Grain Evolution

Formation of Grains

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

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

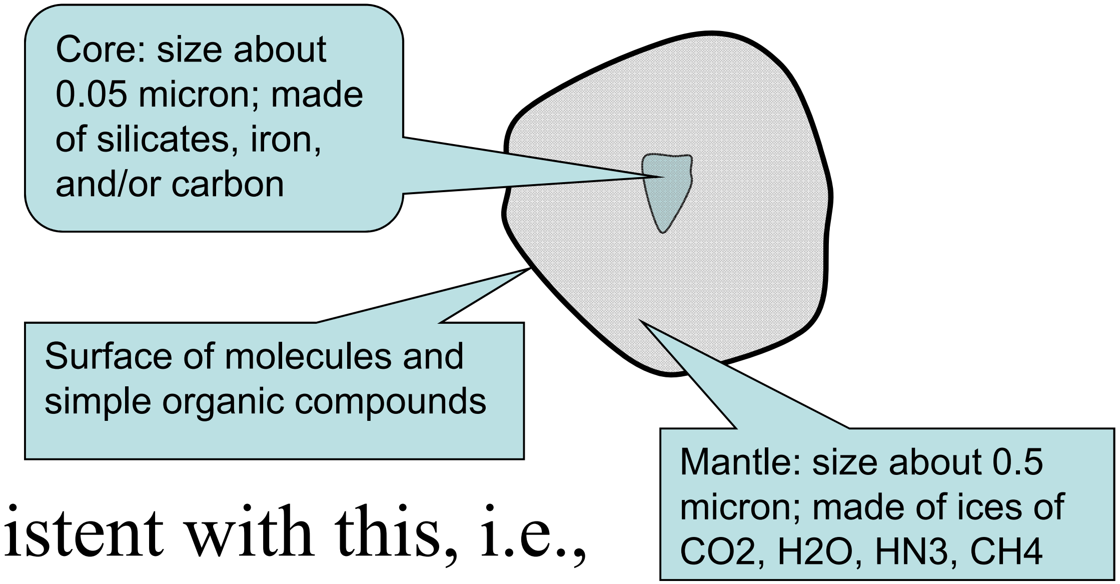
Grains likely formed in (1) atmospheres of cool stars and (2) dark molecular clouds

IR observations detected 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 size (> 1 µm) larger than typical ISM < 0.2-0.5 µm



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

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

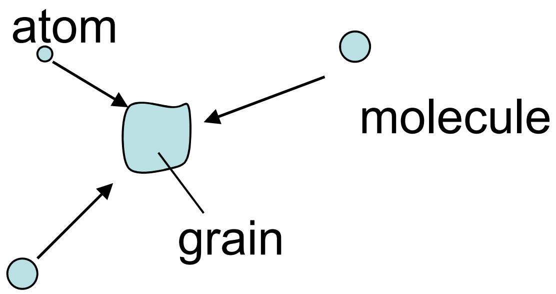
Surface of molecules and simple organic compounds

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

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

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

Grain Growth Rate



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

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

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

$$\begin{aligned}
\frac{da}{dt} &= \frac{(1/4)n\bar{v}m_H A\,\xi}{\rho_s} \\
&= \frac{v\rho_H}{4\rho_s}A\xi \\
&= \frac{10^5\,1.6\times10^{-24}}{4\cdot1}A\xi \\
&= 4\times10^{-20}\,\mathrm{cm\ s^{-1}}\,A\xi \\
&= 15\times10^{-13}\,\mathrm{cm\ yr^{-1}}\,A\xi
\end{aligned}$$

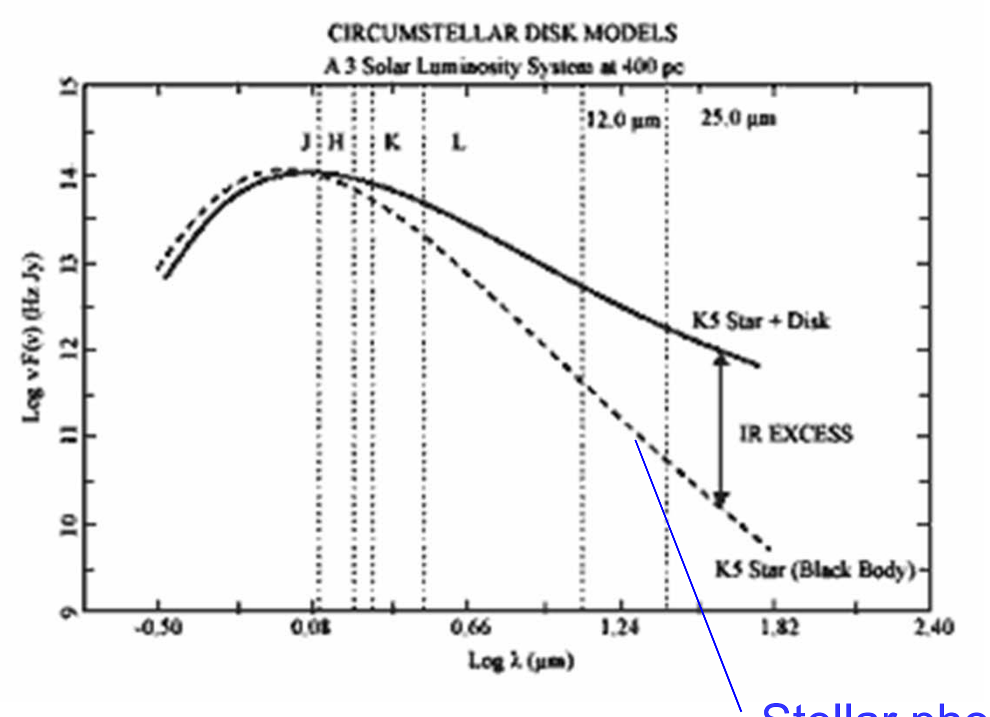
$$t = \frac{a}{da/dt} \sim \frac{10^{-5}}{1.5 \times 10^{-12} A\xi} \sim \frac{10^{7}}{1.5 A\xi}$$

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

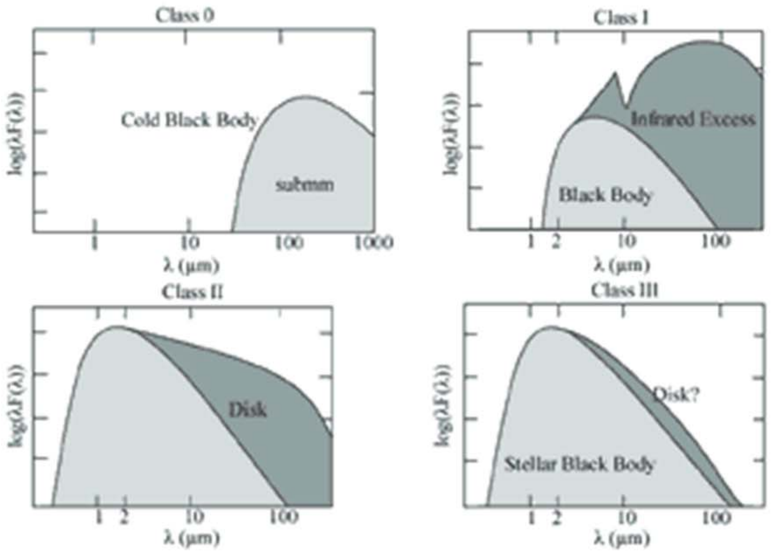
In a much denser environment, e.g., dark clouds, or the envelope of a cool star, the time scale is considerably shorter.

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

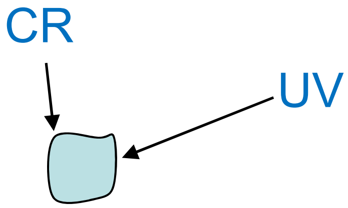


IR excess: reradiation of stellar radiation by heated circumstellar dust

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

Destroy of Grains

1) ***Evaporation***
   CH_4: 20 K; NH_3: 60 K; H_2O: 100 K



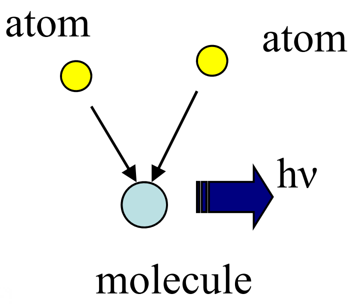
2) ***Sputtering***
   Maybe important in diffuse clouds; grains better shielded in dense clouds

3) ***Grain-grain collision***
   kinetic energy (a few km/s) → dust heated and evaporated; important in shocked media; may not be important in ISM otherwise

4) ***Heating***

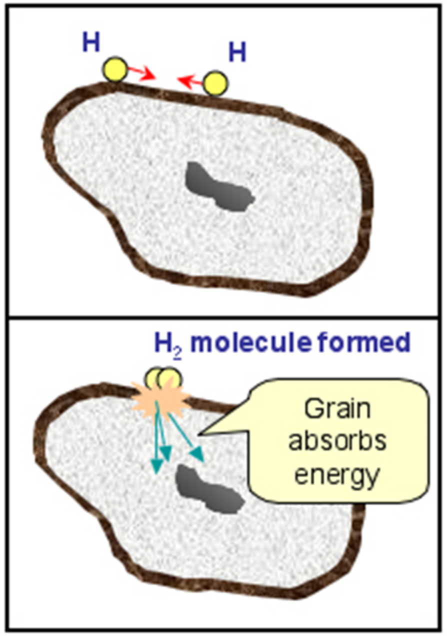
Formation of Molecules

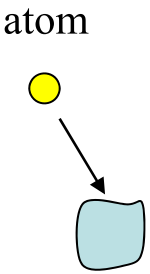
Grains catalyzes the reactions between atoms which otherwise do not meet together (Gould & Salpeter 1963; Hollenbach & Salpeter 1971).



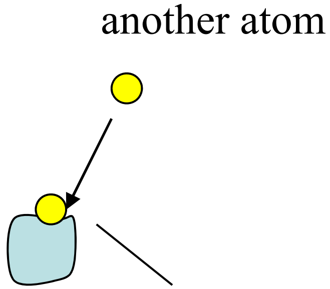
Two-body collision unlikely in ISM

Cannot form H_2 (no dipole)





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



Molecules form on surface; heated, binding energy = 4.47 eV

Take H_2 as an example (Ref: 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

$$[\#\text{ of } H_2 \text{ formed s}^{-1}\text{ cm}^{-3}] = \text{R}\, n_H\, n_H$$

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

2 atoms

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

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

$$\boxed{\text{R} = (1/2)\ \gamma\, n_d / n_H\ v\, \pi a^2}$$

$$= (1/2)\ 1/3\ (4 \text{ x } 10^{-12})/10\ (10^5)\ \pi\ (2 \text{ x } 10^{-5})^2$$
$$= 10^{-17}\ \text{cm}^3\ \text{s}^{-1}$$

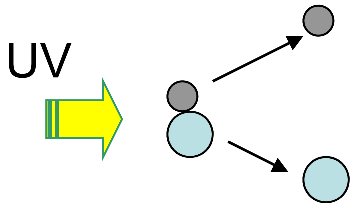
Time scale for H_2 formation is $(\text{R } n_H)^{-1} = 10^{17}/n_H$ [s]

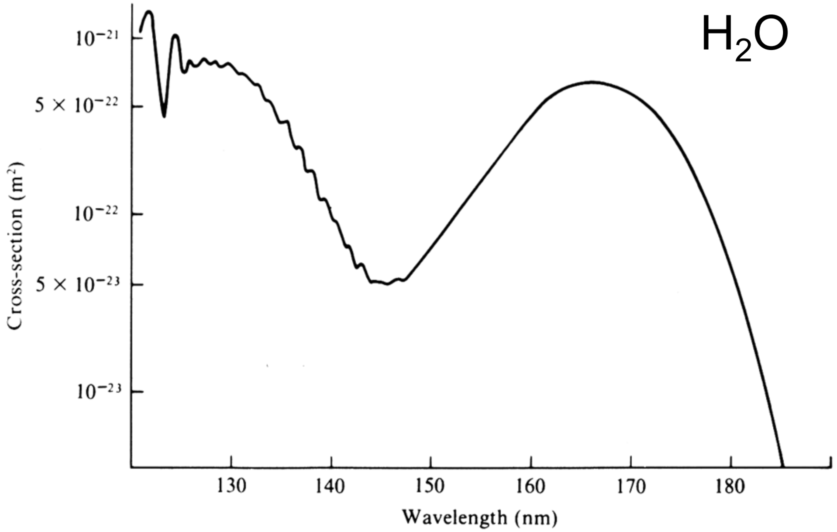
$= 3 \text{ x } 10^9/n_H$ [yr]

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

Ref: Kaplan & Pikelner

Dissociation of Molecules





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

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

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

# of photons $\mathrm{s}^{-1}\ \mathrm{cm}^{-2}$ = $\dfrac{I}{h\nu} = \dfrac{W\,\sigma_B\,T^4}{h\nu}$

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

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

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

➔ need shielding!

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

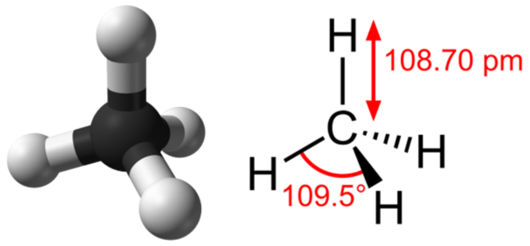
Interstellar Molecules

- 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, and CO.

- Molecules also have term symbols, but they are complicated because of the projection of, e.g., 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**.

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 (O=C=O) or CH_4, do not exhibit rotational spectra, unless they are collisionally excited (molecules “distorted”).
- Even in molecules with permanent dipole moment, selection rules apply for rotational transitions.
- In practice, rotational spectra are always seen in absorption, so J → a higher J



wikipedia

- 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

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

$$\nu_{J \to J+1} = \frac{\hbar}{2\pi I}(J+1)$$

i.e., equally spaced lines.

Vibrational Transitions

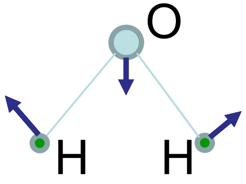
- A molecule does not just rotate, it may vibrate when sufficiently excited → a harmonic oscillator

Vibrational Energy E_v

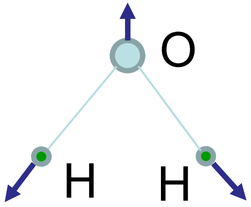
$$E_v = (v + 1/2)\,\hbar\sqrt{\frac{k}{\mu}}$$

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

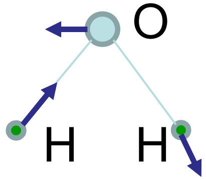
- Selection rule: Δv=+/- 1
- A variety of modes…



symmetric bending



symmetric stretching



asymmetric stretching

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