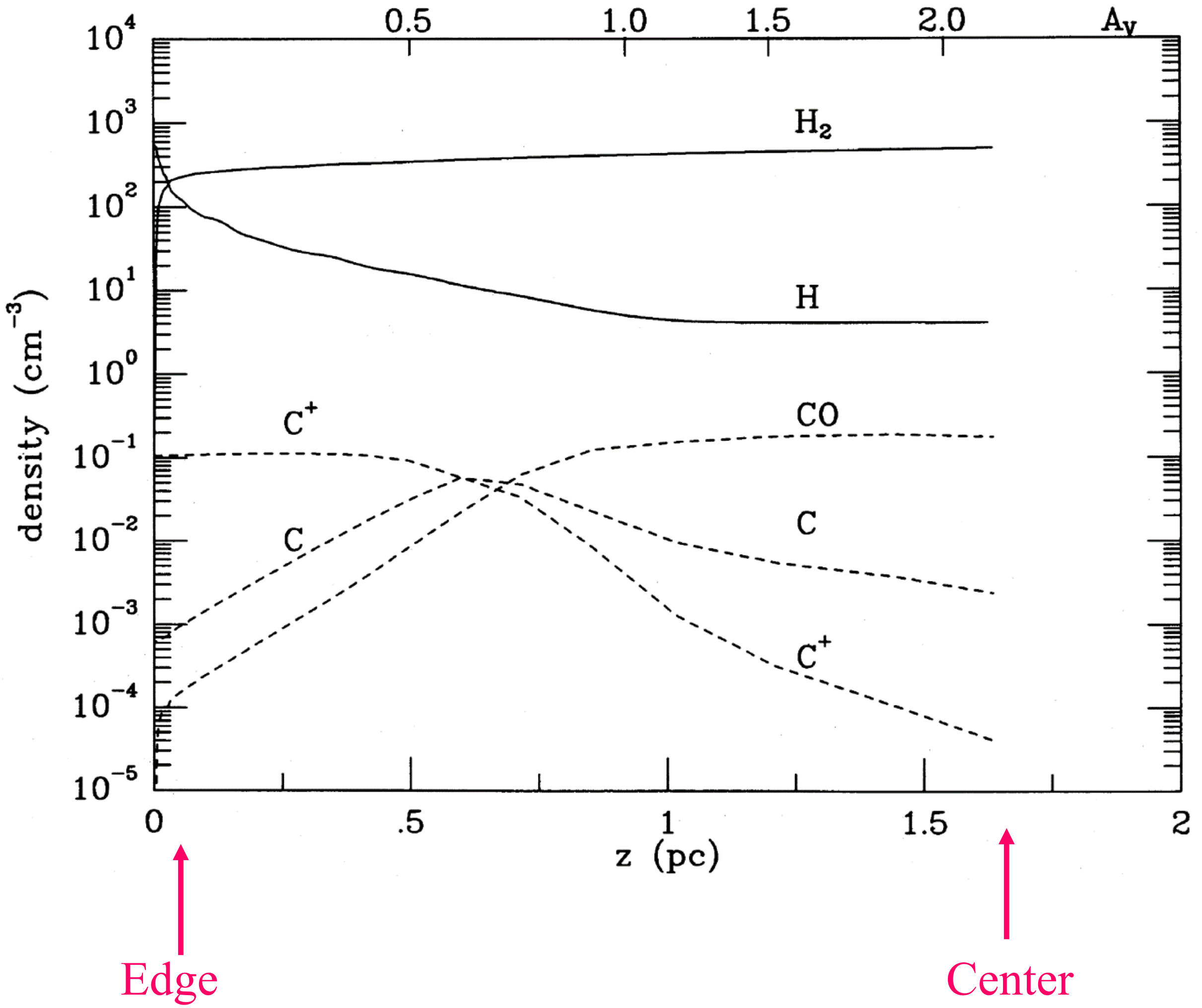
  $\Rightarrow$ complicated UV radiative transfer!
- Note that H_2 and CO photodissociation and C photoionization all occur in the same λ range 912-1100 Å
  - Important to know shape UV radiation field at short λ
- At $A_V \approx$ 1-2 mag, CO / H_2 increases from 10^{-7} to 10^{-4}

Self-shielding of CO and H_2
Photodissociation rates



- Decrease of CO p.d. rate with depth is less steep than that of H_2 because of larger competition with dust for UV photons
- CO self-shielding starts at N(CO)≈10^{15} cm^{-2}

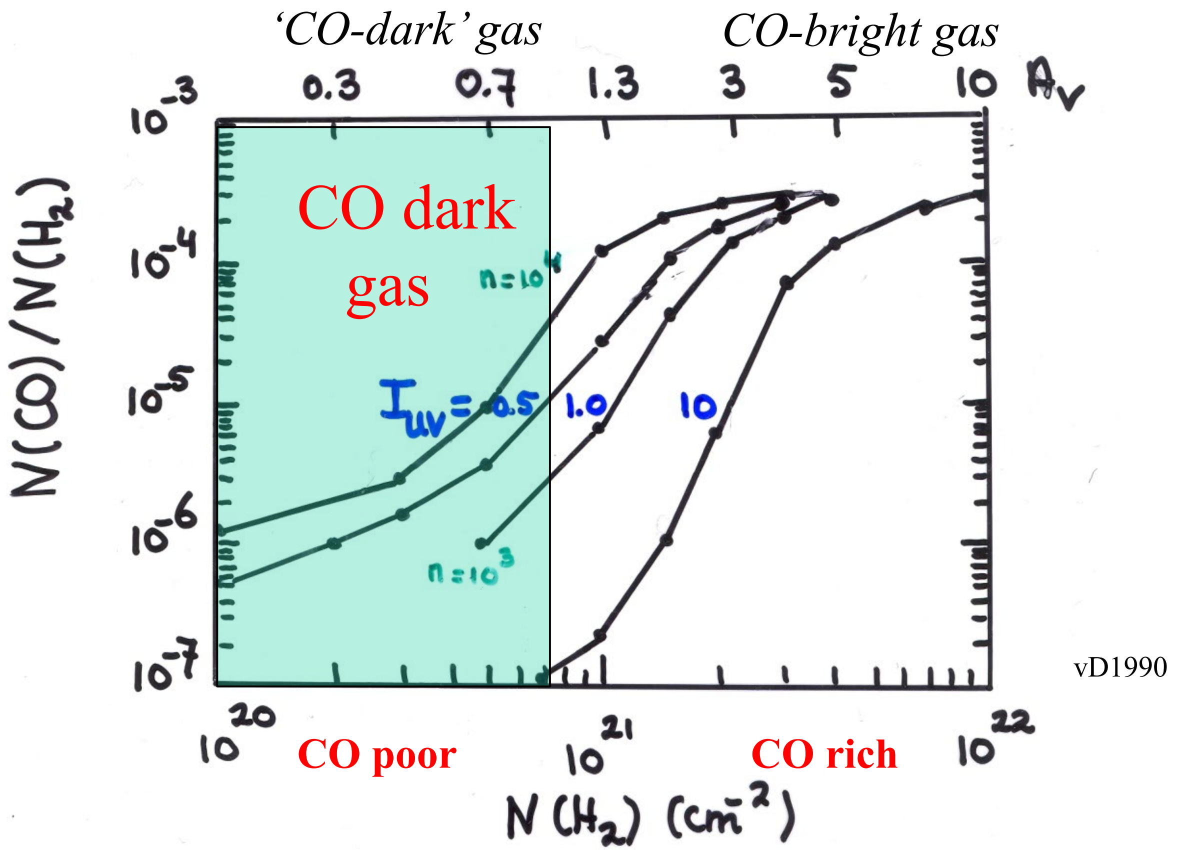
Densities of major species in translucent cloud



T=15 K
n_H=1500 cm^{-3}
I_{UV}=1

- Only column densities are observed => integrate over *z*

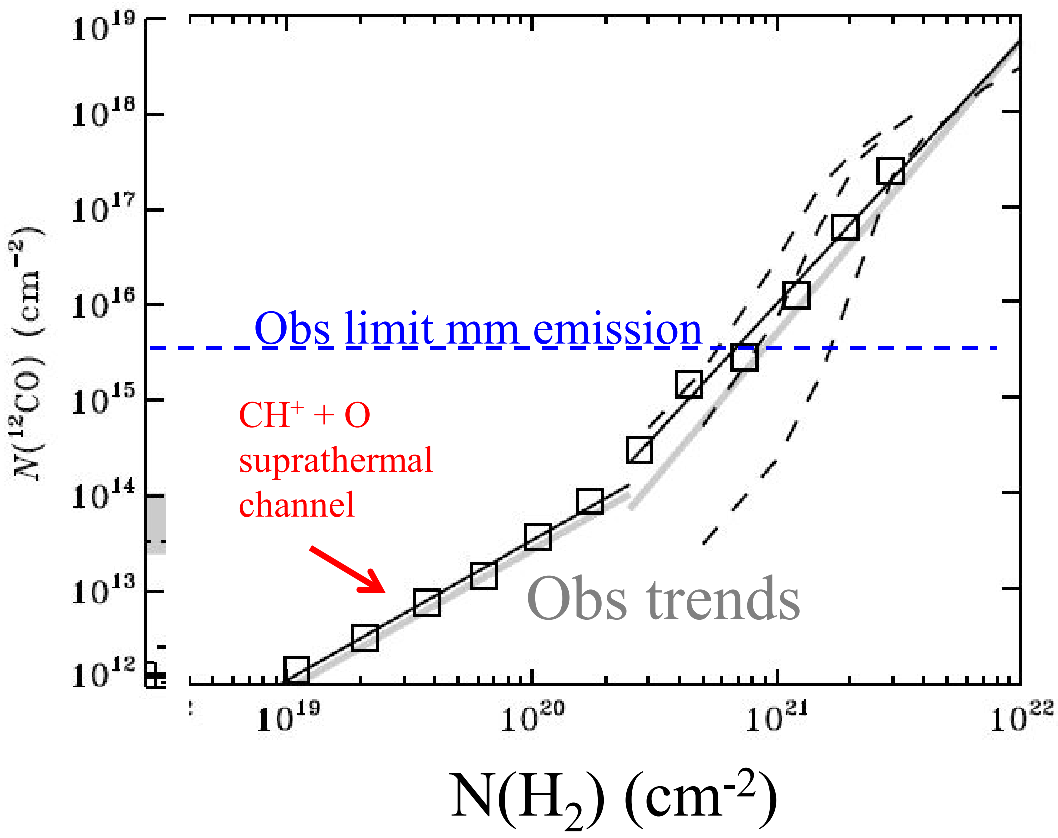
Column densities with N_H or A_V



⇒Increase in CO/H_2 at A_V=1-2 mag from 10^{-7} to 10^{-4}

- Exact location and sharpness transition depend on
  - I_{UV}, n_H, elemental abundances
  - Presence of PAHs, chemistry details (S), ζ, grain details, geometry….

CO vs H_2 column density



Visser et al. 2009
Sheffer et al. 2008

- At low A_V, formation of CH^+ through superthermal chemistry of $C^+ + H_2$ needs to be invoked to fit observations CO in diffuse clouds

Successes models

- Column densities CH, C_2, C_3, CN, OH, HCl O.K. within factor of 2
- Constraints on ζ and [D]/[H]
  - $\zeta=(7\pm3)\times10^{-17}$ s^{-1} (but see below H_3^+, OH^+)
  - $[D]/[H]\approx(1\text{-}2)\times10^{-5}$

Failures models

- CH^+ too low by a factor of 100
- NH too low by factor of 20
- Polyatomic molecules HCO^+, HCN, CH_3, … too low

Possible remedies

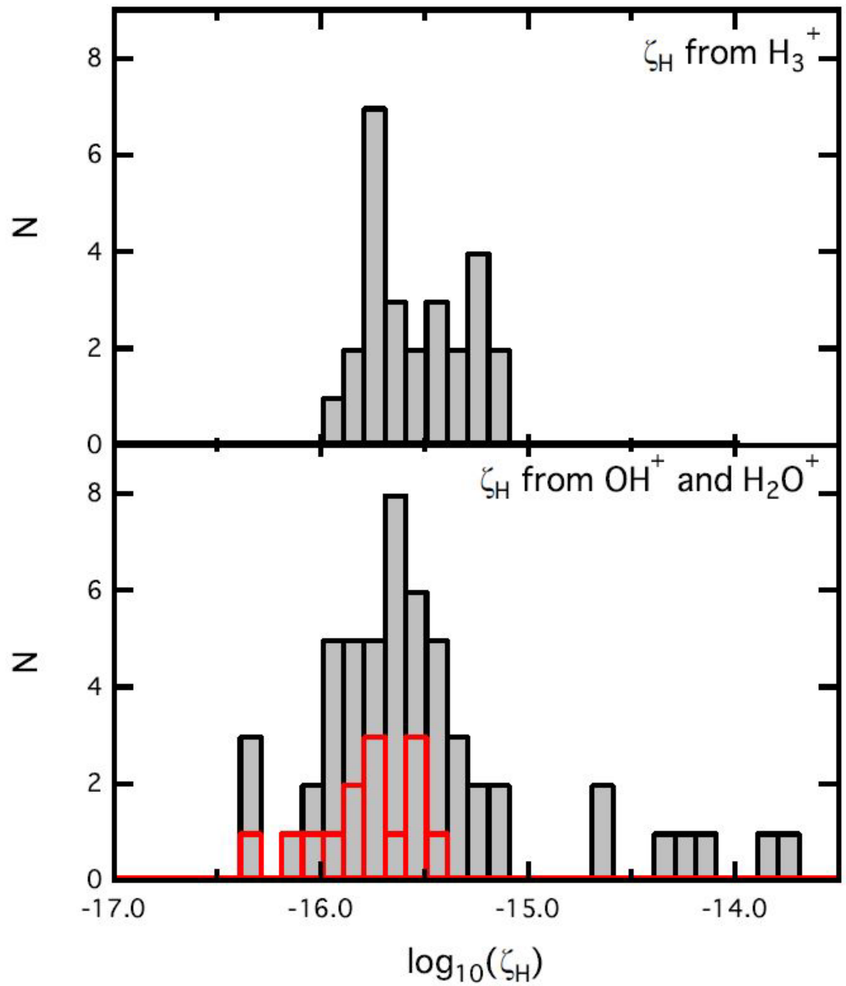
- Weak shocks or turbulence
  - CH^+: TDR models Godard et al. 2016
    - see also Chapter 5
  - HCO^+, HCN, CO, CH_3 enhanced if CH^+ enhanced
- Surface chemistry
  - NH, CH_3?
- Cloud structure: clumpy, high H/H_2, ...
  - CO
  - OH^+, H_2O^+, ArH^+

H_3^+ as probe of ζ

- Large column densities of $\sim 10^{14}$ cm^{-2} found in several diffuse clouds (Galactic Center , ζ Per, others)
- $n(H_3^+) = (\zeta / k_{DR}) n(H_2) / n(e)$
- $N(H_3^+) = n(H_3^+) L$ $\quad L$=pathlength
- $n(e)/n(H_2) \approx N(e)/N(H_2) \approx N(C^+)/N(H_2) \approx 3.8\times10^{-4}$ observed ζ Per
- $k_{DR} = 2.6\times10^{-7}$ cm^3 s^{-1} from exp
- $\underbrace{N_H}_{\text{obs}} = 1.6\times10^{21}$ cm^{-2}, $\underbrace{\langle n_H \rangle}_{\text{obs}} = 250$ cm^{-3} $\Rightarrow L = 2.1$pc
- $\Rightarrow$ **$\zeta = 1\times10^{-15}$ s^{-1},** factor of 10-20 larger than 'canonical value'
- Survey gives range of 10^{-16}-10^{-15} s^{-1} for number of sources

McCall et al. 2003
Le Petit et al. 2004
Indriolo et al. 2007

Cosmic ray ionization rate



Indriolo et al. 2015
Neufeld et al. 2017

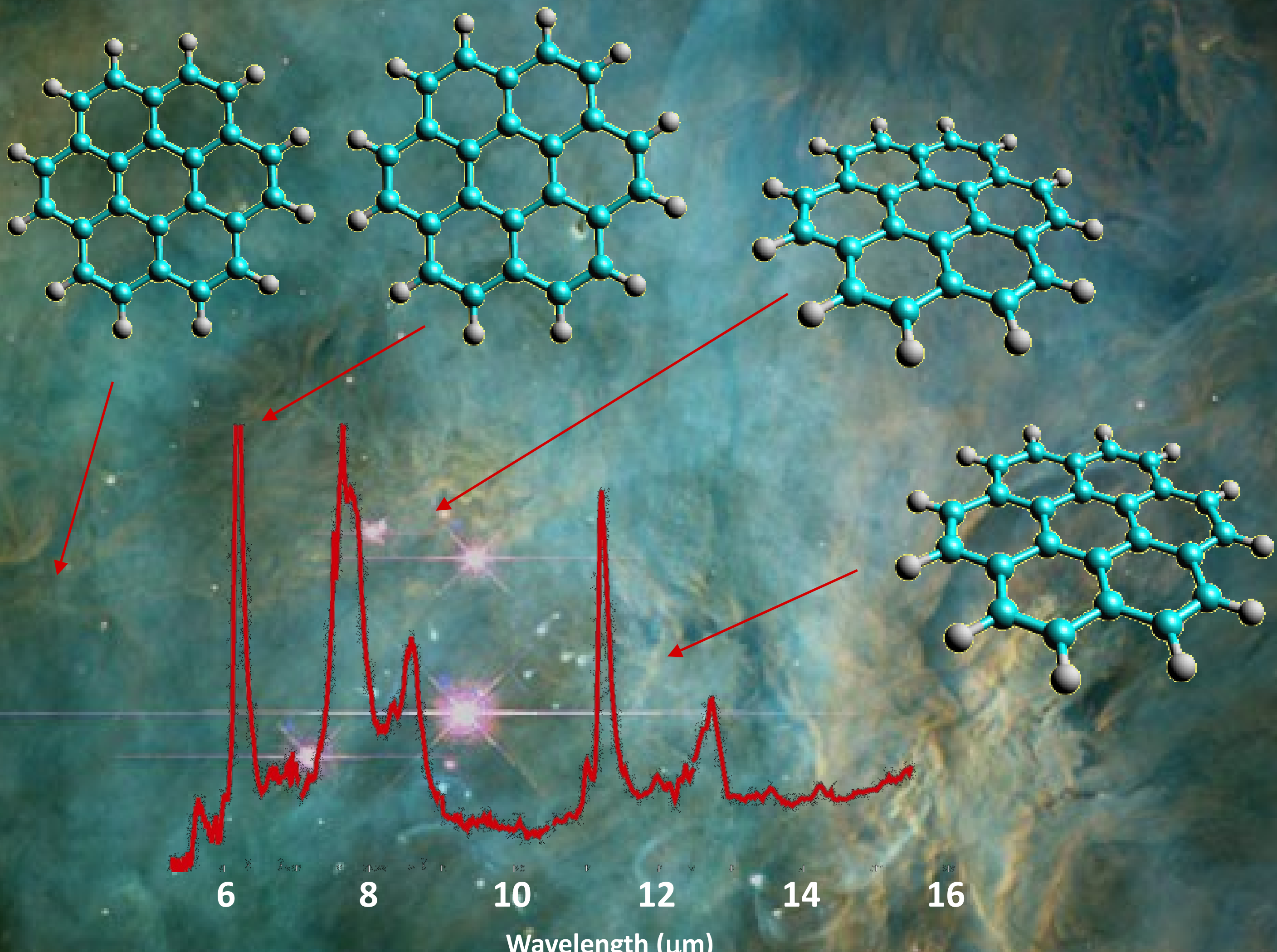
Use both H_3^+ and OH^+, H_2O^+ as probes

4.4 Photon-dominated regions (PDRs)

Tielens Chap 11
Hollenbach & Tielens 1997

- Diffuse and translucent clouds are examples of PDRs, i.e., clouds in which UV photons control the physical and chemical state of the cloud
- Traditionally, PDRs are dense molecular clouds located close to an OB star, in which the UV radiation field is enhanced by a factor of 10^5 w.r.t. average interstellar radiation field (ISRF)
  - Example: Orion Bar
- PDRs show very strong atomic fine-structure lines
  - E.g. [C II] 158 μm, [C I] 610 μm, [O I] 63 μm
- And submillimeter lines of molecules
  - E.g. CO 7-6, HCO^+ 4-3
- And strong H_2 mid- and near-IR lines and PAH features

PAH vibrational modes



"Unidentified infrared emission bands"

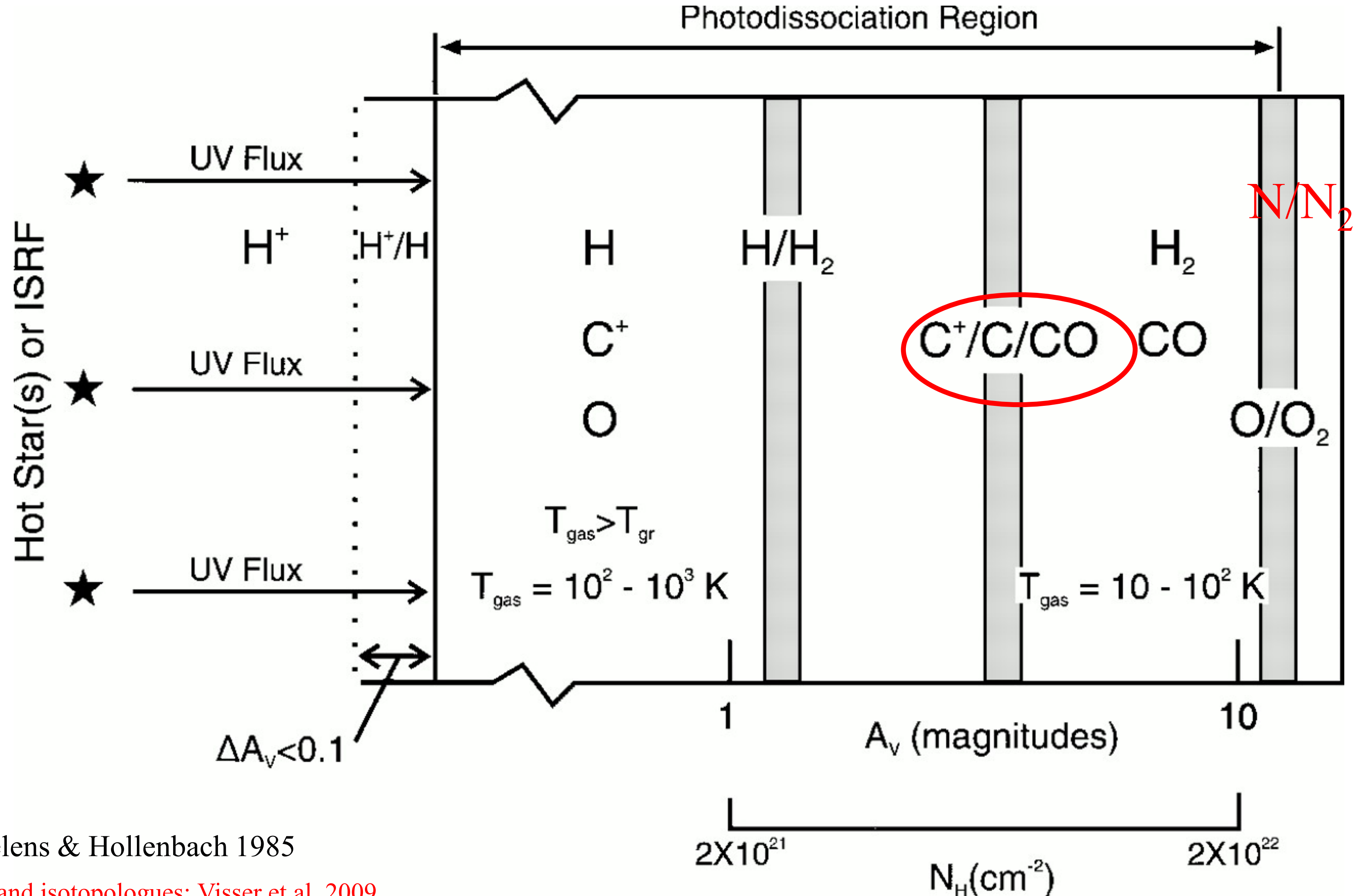
PAHs heat gas through photoelectric effect

Slide by Jos Oomens

Horsehead nebula as a PDR

AAT

PDR structure

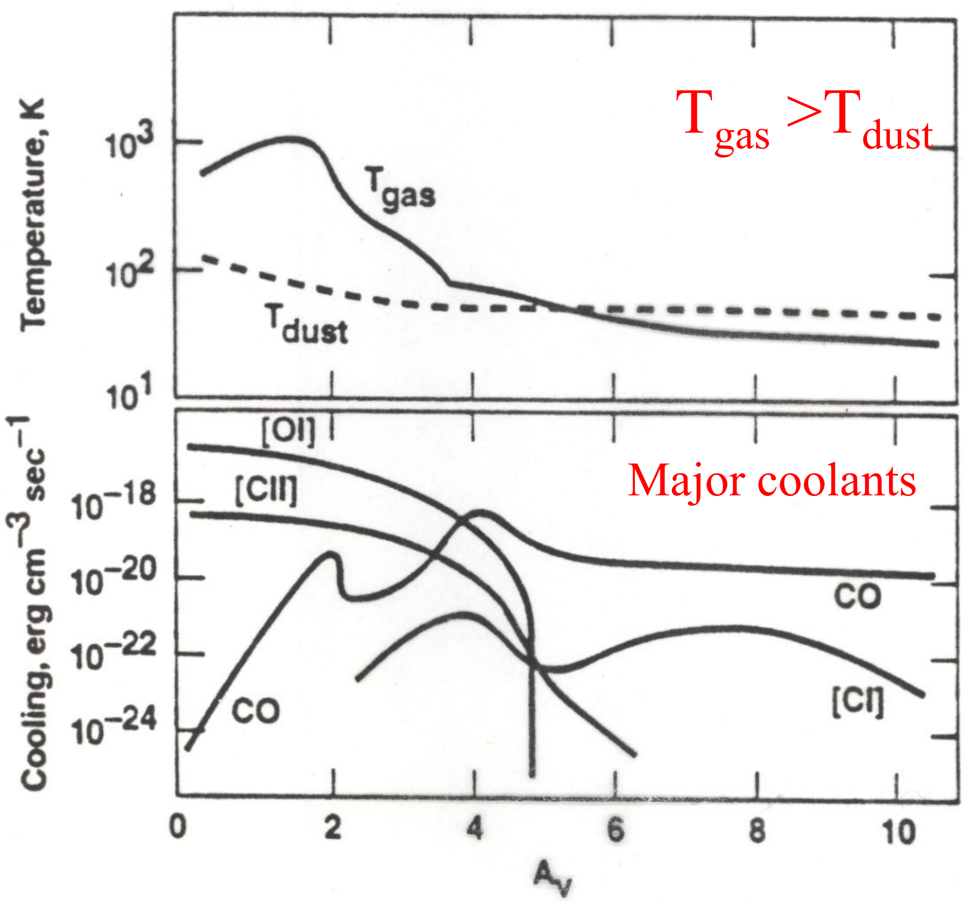


Tielens & Hollenbach 1985

CO and isotopologues: Visser et al. 2009

Hollenbach & Tielens 1997

Orion PDR physical structure



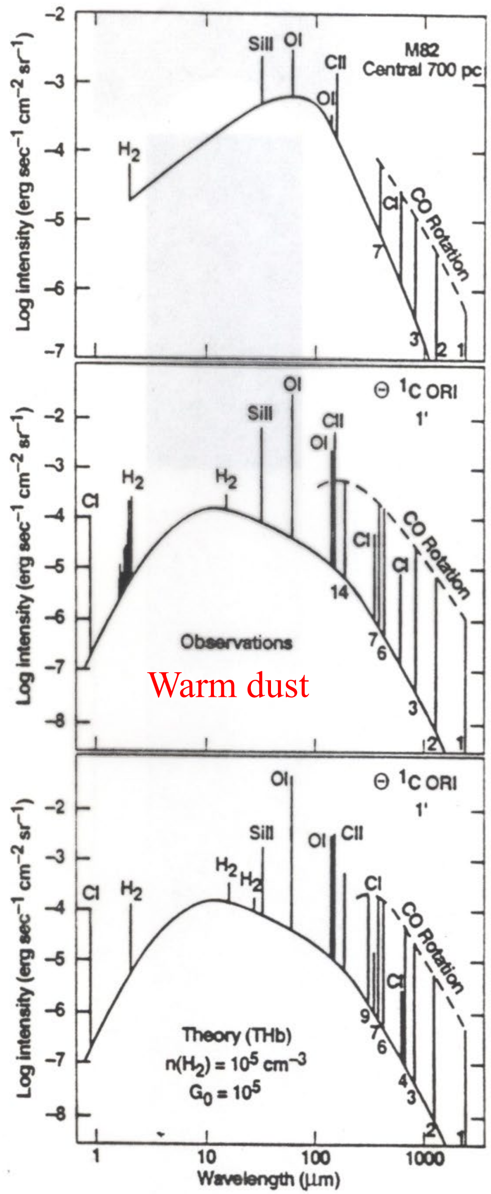
$n_H = 10^5$ cm^{-3}

$I_{UV} = 10^5$

Tielens & Hollenbach 1985

High temperature at edge allows $O + H_2 \rightarrow OH + H$ and $C^+ + H_2 \rightarrow CH^+ + H$ reactions to proceed, in contrast with low density diffuse clouds

Global PDR emission



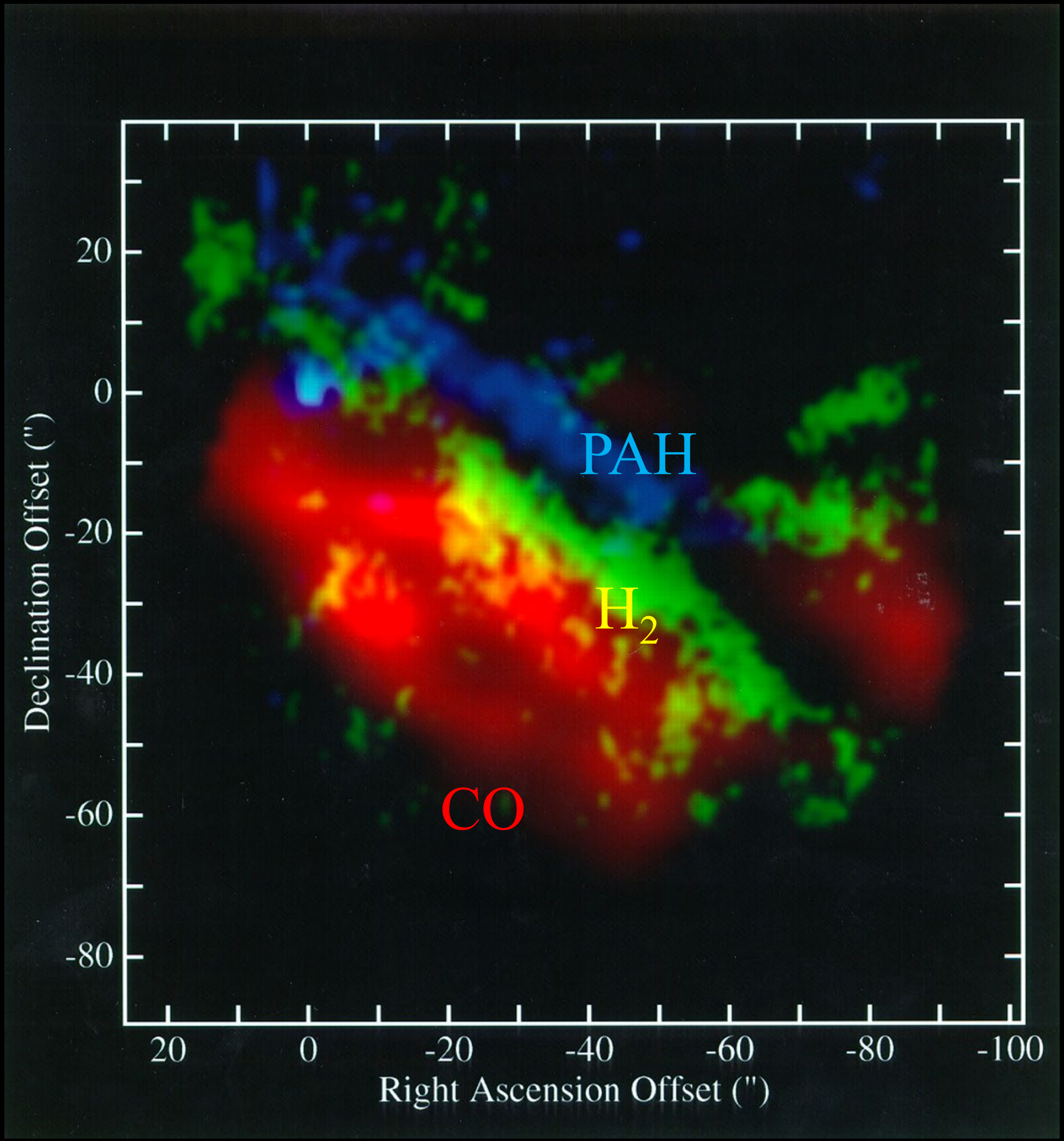
M 82 galaxy

Orion

Dense PDR model

Genzel et al. 1989

Orion Bar PDR



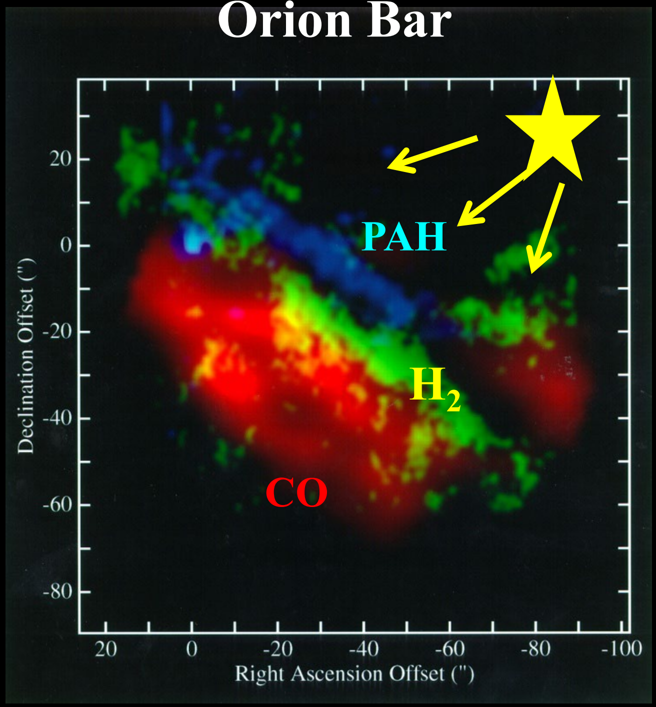
Yellow: H_2 v=1-0
Blue PAH
Red: CO

(0,0)=Θ^2A Ori

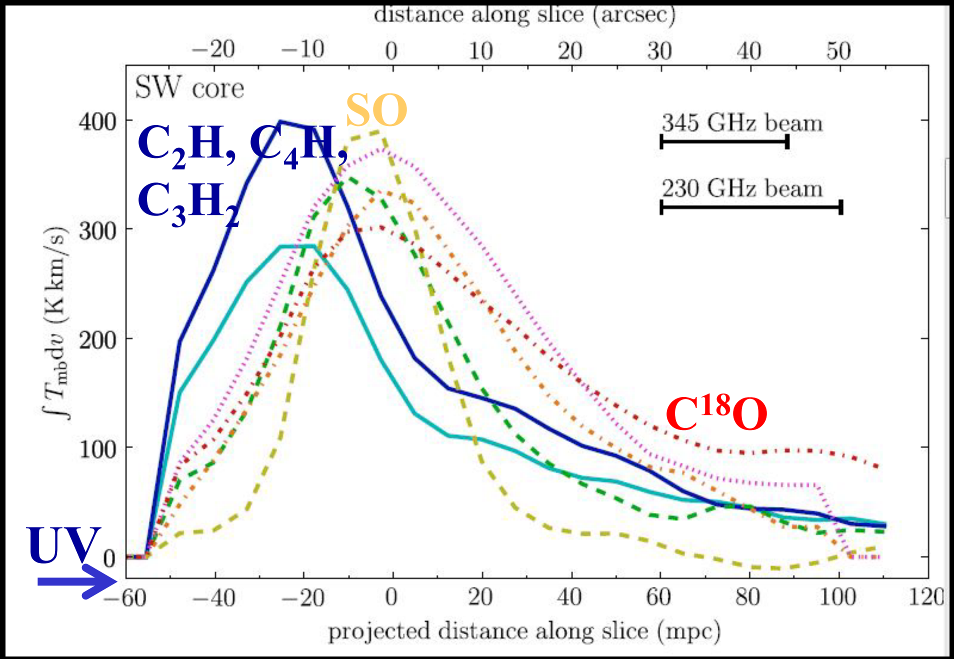
Note layered structure!

Tielens et al. 1993

Layered structure PDRs



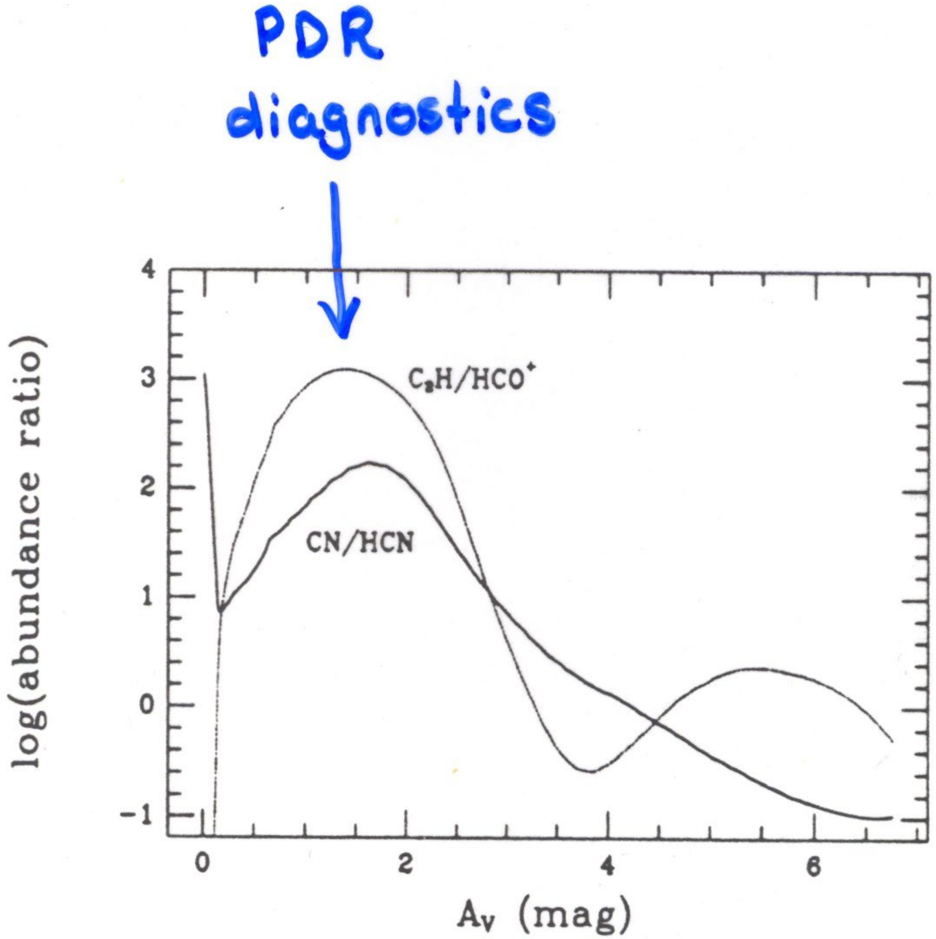
Tielens et al. 1993



Hogerheijde et al. 1995, van der Wiel et al. 2009

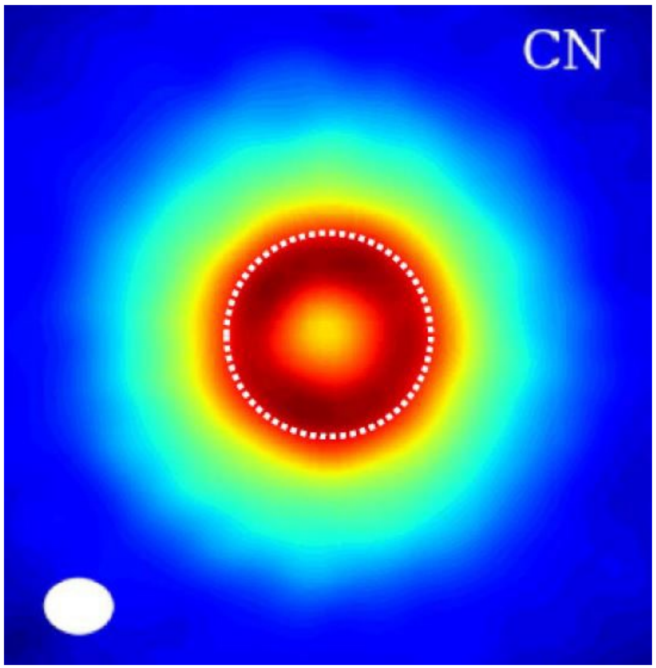
- Radicals C_2H, CN peak at $C^+ \rightarrow C$ transition
- Stable HCN, CO peak deeper into cloud

PDR diagnostics: CN/HCN



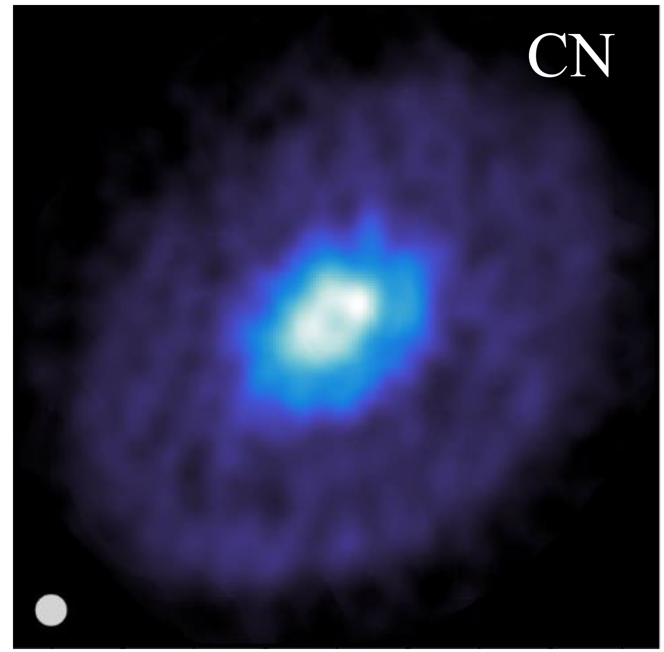
Jansen et al. 1995

4.5 Other examples PDRs: Protoplanetary disks



TW Hya disk

Teague et al. 2016,
Cazzoletti et al. 2018



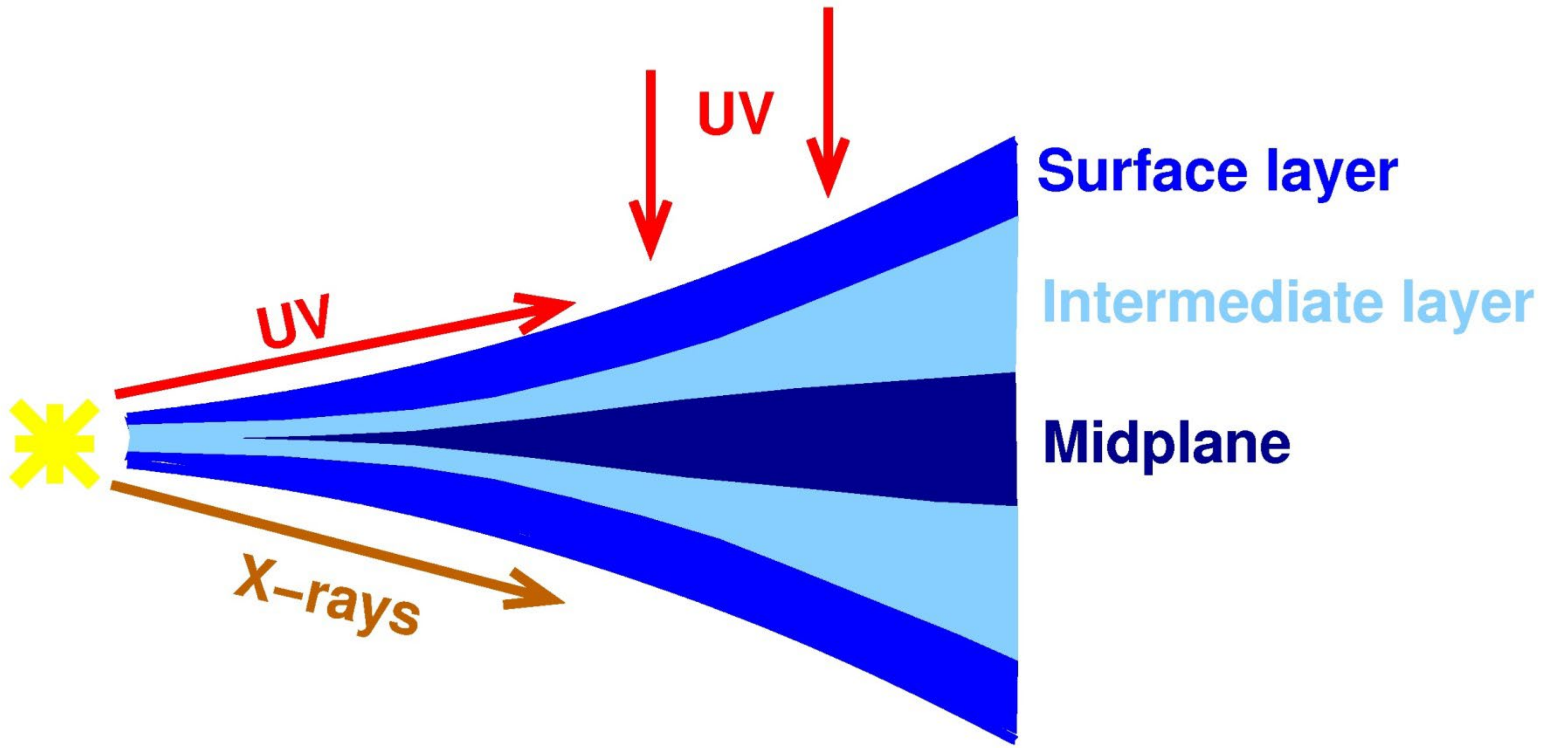
HD 163296 disk

Bergner et al. 2021, MAPS

Ring-like CN emission on ~100 AU scales

2D flaring protoplanetary disks

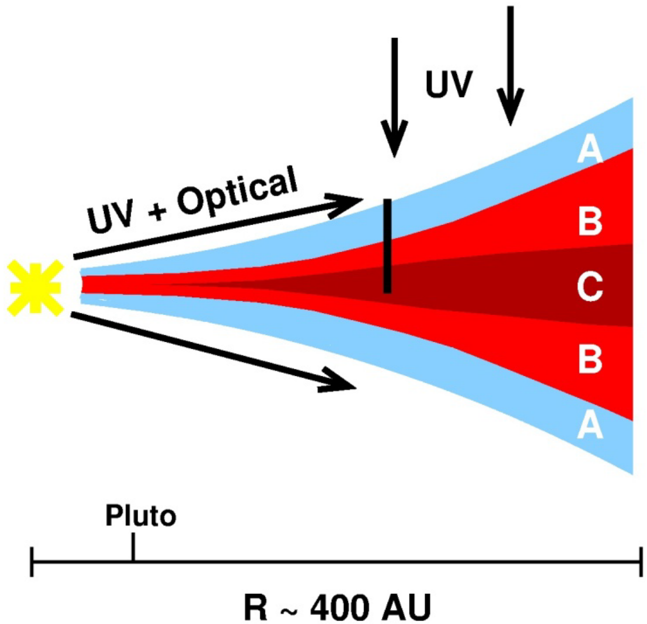
- Surface layer: molecules dissociated by UV photons
- Warm intermediate layer: molecules not much depleted, rich chemistry
- Cold midplane: molecules heavily frozen out

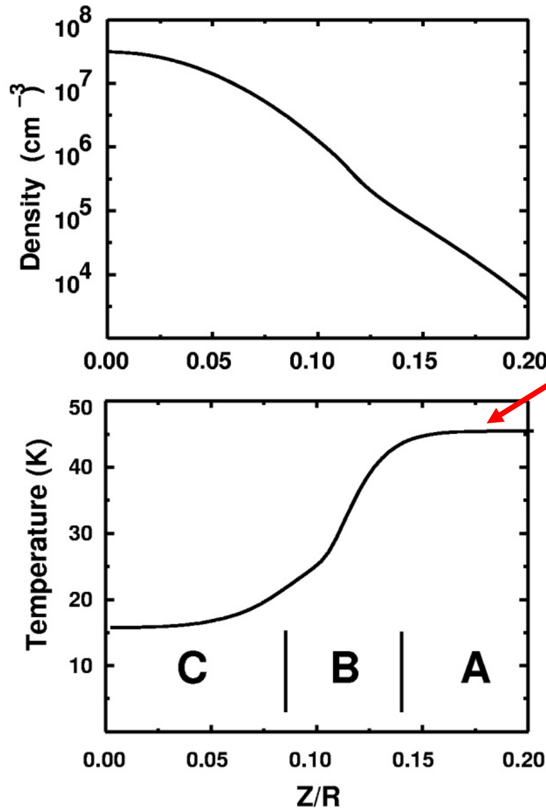


PDR-like structure but with large density gradients and very intense UV (up to 10^6 x ISM)

Aikawa et al. 2002
Bergin et al. 2007, PPV
+ many other groups

Vertical structure



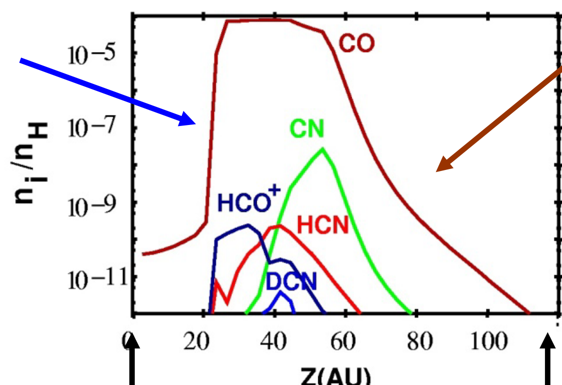


R=200 AU

T_{gas} is larger

Freeze-out

Photodissociation



midplane

surface

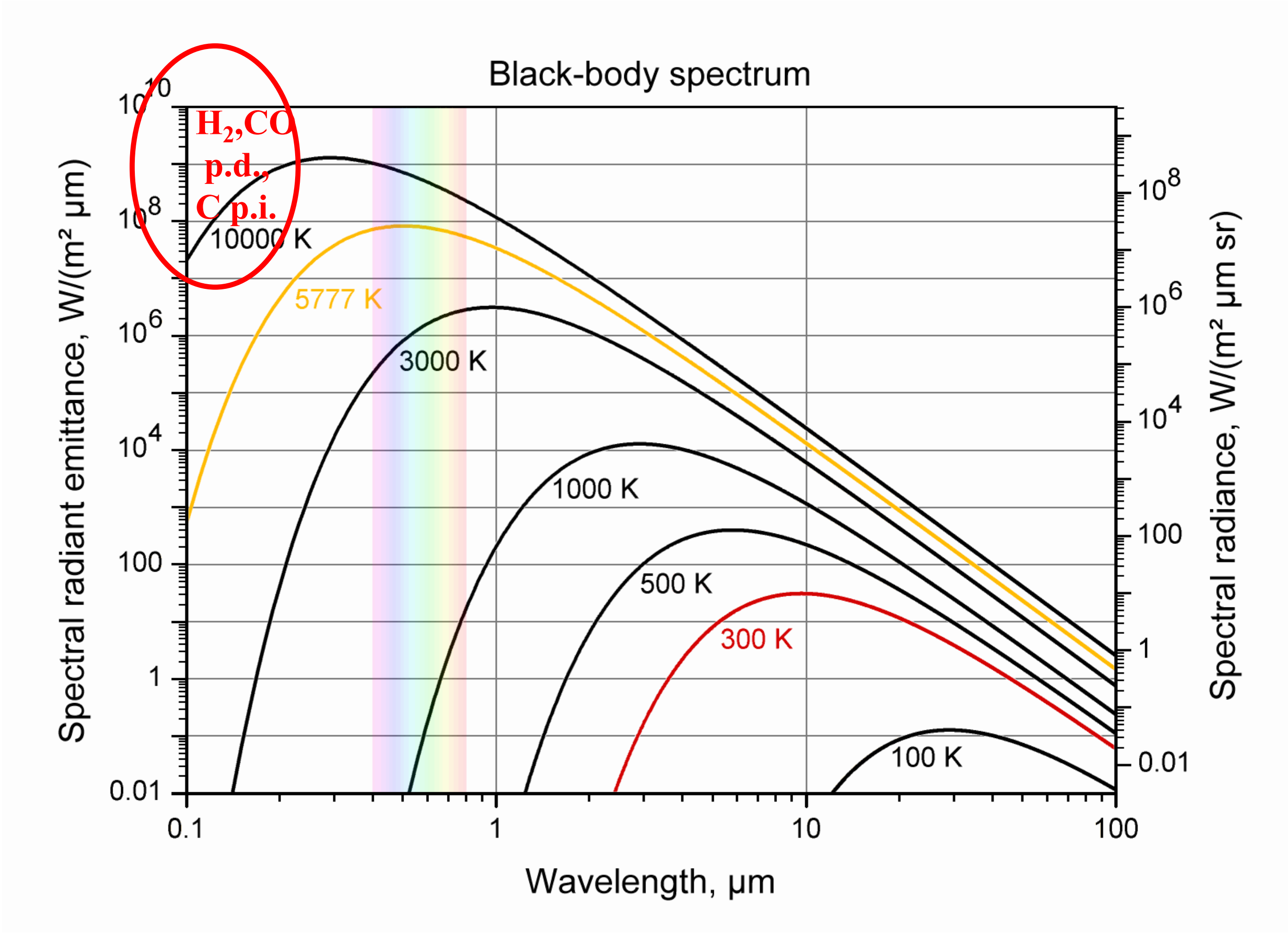
Ionization fraction:

- Surface: 10^{-4} (C^+)
- Intermediate: 10^{-9} (HCO^+)
- Midplane: $\sim 10^{-11}$ (H_3^+, H_2D^+)

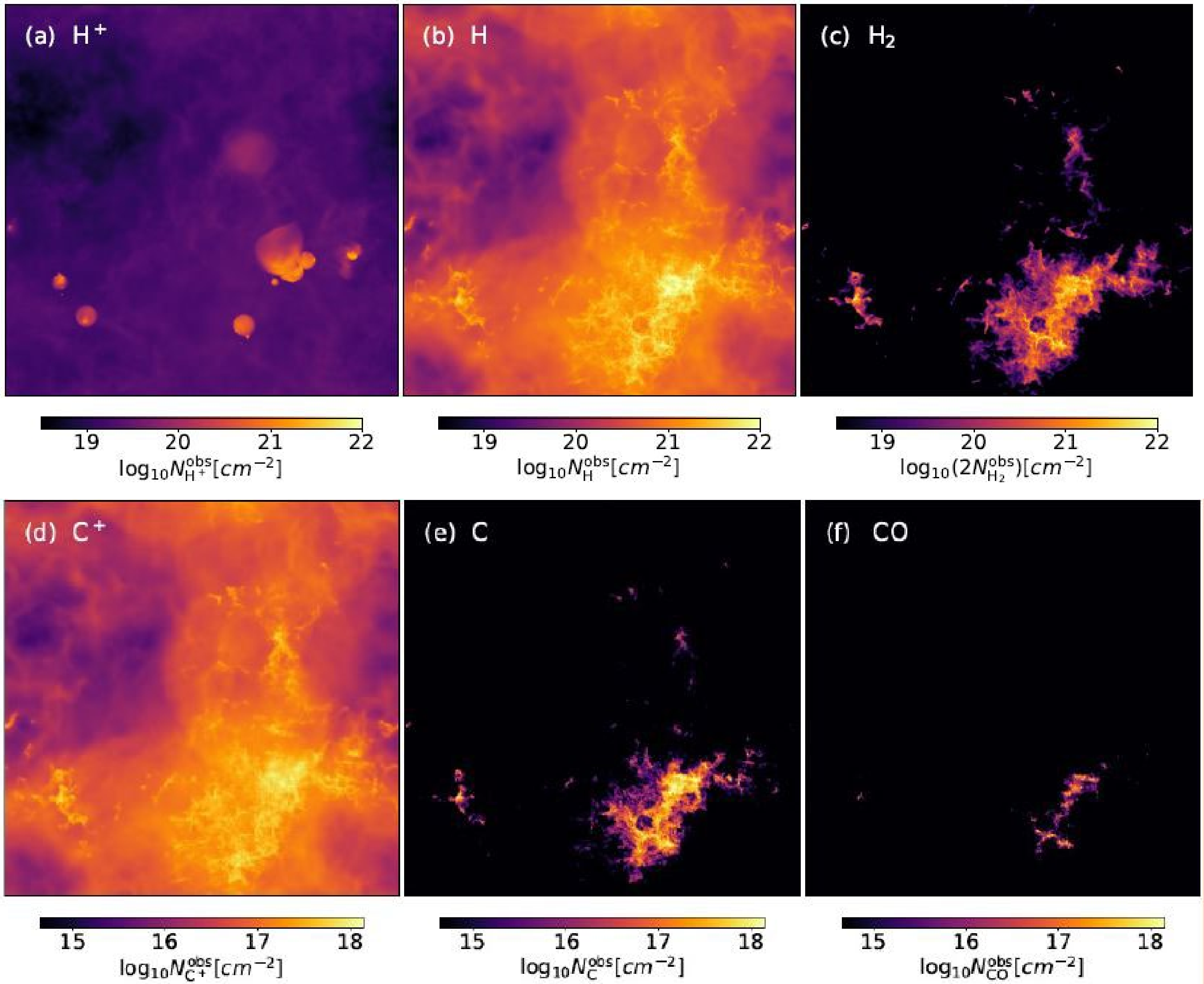
Beyond the standard model

- Cool PDRs
  - Clouds exposed to A, F, … stars with T_{eff}=6000-10000 K ⇒ fewer photons between 11 and 13.6 eV to dissociate H_2 and CO
- Metal poor PDRs
  - Regions with C, O, … depleted by factors >4. Large gas/dust ratios (ex: LMC, SMC)
- Inhomogeneous, clumpy PDRs
  - Regions with large density contrasts and small filling factors clumps
- Time-dependent PDRs
  - Regions with evolving radiation field (e.g., planetary nebulae) or flowing gas (e.g., expanding HII region)
- XDRs
  - Regions exposed to X-rays, which can ionize H, He and multiply ionized atoms (e.g., S^{++}). Penetrate farther into cloud than UV

Cool radiation fields



Extragalactic multiphase ISM



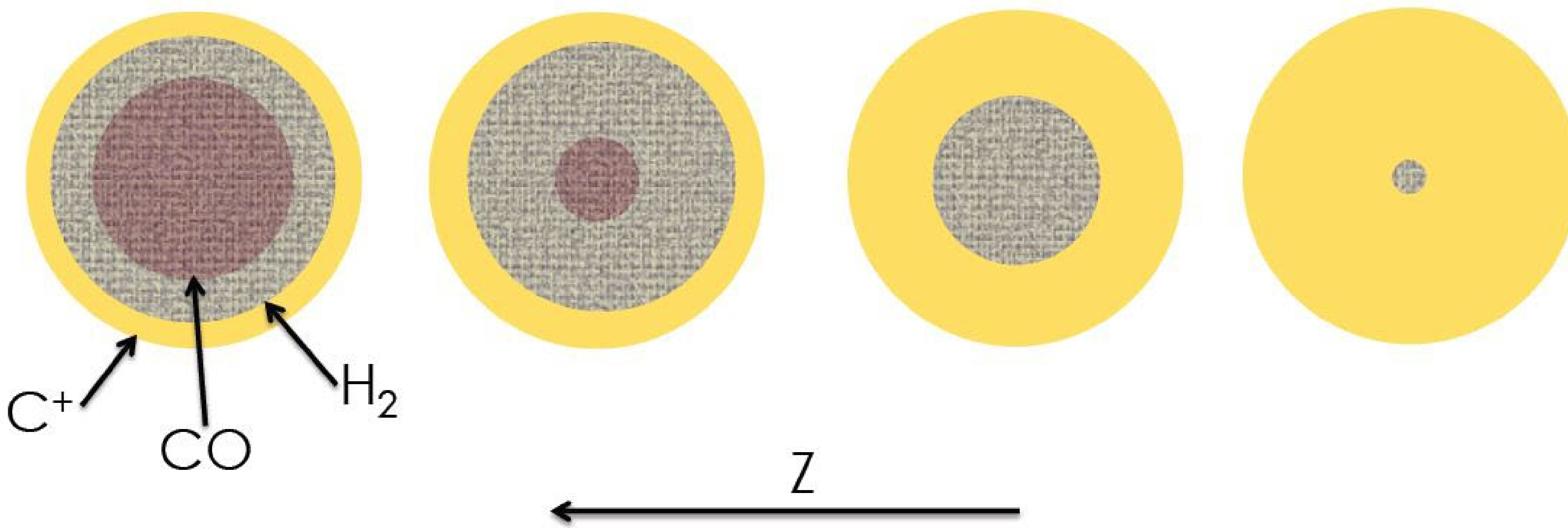
kpc scales

Incl. supernova feedback

Note CO limited to small patch

Hu, Sternberg, vD 2021

Low metallicity ISM



Pak et al. 1998
Wolfire et al. 2010

- At low metallicity, less dust and less C → less shielding
- Larger fraction of the cloud is atomic at low Z

Summary Lecture 4

- Diffuse and translucent clouds are unique laboratories for testing gas-phase chemistry
- New data and insight from mm+FIR absorptions
  - Herschel, ALMA
- Several successes, but also some problems
  - Sometimes physics rather than chemistry not understood (e.g., turbulence)!
- Structure diffuse and translucent clouds as well as dense PDRs controlled by $H \rightarrow H_2$, and $C^+ \rightarrow C \rightarrow CO$ transitions

Appendix: equivalent width of spectral lines

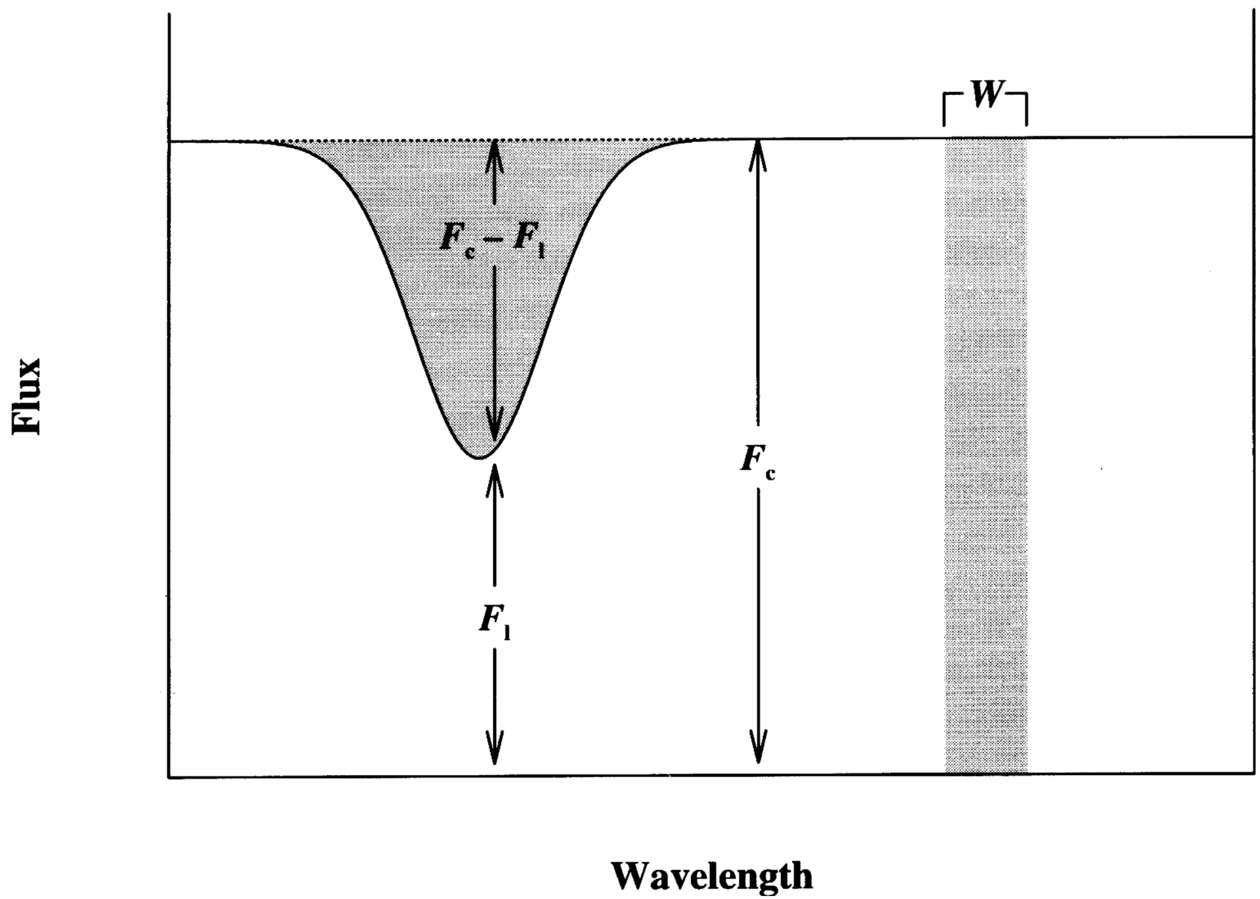
- In practice, resolution at optical wavelengths often insufficient to resolve line $\Rightarrow$ measure only line strength or equivalent width
- Definition of equivalent width of line:

$$W_\nu = \int_{-\infty}^{\infty} \left(1 - e^{-\tau_\nu}\right) \mathrm{d}\nu = \int_{-\infty}^{\infty} \left[\frac{I_\nu(0) - I_\nu}{I_\nu(0)} \right] \mathrm{d}\nu \quad \text{Hz}$$

- W_ν is the width of a rectangular profile from 0 to $I_\nu(0)$ that has the same area as actual line
- W_ν measures line strength, but units are Hz
- In wavelength units

$$W_\lambda = \frac{\mathrm{d}\lambda}{\mathrm{d}\nu} W_\nu = \frac{\lambda^2}{c} W_\nu \ \text{ cm}$$

Schematic drawing of equivalent width of line



Column density $N \propto W/f$ if line optically thin
with f = oscillator strength