

Grains and Molecules

Formation of Grains

Atoms → diatomic molecules (e.g., CH, CO, CN)
→ 10 to 20 atoms as condensation nuclei
→ growth by accretion

In HI clouds, $n_H \approx 10 - 100 \text{ cm}^{-3}$ → 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

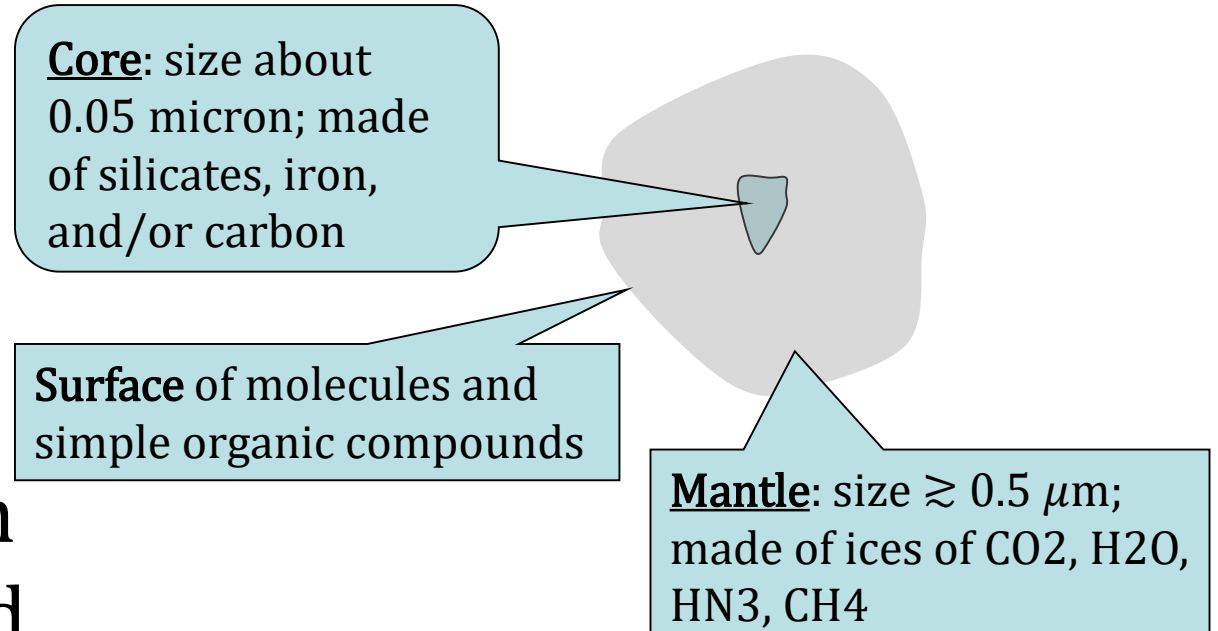
With condensation nuclei (small, refractory particles), volatile materials such as CO_2 , CH_4 , NH_3 , H_2O condense as mantles

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

A large number $a < 0.015 \mu\text{m}$

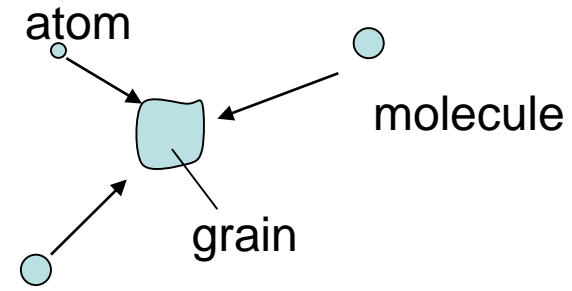
C, N, O depletion consistent with this, i.e., these elements locked into ices on the grains

ISM grain (nuclei, mantles) \rightarrow grain growth \rightarrow planetesimals \rightarrow planets



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

Grain Growth Rate



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

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

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

$$\frac{da}{dt} = \frac{(1/4)n\bar{v}m_H A \xi}{\rho_s}$$

$$= \frac{v\rho_H}{4\rho_s} A\xi$$

$$= \frac{10^5 1.6 \times 10^{-24}}{4 \cdot 1} A\xi$$

$$= 4 \times 10^{-20} \text{ cm s}^{-1} A\xi$$

$$= 15 \times 10^{-13} \text{ cm yr}^{-1} A\xi$$

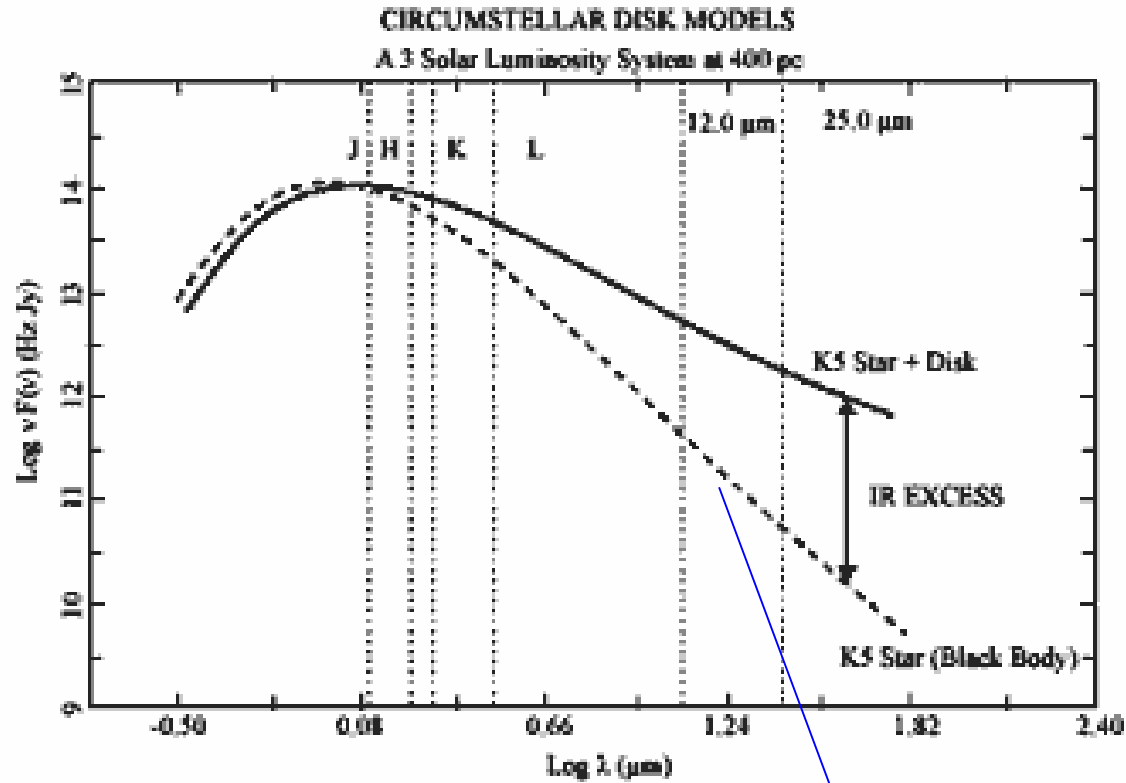
$$t = \frac{a}{da/dt} \sim \frac{10^{-5}}{1.5 \times 10^{-12} A \xi} \sim \frac{10^7}{1.5 A \xi}$$

Take $A = 1$, $\xi = 1$, then $t = 10^7 - 10^9$ yr to grow to $0.1 \mu\text{m}$.

In much denser environments, e.g., inside dark clouds, or in 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

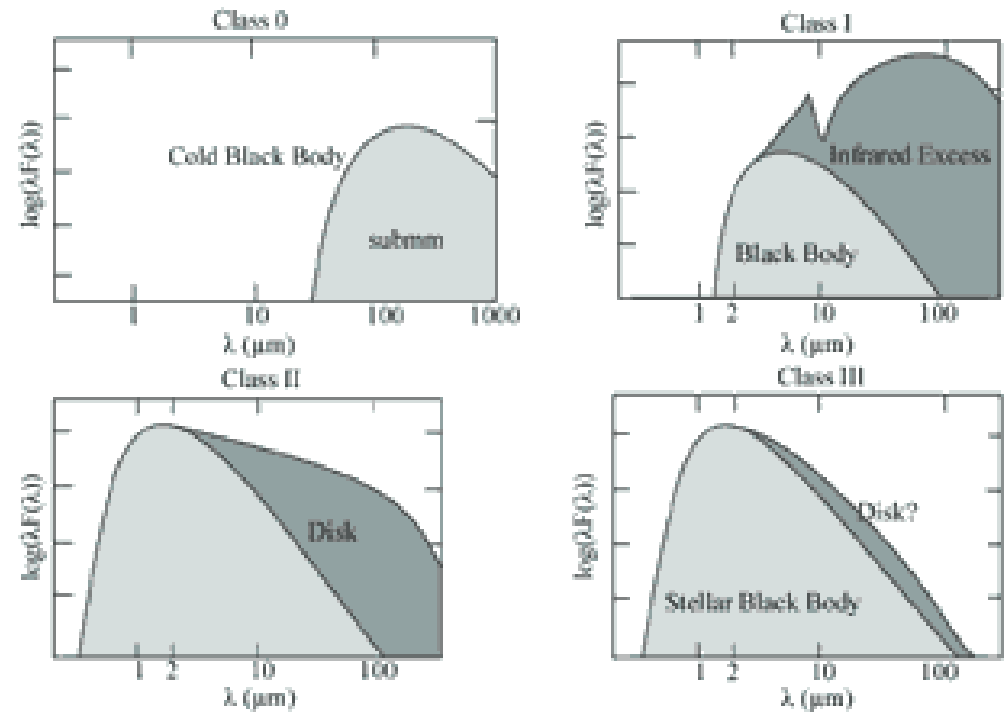
We indeed see evidence of dust in all these objects.

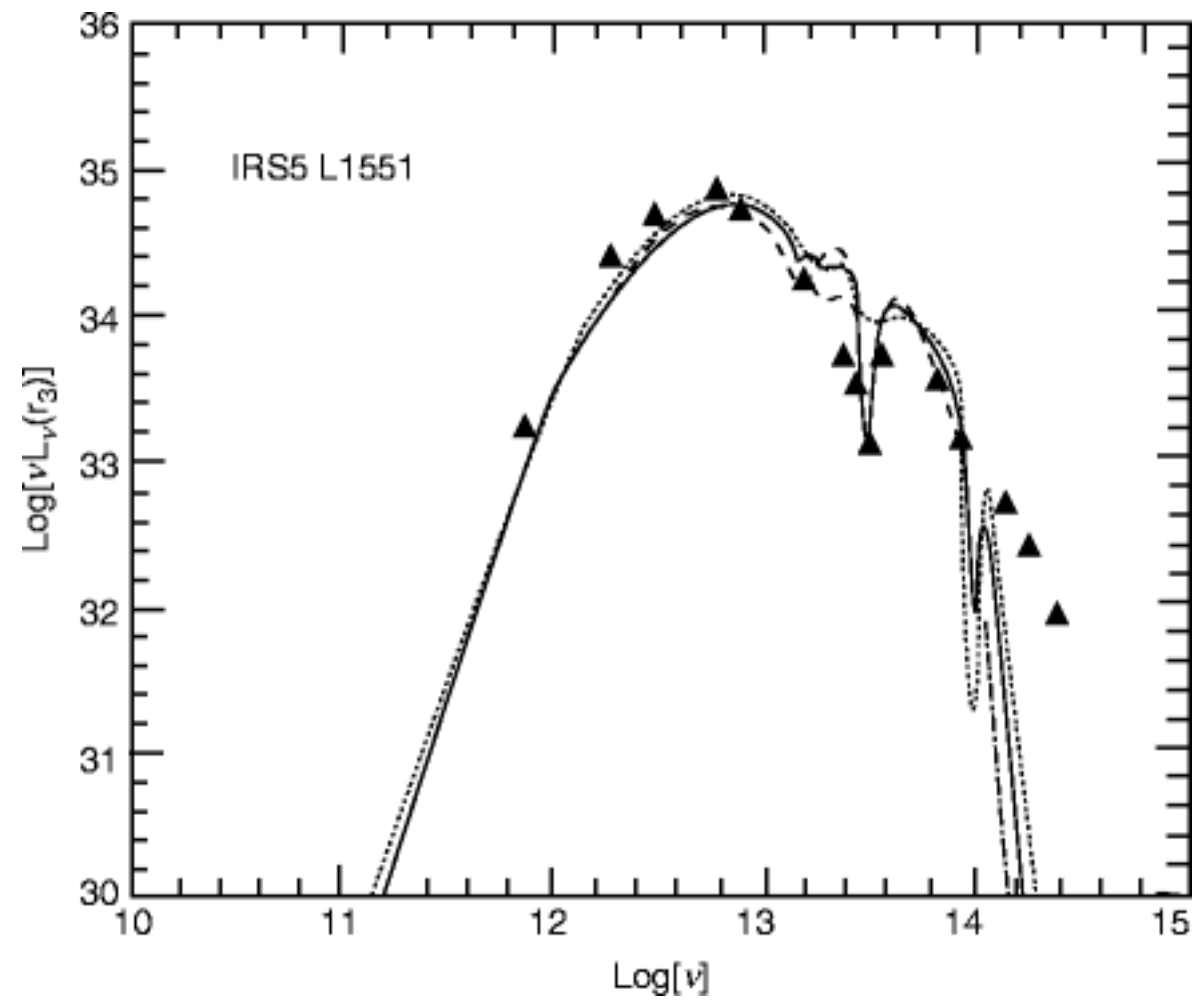
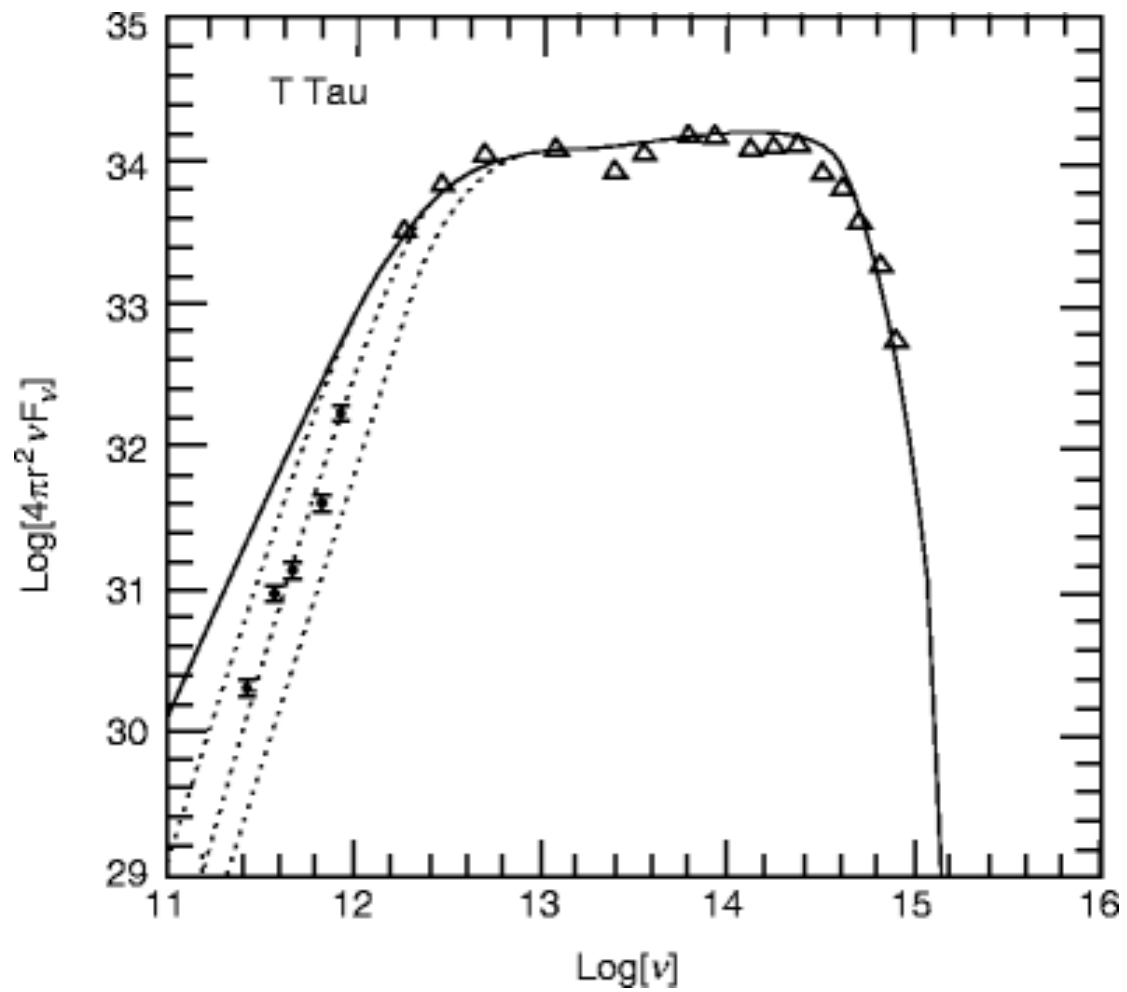


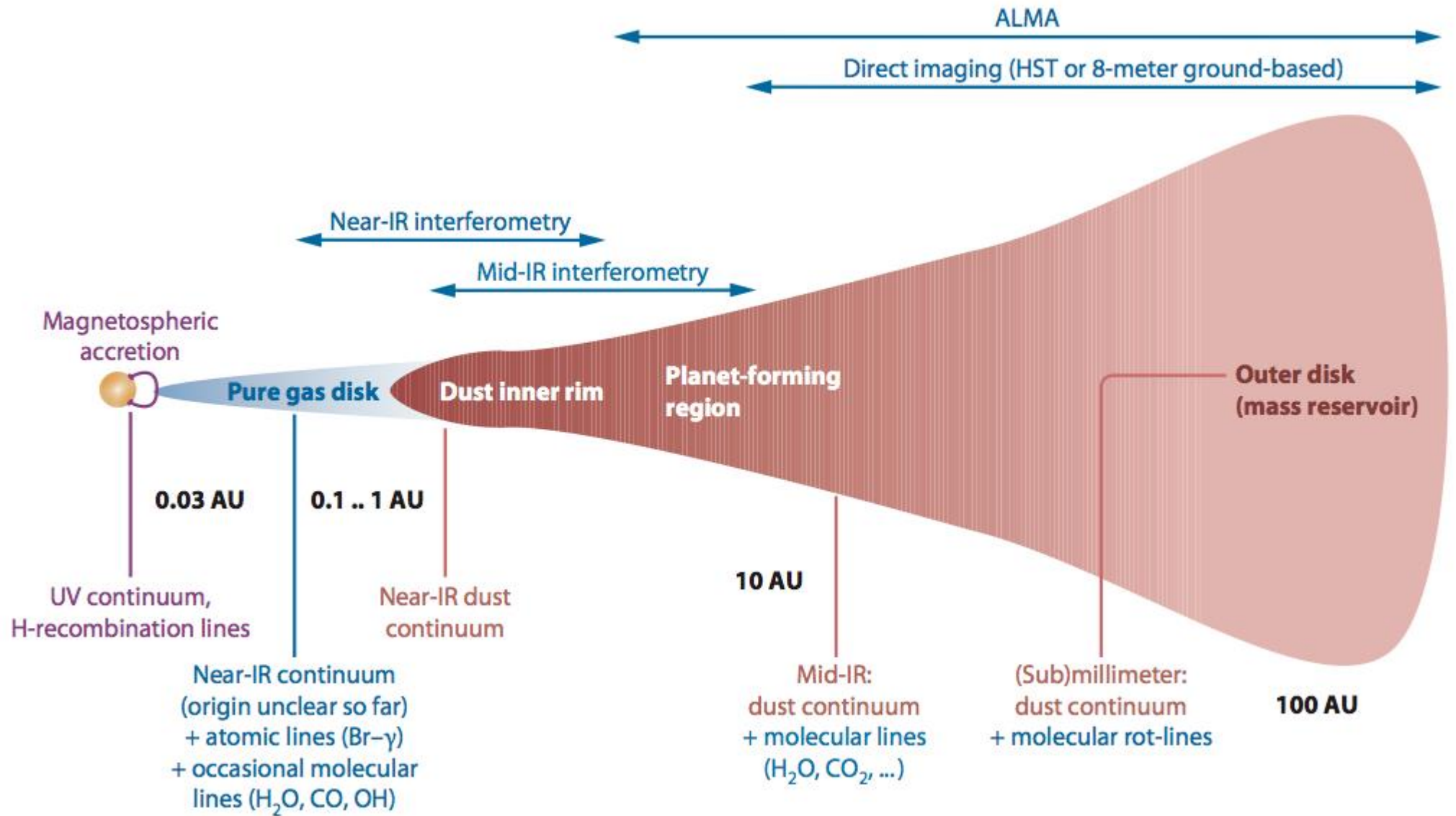
Stellar photosphere

IR excess: reradiation of stellar radiation (UV and optical) by heated circumstellar dust (in IR)

A distribution of $T_{\text{dust}} \rightarrow$ superposition of bb spectra







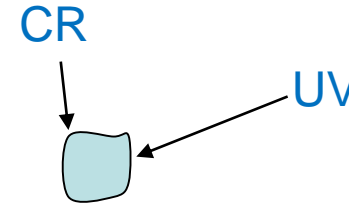
Destruction of Grains

Evaporation

CH₄: 20 K; NH₃: 60 K; H₂O: 100 K

Sputtering

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



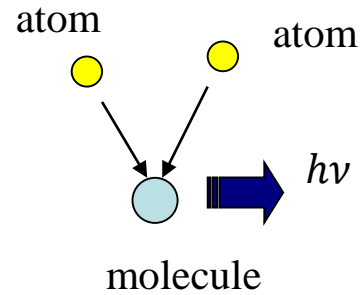
Grain-grain collision

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

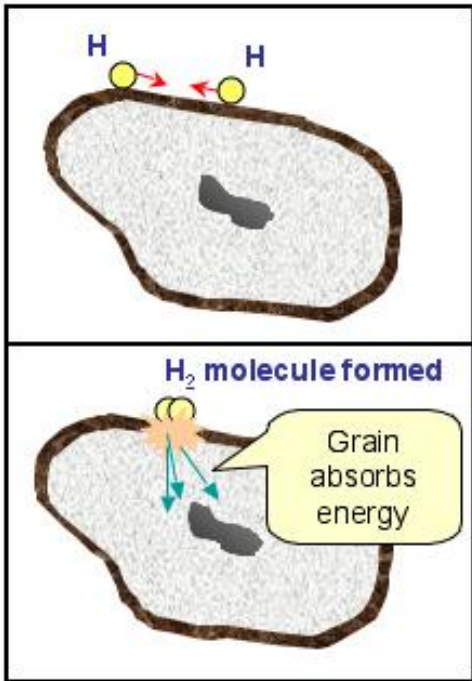
Heating

Formation of Molecules

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



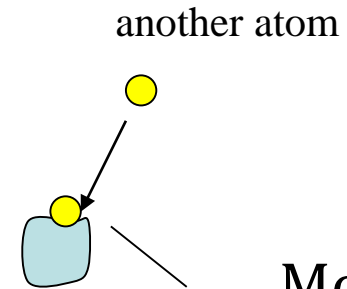
Two-body collision unlikely in ISM
Cannot form H_2 (no dipole)



atom
atom
molecule
 $h\nu$

atom

$\sim 1 \text{ keV}$ to expel, $>$ general E_{kin} in HI clouds \rightarrow sticking



Molecules form on surface; binding energy = 4.47 eV \rightarrow heating

Take H₂ 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 H₂

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

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

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

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

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

2 atoms

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

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

$$= (1/2) (1/3) (4 \times 10^{-12}) / 10 (10^5) \pi (2 \times 10^{-5})^2$$

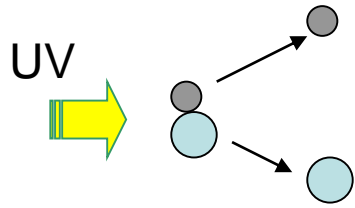
$$= 10^{-17} [\text{cm}^3 \text{s}^{-1}]$$

Time scale for H₂ formation is $(R n_H)^{-1} = 10^{17} / n_H$ [s]

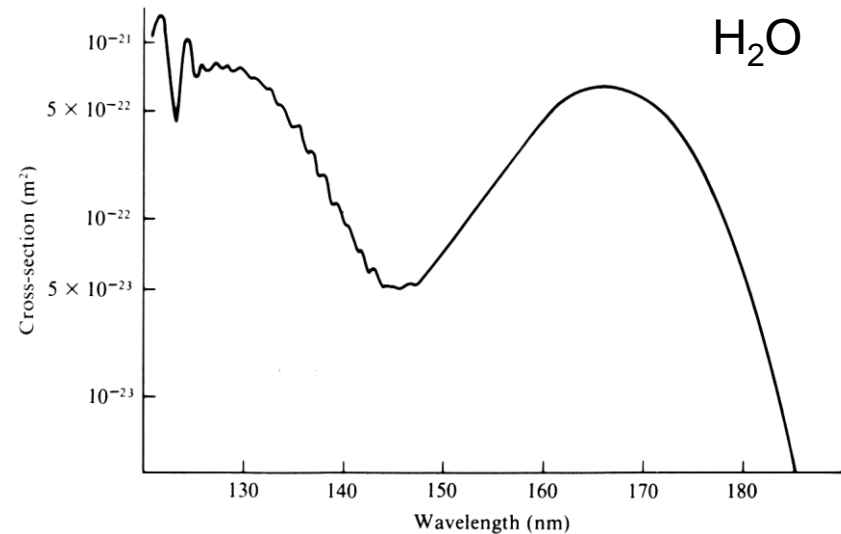
$$= 3 \times 10^9 / n_H$$
 [yr]

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

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 ($6 \text{ eV} < E < 13.6 \text{ eV}$), not energetic enough to ionize hydrogen, but can dissociate most molecules (e.g., H_2 , CO)

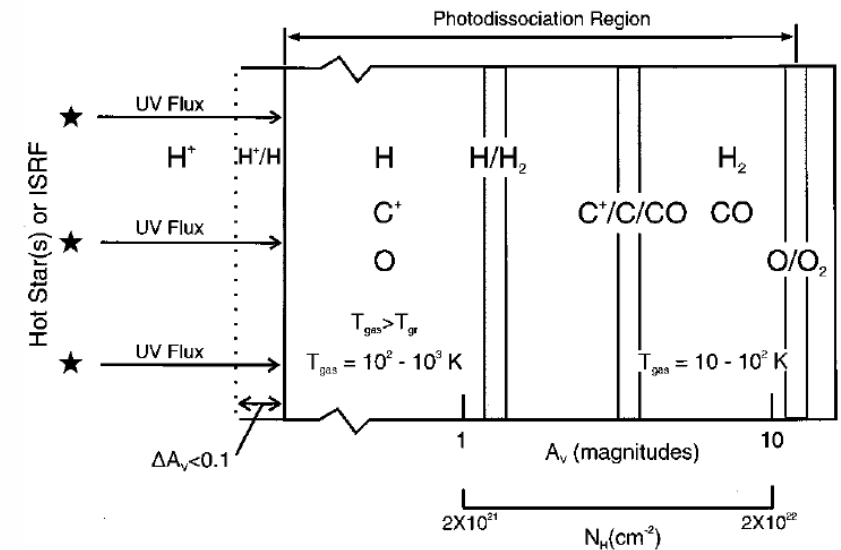
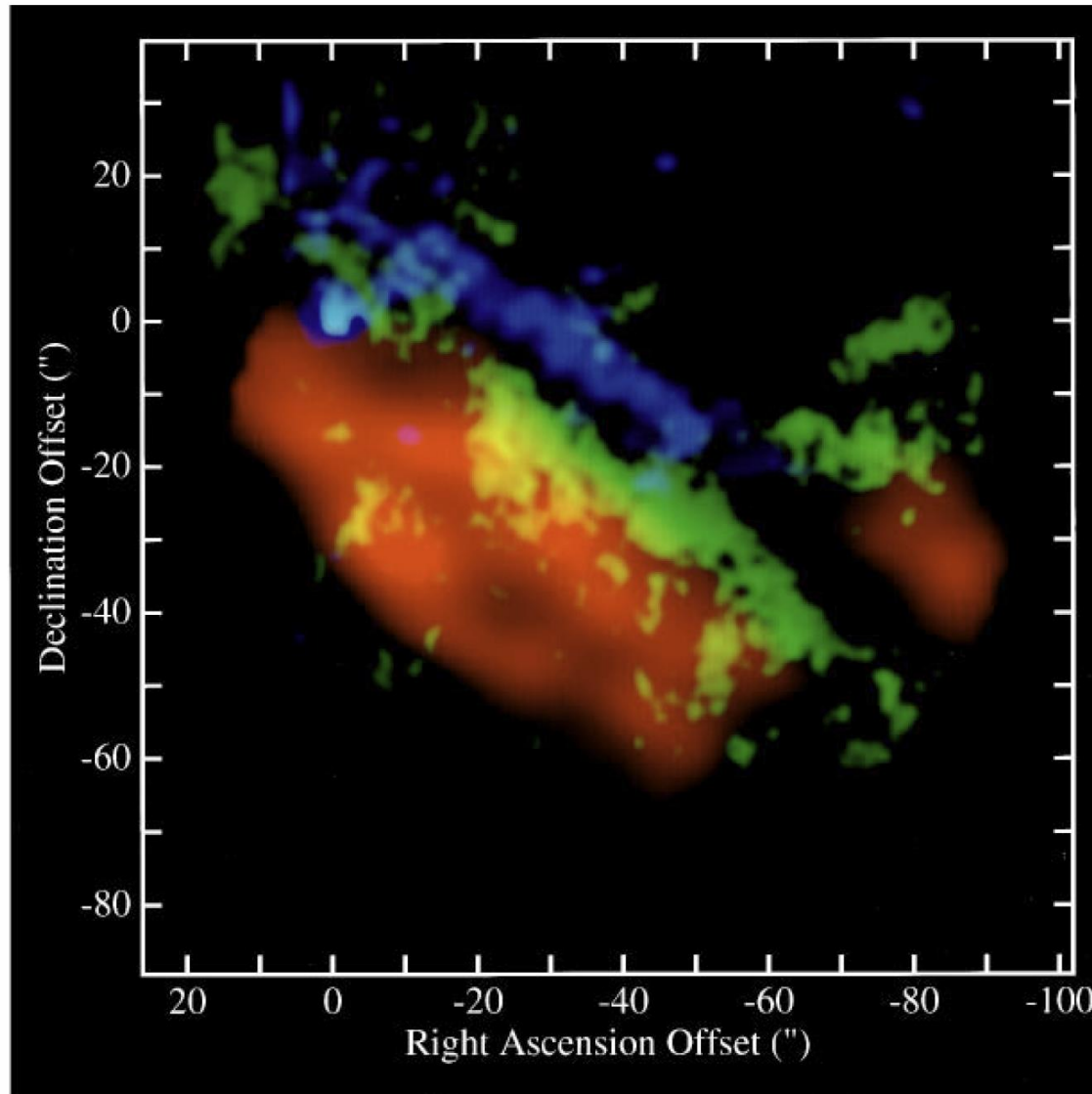


FIG. 3. A schematic diagram of a photodissociation region. The PDR is illuminated from the left and extends from the predominantly atomic surface region to the point where O_2 is not appreciably photodissociated ($A_V \approx 10$). Hence the PDR includes gas whose hydrogen is mainly H_2 and whose carbon 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. Phys, 71, 173

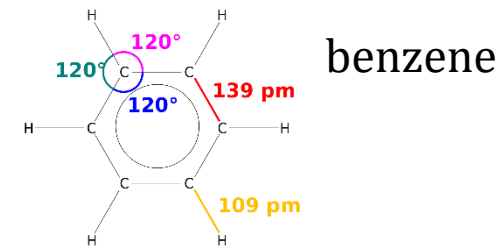
The PDR region in the Orion Bar region, seen edge-on



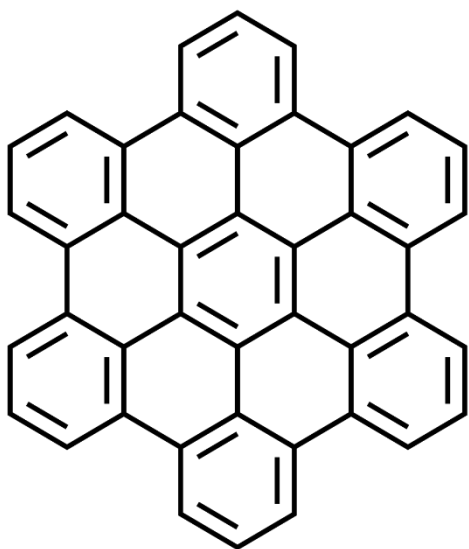
Blue PAH
Yellow H₂
Red CO

FIG. 2. (Color) The Orion Bar region mapped in the 3.3- μm PAH feature (blue), H₂ 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 $\approx 10''$ is seen between the PAH emission and the H₂ emission, and between the H₂ emission and the CO emission, as predicted by PDR models (see text).

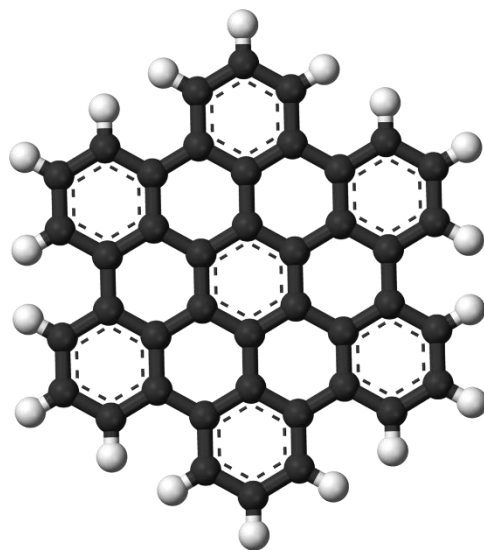
Polycyclic aromatic hydrocarbon



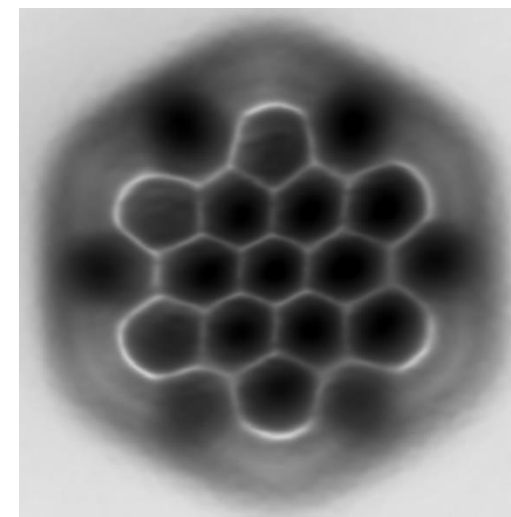
Chemicals contains C and H only, with multiple aromatic rings (ring-shaped and planar, e.g., benzene C₆H₆; very stable)



Line-angle schematic

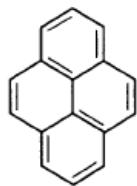


Ball-and stick model



Microscopy image

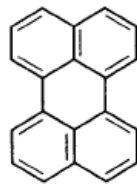
PERICONDENSED



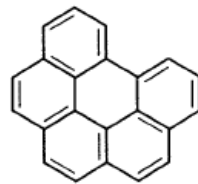
Pyrene
C₁₆H₁₀



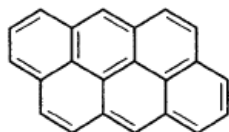
Coronene
C₂₄H₁₂



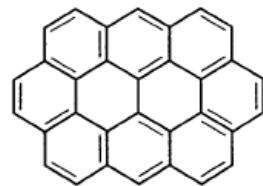
Perylene
C₂₀H₁₂



Benzo[ghi]perylene
C₂₂H₁₂

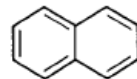


Anthanthrene
C₂₂H₁₂

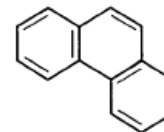


Ovalene
C₃₂H₁₄

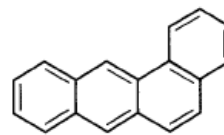
CATACONDENSED



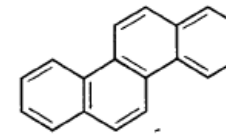
Naphthalene
C₁₀H₈



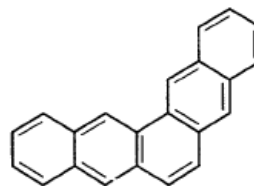
Phenanthrene
C₁₄H₁₀



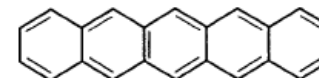
Tetraphene
C₁₈H₁₂



Chrysene
C₁₈H₁₂



Pentaphene
C₂₂H₁₄



Pentacene
C₂₂H₁₄

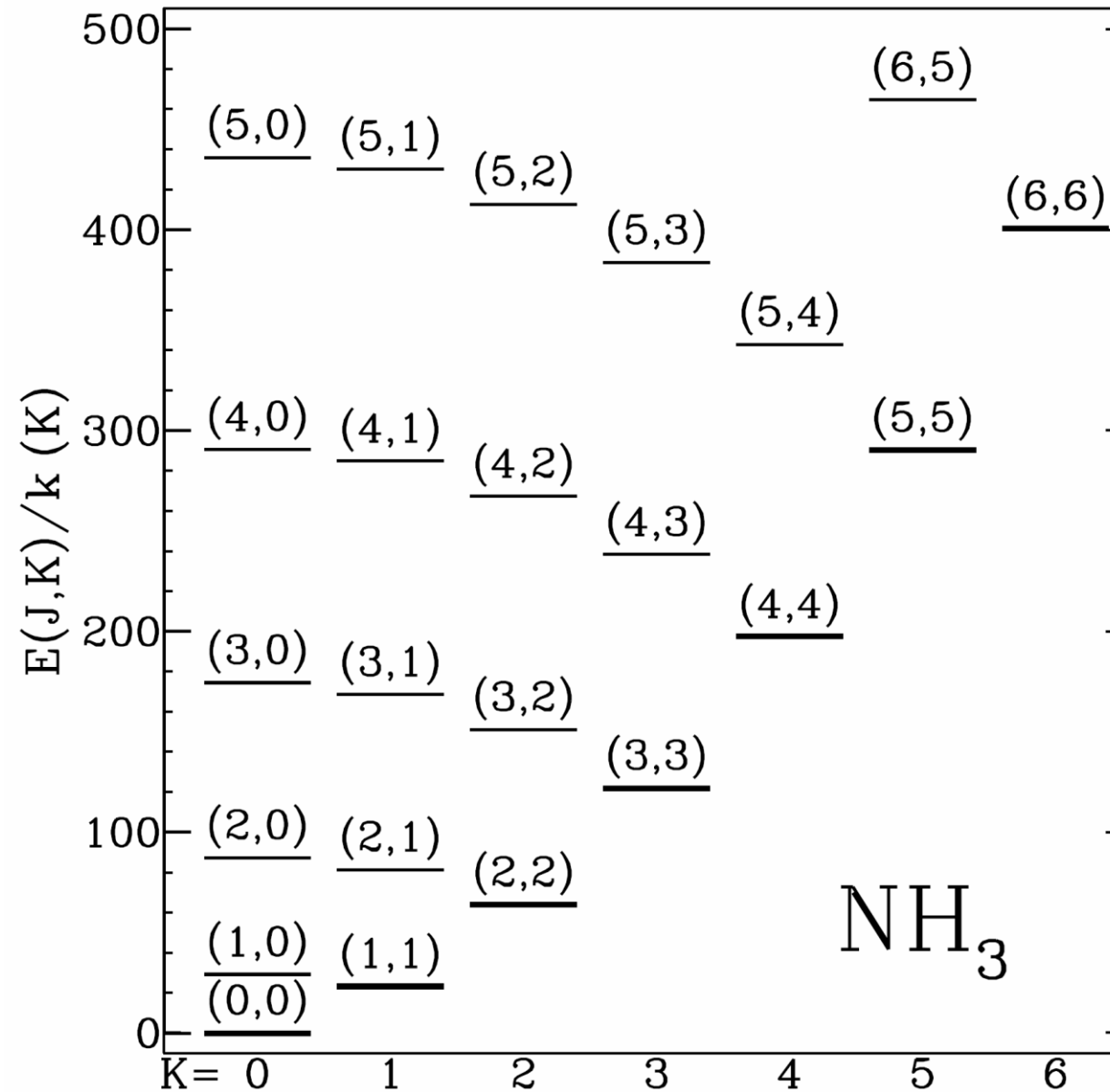
FIG. 1.—Structures of some representative pericondensed and catacondensed polycyclic aromatic hydrocarbons (PAHs). Hydrogen atoms, located on the periphery, are not represented.



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 , oxomethylion ion HCO^+ , alcohol CH_3OH
- Diatomic molecules with identical nuclei, e.g., H_2 , N_2 , O_2 , are called **homonuclear** (同核), as oppose to **heteronuclear** (異核) 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 \rightarrow **para- H_2** ;
if two protons are parallel, with total spin 1 \rightarrow **ortho- H_2** .



Rotational Transitions

- Rotational spectra arise from transitions between rotational energy states.
- Only molecules with electric dipole moments can absorb or emit photons in such transitions. Non-polar diatomic molecules, e.g., H_2 , and symmetric polyatomic molecules, e.g., CO_2 ($\text{O}=\text{C}=\text{O}$) or CH_4 , do not exhibit rotational spectra, unless they are collisionally excited (molecules “distorted”).
- Even in molecules with a permanent dipole moment, selection rules apply for rotational transitions.
- In practice, rotational spectra are always seen in absorption, so $J \rightarrow$ a higher J

- H_2 has no permanent electric dipole moment, and the vibrational states and the rotational states radiates very weakly, via the time-variation of the electric quadrupole moment as the molecule vibrates or rotates.
- Often one uses, e.g., CO, as the tracer of molecular species. This is valid if collisional equilibrium is established.

- Rotational energy

$$E_J = \frac{1}{2} I \omega^2 = \frac{L^2}{2I} = \frac{J(J+1)}{2I}$$

That is, $\nu_{J \rightarrow J+1} = \frac{\hbar}{2\pi I} (J+1)$; with equally spaced lines.

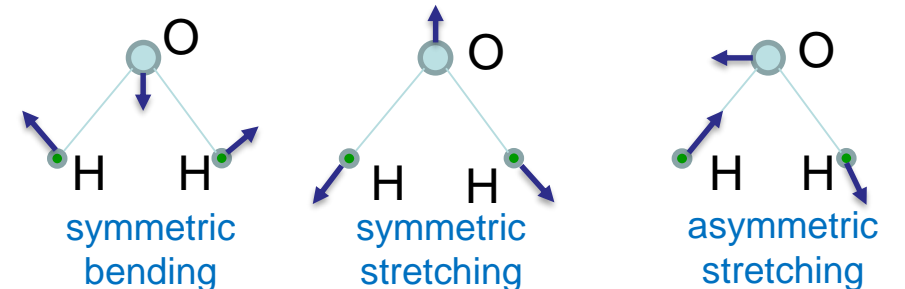
Vibrational Transitions

- A molecule not only rotates, it also vibrates when sufficiently excited → a harmonic oscillator
- Vibrational energy

$$E_v = (v + 1/2) \hbar \sqrt{\frac{k}{\mu}}$$

where v is the vibrational quantum number, k is the vibrational force constant, and μ is the reduced mass.

- Selection rule: $\Delta v = \pm 1$
- A variety of modes...



Types of Molecular Clouds

Type	A_v (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

IRDCs discovered in 1996 by the ISO = formation sites of massive stars?

