Grains and Molecules

Formation of Grains

Atoms → diatomic molecules (e.g., CH, CO, CN)
→ 10 to20 atoms as condensation nuclei
→ growth by accretion

In HI clouds, $n_H \approx 10 - 100\ \mathrm{cm}^{-3}$ → molecules form too slowly

Grains likely formed in (1) atmospheres of cool stars, or
(2) dark molecular clouds

IR observations detect grains in both.

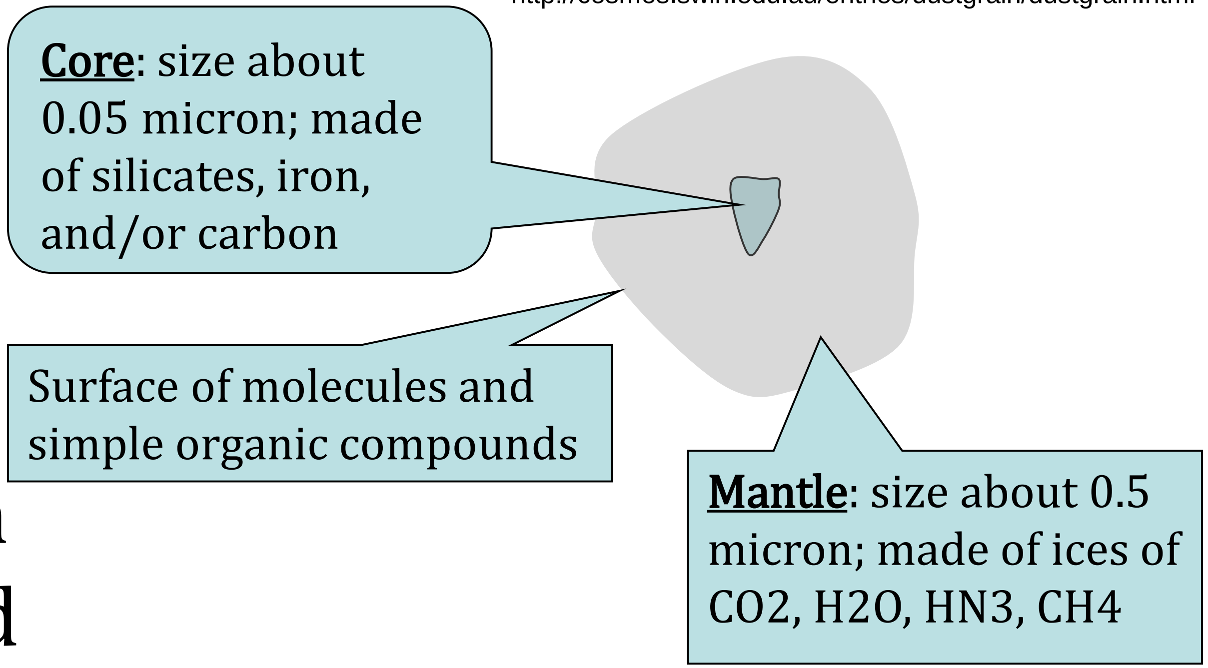
Generally, depletion of elements → grain formation
Those with higher condensation temperatures condense first, so condense/deplete more

With condensation nuclei (small, refractory particles), volatile materials such as CO_2, CH_4, NH_3, H_2O condense as mantles

Dark clouds show grain sizes ($a \gtrsim 1\ \mu$m), larger than typical ISM $a < 0.2 - 0.5\ \mu m$

A large number $a < 0.015\ \mu m$

C, N, O depletion consistent with this, i.e., these elements locked into ices on the grains



http://cosmos.swin.edu.au/entries/dustgrain/dustgrain.html

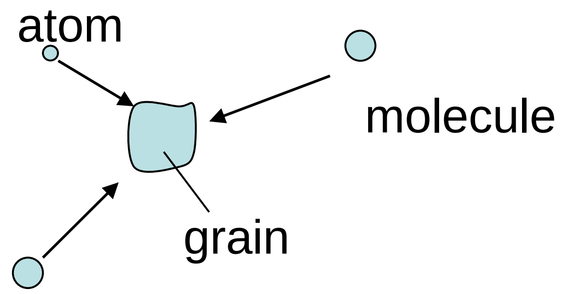
Core: size about 0.05 micron; made of silicates, iron, and/or carbon

Surface of molecules and simple organic compounds

Mantle: size about 0.5 micron; made of ices of CO2, H2O, HN3, CH4

ISM grain (nuclei, mantles) → grain growth → planetesimals → planets

Grain Growth Rate



$$\frac{dm}{dt} = (\frac{1}{4} n \bar{v})(m_H\, A)\, \xi\, (4\pi a^2)$$

Sticking coefficient (probability) $\xi \lesssim 1$

$$\frac{dm}{dt} = \rho_s 4\pi a^2\, \frac{da}{dt}$$

$$\begin{aligned}
\frac{da}{dt} &= \frac{(1/4) n \bar{v} m_H A\, \xi}{\rho_s} \\
&= \frac{v \rho_H}{4 \rho_s} A\xi \\
&= \frac{10^5\, 1.6 \times 10^{-24}}{4 \cdot 1} A\xi \\
&= 4 \times 10^{-20}\, \mathrm{cm\ s}^{-1}\, A\xi \\
&= 15 \times 10^{-13}\, \mathrm{cm\ yr}^{-1}\, A\xi
\end{aligned}$$

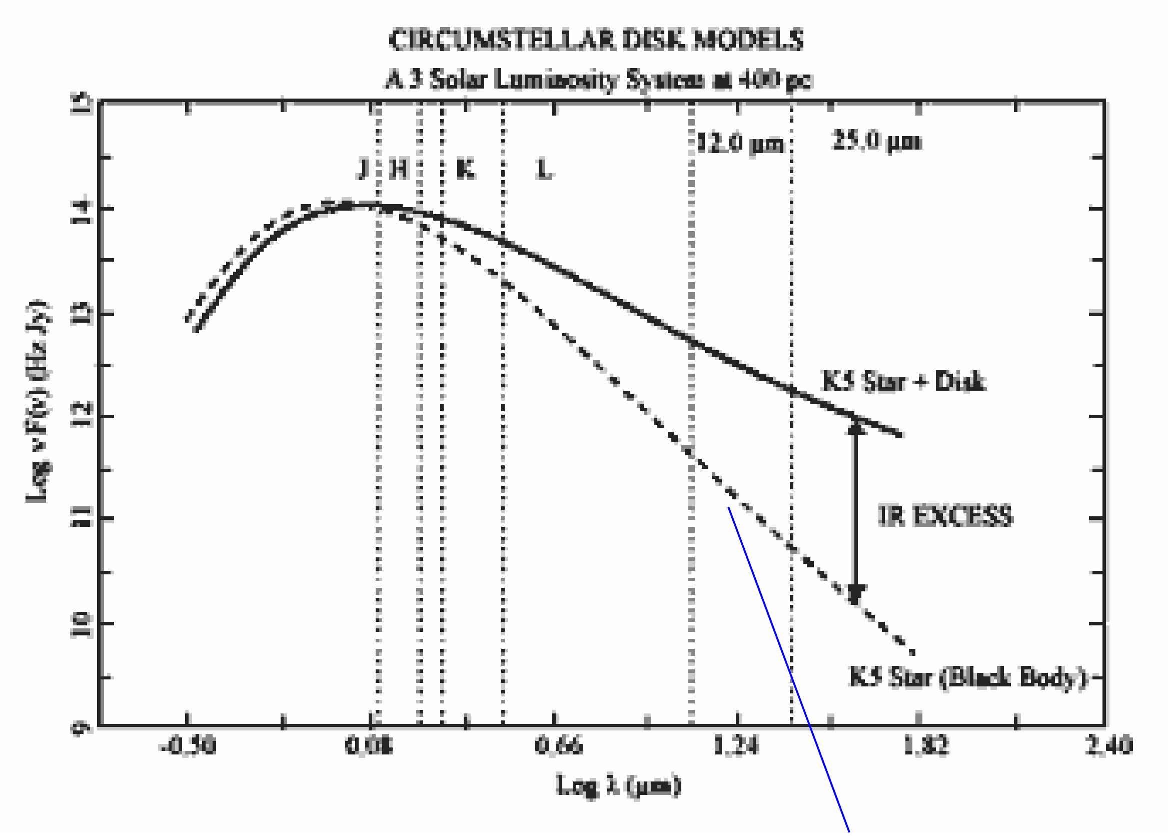
$$t = \frac{a}{da/dt} \sim \frac{10^{-5}}{1.5 \times 10^{-12} A\xi} \sim \frac{10^{7}}{1.5 A\xi}$$

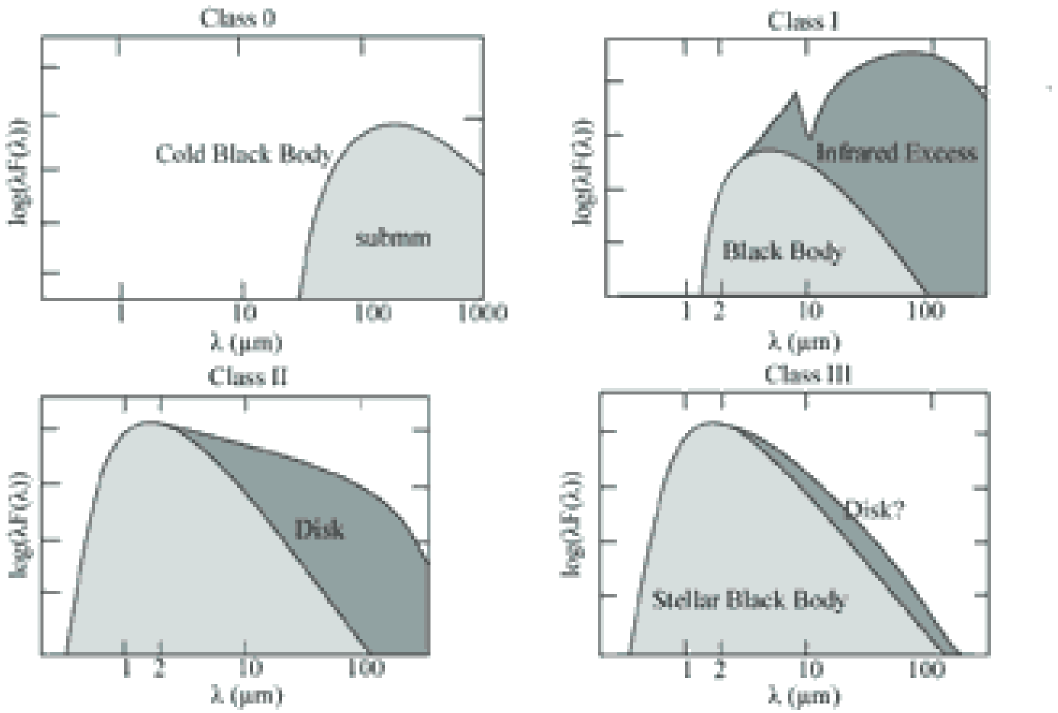
Take $A = 1$, $\xi = 1$, then $t = 10^7$–10^9 yr to grow to 0.1μm.

In much denser environments, e.g., inside dark clouds, or the envelopes of cool stars, the time scales are considerably shorter.

The initial nucleation is extremely slow; general diffuse ISM cannot do it ➔ Need high densities (1) star-forming regions (2) cool stellar atmospheres, (3) (super)novae or PNe: expanding gas shells

We indeed see evidence of dust in all these objects.





Stellar photosphere

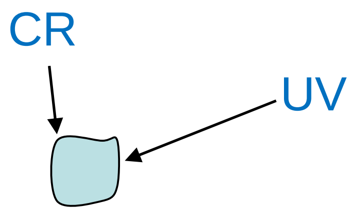
IR excess: reradiation of stellar radiation by heated circumstellar dust

A distribution of T_{dust} → superposition of bb spectra

Destruction of Grains

Evaporation

CH_4: 20 K; NH_3: 60 K; H_2O: 100 K



Sputtering

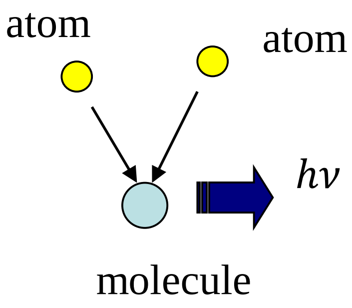
Maybe important in diffuse clouds;
grains otherwise better shielded in dense clouds

Grain-grain collision

Kinetic energy (a few km/s) → dust heated
and evaporated; important in shocked media;
may not be important in ISM otherwise

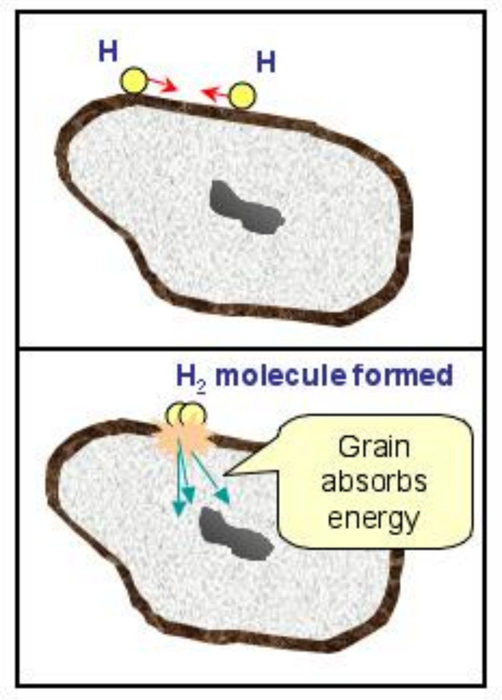
Formation of Molecules

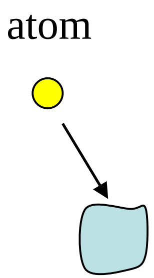
Grains catalyze the reactions between atoms which otherwise do not meet together (Gould & Salpeter 1963; Hollenbach & Salpeter 1971).



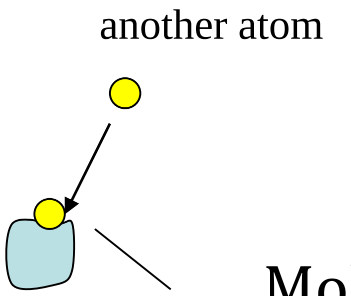
Two-body **collision** unlikely in ISM

Cannot form H_2 (no dipole)





~ 1 keV to expel, which > general E_{kin} in HI clouds → sticking



Molecules form on surface; binding energy = 4.47 eV → heating

Take H_2 as an example (Hollenbach & Salpeter, 1971, ApJ, 163, 155)

Fraction of H atoms that stick: s
…………………… move across and find another H: ξ
…………………… react: ζ
…………………… come off the grains: η

Overall, rate γ: fraction that hit and then make an H_2

$$\gamma = s\,\xi\,\zeta\,\eta$$

In the lab, $s \sim 1/3$, and for H, ξ, ζ, η all ~ 1

$$[\#\ \text{of H}_2\ \text{formed s}^{-1}\text{cm}^{-3}] = R\, n_H n_H$$

$$= (1/2)\, \gamma\, n_H\, n_d\, v\, \pi\, a^2$$

2 atoms

where R [cm^{3}s^{-1}]

$$n_d \frac{4}{3}\pi a^3 \rho_s = \rho_d = \frac{\rho_{gas}}{100} = \frac{10 \times 1.6 \times 10^{-24}}{100}$$

$$\begin{aligned} R &= (1/2)\, \gamma\, n_d/n_H\, v\, \pi\, a^2 \\ &= (1/2)\,(1/3)\,(4 \times 10^{-12})/10\,(10^5)\,\pi\,(2 \times 10^{-5})^2 \\ &= 10^{-17}\ [\text{cm}^3\ \text{s}^{-1}] \end{aligned}$$

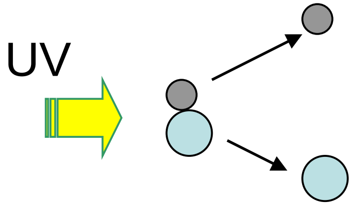
Time scale for H$_2$ formation is $(R\, n_H)^{-1} = 10^{17}/n_H$ [s]

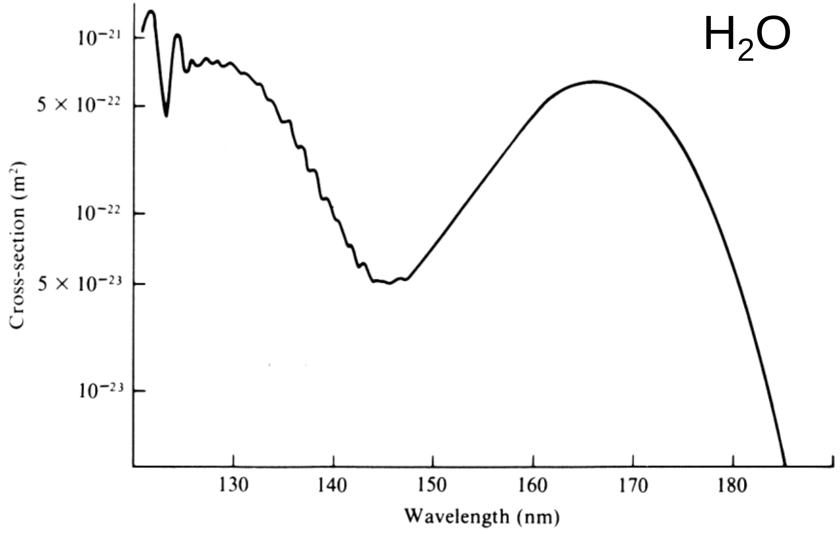
$$= 3 \times 10^9/n_H\ [\text{yr}]$$

e.g., for $n_H = 100$ cm^{-3}, then $(R\, n_H)^{-1} \approx 3 \times 10^7$ yr

Ref: Kaplan & Pikelner

Dissociation of Molecules





$$\sigma_{dis} \sim 10^{-20} - 10^{-18} \text{ cm}^2$$

General ISM stellar radiation is equivalent to 10,000 K diluted by $W \sim 10^{-14}$

$$I = W\,\sigma_B\,T^4$$

$$\text{\# of photons } [\text{s}^{-1}\ \text{cm}^{-2}] = \frac{I}{h\nu} = \frac{W\,\sigma_B\,T^4}{h\nu}$$

$$\text{\# of dissociation } [\text{s}^{-1}] = \frac{W\,\sigma_B\,T^4}{h\nu}\,\sigma_{dis} \approx (1/3) \times 10^9 \text{ s}^{-1}$$

$\tau_{\text{dissociation}} \sim 3 \times 10^9 \text{ s} \approx 100 \text{ yrs}$

So it takes some 10^7 years to form an H_2 molecule, but it is destroyed in 100 years.

➔ need shielding!

- Photodissociation is the main process to destroy IS H_2.
- Usually stronger lines have stronger self-shielding.

Photodissociation Region (PDR)

- Far-UV photons (6 eV < E<13.6 eV), not energetic enough to ionize hydrogen, but can dissociate most molecules (H_2, CO, and others)

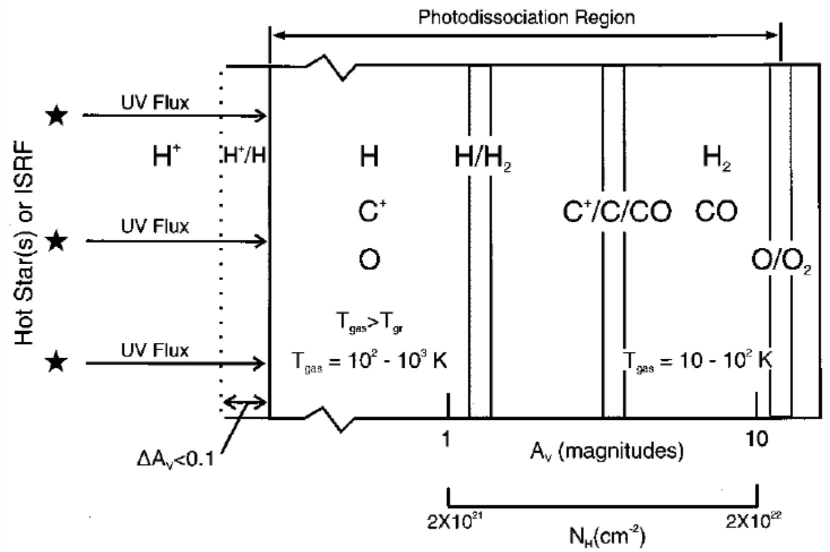
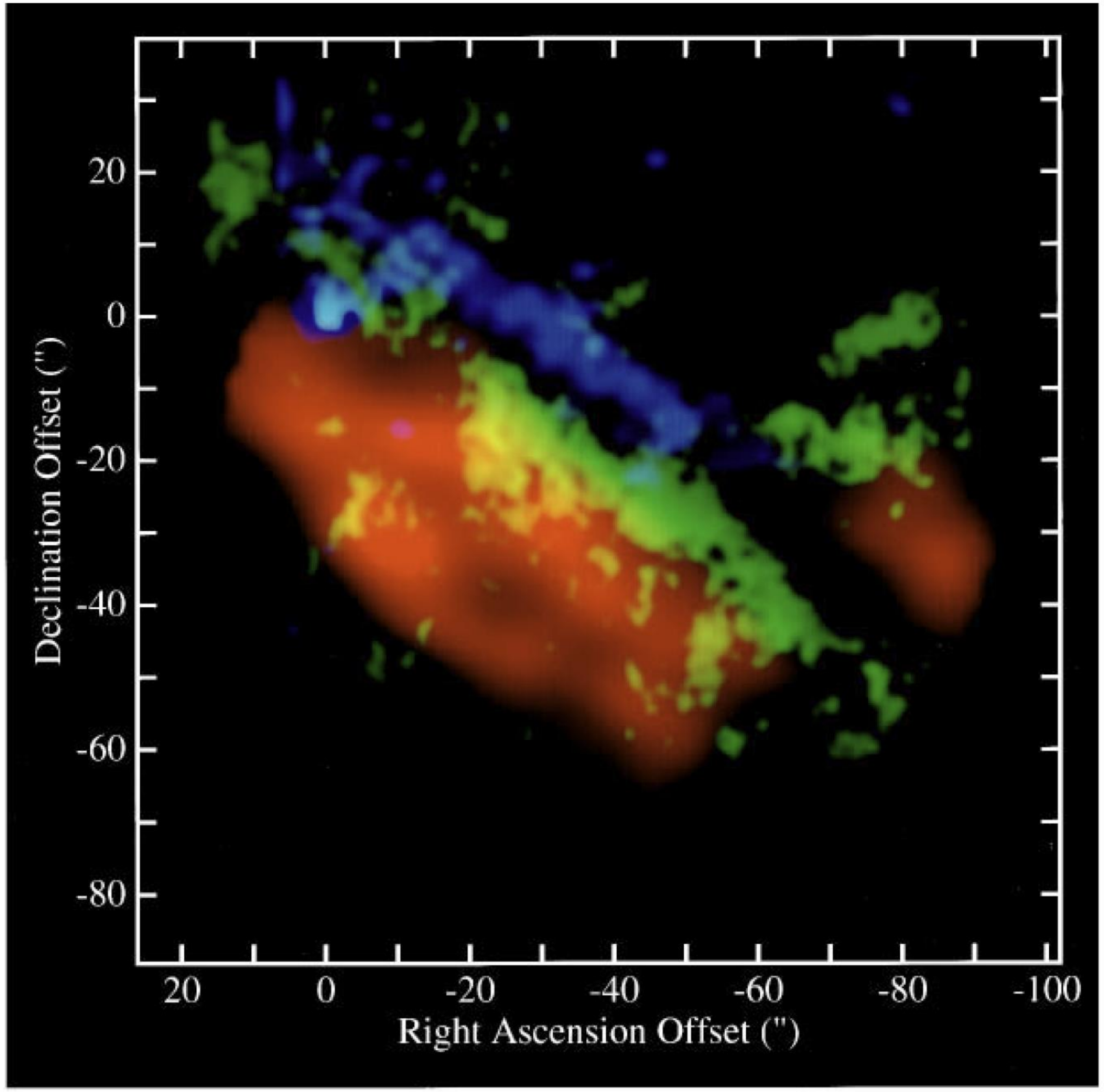


FIG. 3. A schematic diagram of a photodissociation region. The PDR is illuminated from the left and extends from the predominantly atomic surface region to the point where O_2 is not appreciably photodissociated ($A_V \simeq 10$). Hence the PDR includes gas whose hydrogen is mainly H_2 and whose carbon is mostly CO. Large columns of warm O, C, C^+, and CO, and vibrationally excited H_2 are produced in the PDR.

Hollenback & Tielens, 1999, Rev. Mod. Phy, **71**, 173

The PDR region in the Orion Bar region, seen edge-on



Blue PAH
Yellow H_2
Red CO

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).

Hollenback & Tielens (1999)

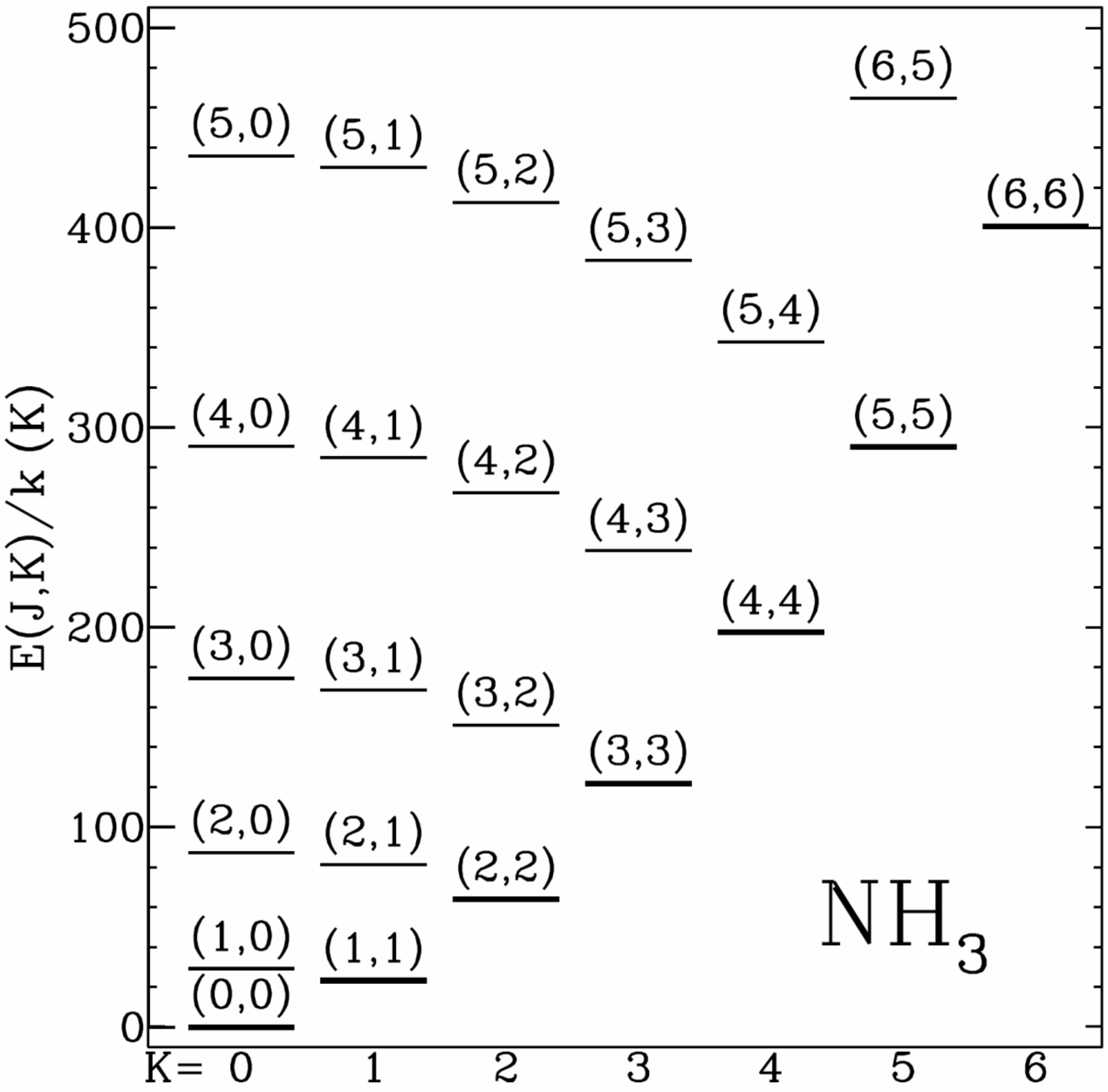
Interstellar Molecules

- All from abundant elements (H, C, N, O, S, Si) + simple molecules (H_2CO, CH, OH radicals)
- There are diatomic, triatomic, and more complicated polyatomic molecules, such as ammonia NH_3, water H_2O, hydrogen cyanide HCN, methanal (**甲醛**) H_2CO, oxomethylium ion HCO^+, alcohol CH_3OH
- Diatomic molecules with identical nuclei, e.g., H_2, N_2, O_2, are called **homonuclear**, as oppose to **heteronuclear** molecules, such as HD, OH, or CO.

- Molecules also have term symbols, but they are complicated because of the projection, e.g., of the angular momentum onto the internuclear axis.

- The ground term of H_2 is $^1\Sigma_g^+$; it has zero electronic orbital angular momentum, has zero electron spin, is symmetric under reflection through the center of mass (*g*), and is symmetric under reflection through planes containing the nuclei (+).

- If the protons have spin 0 → **para-H_2**;
  if two protons are parallel, with total spin 1 → **ortho-H_2**.

E(J,K)/k (K)
500
400
300
200
100
0
K= 0
1
2
3
4
5
6
(0,0)
(1,0)
(2,0)
(3,0)
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NH_3

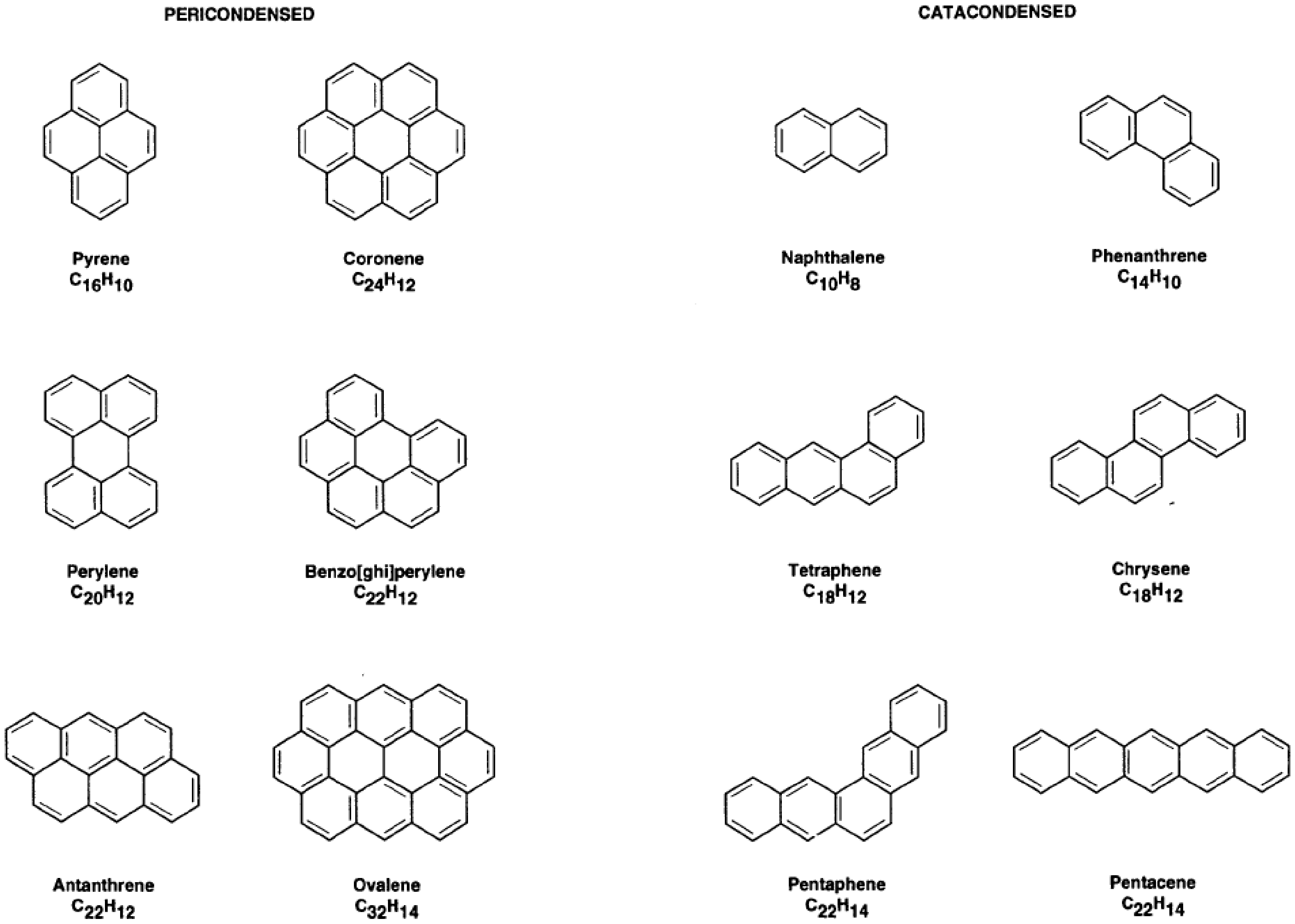

FIG. 1.—Structures of some representative pericondensed and catacondensed polycyclic aromatic hydrocarbons (PAHs). Hydrogen atoms, located on the periphery, are not represented.

Types of Molecular Clouds

Type	Av (mag)	Examples
Diffuse Molecular Cloud	< 1	Rho Oph
Translucent Cloud	1 to 5	HD 24534 cloud
Dark Cloud	5 to 20	B 335
Infrared Dark Cloud	20 to > 100	IRDC G028.53-00.25