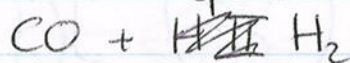ISM   28 - 10 - 2019

• Full understanding of ~~HII~~, CO, H_2
• Realisation that there are many other ~~molee~~ molecules that are more complicated to underst- and. Draine ch 5 and 31

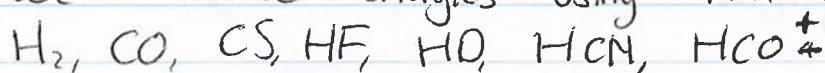Born - Oppenheimer approximation: we can seperate nuclear motion from general motion
- electrons in ground state and nulei can rotate, vibrate, etc
- electronic cloud in excited state and nuclei rotate, vibrate, etc.
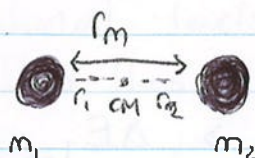
Transitions

Rotational spectrum
   CO + ~~HII~~ H_2
   We'll derive energies using non - QM physics
   H_2, CO, CS, HF, HO, HCN, HCO$^{\pm}$
                          ↑

                      CN acts kind of as one nuclei.

All these are linear atoms, but ∅ this derivation does not work for every linear molecule. ₅

$$\begin{cases} r_1 = \dfrac{r_m \, m_2}{m_1 + m_2} \\[2mm] r_2 = \dfrac{r_m \, m_1}{m_1 + m_2} \end{cases}$$

Classical rigid rotor !
                       o

   has energies $E = \dfrac{1}{2I} J^2$
                          ↗
                      inertia

Now quantum physics variant

$$E_{rot} = \frac{\hbar^2}{2 m_r^2 m_r} J(J+1)$$

↗ reduced mass $\quad m_r = \frac{m_1 m_2}{m_1 + m_2}$

Rotational levels
for simple (linear) molecules
More massive molecules have closer levels

Now: $\quad E_{rot}(J) = B_r \, J(J+1) \quad \left(\propto J^2 \text{ roughly!} \right)$

$$B_r = \frac{\hbar^2}{2 m_r \, r_n^2}$$

↳ rot. constant

Some numbers:

$$\frac{E_{rot}}{k_B} \approx 24 k \, \frac{m_H}{m_r} \left(\frac{1 \overset{\circ}{A}}{r_n} \right) J(J+1)$$
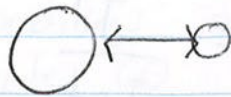
Thus few ~ 10's of kelvin.

∇
0
$\Rightarrow H_2 : \quad \frac{E_{rot}}{k_B} = \frac{m_H}{\left(\frac{m_H}{2} \right)} \rightarrow \Delta E_{J=1\to 0} = 170 \, k$

2

CO: $\quad m_r = 6.9 \, m_H$ $\quad \rightarrow \Delta E_{J=1\to 0} = 5.5 \, k$
$H_2 : \quad m_r = \frac{m_n^2}{2 m_n} = \frac{1}{2} m_H = 2 m_H$

We thus do not easily observe H_2, since
$170 \, k \gg \sim 20 \, k$ (Temperature of molecular clouds). CO
is easily to trace, since it's excitation T is low.
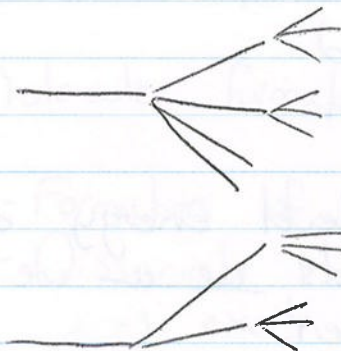
Vibrational levels : classicaly and insert QM

Classic : k both connected by ~~string~~ `spring`.
The energy depends on the bonding constant. ~~Har~~
Quantum harmonic oscillator.

$$E(v) = h\nu_0 \left(v + \tfrac{1}{2}\right)$$

characteristic frequency

$$E_{tot} = E_{el} + \cancel{E} \, h\nu_0 \left(v + \tfrac{1}{2}\right) + B_0 \, J(J+1)$$

Q : $\Delta J = 0$
P : $\Delta J = -1$
R : $\Delta J = +1$

H_2 potential curves : All vibrational levels are split
in rotational levels. Vibrational bands depend on chemical
~~bond~~ This thus tells us what molecule we have.
  eg 3.3 μm : C-H

Collissional de-excitation in atmosphere causes
greenhouse effect

$$n_{crit} = \frac{A_{ij}}{k_{ij}}$$

$$A_{J, J-1} = \frac{128\pi^3}{3\hbar} \left(\frac{B_v}{hc}\right)^3 \nu^2 \frac{J^4}{J+\frac{1}{2}}$$

and / where $\Delta J = \pm 1$

$$\underset{\approx}{\propto} J^3$$

CO: $A_{J, J-1} = 1.07 \cdot 10^{-37} \; J^3 \, s^{-1}$

Quadrupole transitions

Two seperate species : odd J and even J for H_2 as $\Delta J = 2$

H_2 : ortho $-H_2$: J odd

para $- H_2$: J even

Lowest transition has upper level energy of $\sim 500k$

Therefore, in bulk molecular gas ~~ce a~~ we cannot observe (cold) molecular hydrogen.

∇_0 $\Big\{$ #1 arg : need to excite level at $T > 500 \, k$

#2 : line is faint becaus quadrupole

#3 : only observcable from space = expensive

CO: $n_{crit} = \frac{A_{ij}}{k_{ij}} \underset{\approx}{\propto} J^3$

$E_{upper} \underset{\approx}{\propto} J^2$

Higher $\Rightarrow n$: higher T and higher density. We thus have no clean T or n probe. No matter where we are at rotational level, we will probe higher T and n with higher transition $\mapsto$ bias!

$J=1$: $n_{crit} \sim$ few 100 cm^{-3}. So CO has
right T, right n_{crit}, etc. So CO is good tracer
and conditions in molecular ISM are very suitable
to excite CO.

~~J selects basically at~~

HCN : $n_{crit} = \sim 10^5$ cm^{-3} for $J=1$

know
$\left\{\begin{array}{l}\text{– what is probed by what?} \\ \quad \text{– eg to | probe cold, low density, we need CO} \\ \text{– higher density} \\ \quad \text{– HCN} \\ \text{etc}\end{array}\right.$

$\int_0^1$

CO is a probe for H_2.

Molecule formation and dissociation

  – Formation of H_2
  – Dissociate H_2
     • 1 excite molecule to excited electronic state
     • 2 spontaneous decay leading to dissociation
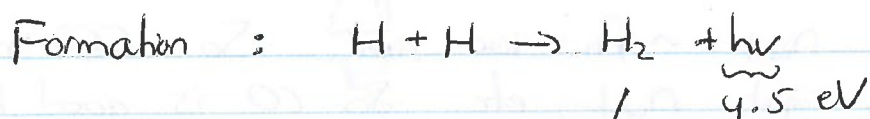 $\hookrightarrow$ ~~&~~ $912 < \lambda < $ ~~12~~ 1100 Å   UV photons

  Line process : need γ of exact right energy.

  • Destruction rate for H_2 :

$$\frac{dn_{H_2}}{dt} = - \int_{diss} n_{H_2}$$

$\uparrow$

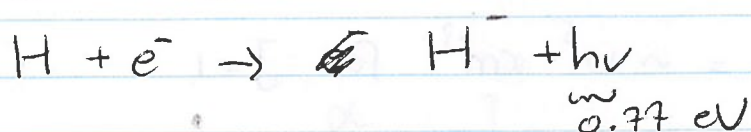depends on radiation ~~coeffici~~ field.
= $4 \cdot 10^{-11}$ s^{-1} in ISRF

Formation : $\quad H + H \rightarrow H_2 + h\nu$

$$4.5 \text{ eV}$$

homonuclear molecule, cannot
radiate very well.

~~Only one gas pha~~

$$H + e^- \rightarrow \cancel{} \quad H^- + h\nu$$

$$0.77 \text{ eV}$$

$$H^- + H \rightarrow H_2 + e^-$$

electron acts as catalyst for the reaction. First
H_2 molecule in universe is produced in this way.

$$\frac{dn_{H_2}}{dt} = R \, n_H^2$$

Now for 'statistical balance'

$$R \, n_H^2 = \frac{1}{2} \int_{diss} n_{H_2}$$

$$\qquad\qquad 4 \cdot 10^{-11} \, s^{-1} \, @ \, ISRF$$

$$R = \frac{n_{H_2} \int_{diss}}{\frac{1}{2} \, n_H^2}$$

$$\underline{\underline{= 3 \cdot 10^{-17} \, cm^3 \, s^{-1}}}$$

We can also try to derive $\cancel{R}$ R from QM
for the reaction path. This R is 8 magnitudes
lower. So we understand how to dissociate H_2 but
we do not know how to form H_2. We can
however also have chemistry on grain surfaces!

Rate for dust hydro H_2 formation

$$R = 3 \cdot 10^{-17} \left(\frac{T}{70k} \right)^{1/2} \text{ cm}^3 \text{ s}^{-1}$$

So right order of magnitude. Can work out eq. wit equilibrium abundance.

$$\frac{n_{H_2}}{n_H} = \frac{R_{gr} \, n_H}{\int_{diss}} = 2.3 \cdot 10^{-5} \frac{n_H}{30 \text{ cm}^{-3}}$$

Very low molecular abundance. We must have missed / overlooked something. Lines however become optically thick very fast. Thus the value just above is the dissociation rate at the surface of the cloud.

dissociation
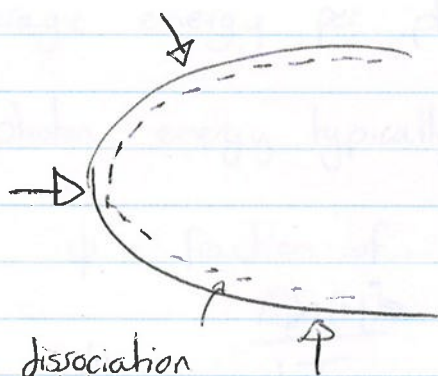
at edge of cloud → H_2 at edge. Self-shielding ↗ CO is also a self-shielding molecule.

We could calculate the thickness of the layer. Lines become optically thick at H_2 column density of $N_{H_2} \geq 10^{17} \text{ cm}^{-2}$?

$$N(HI) \, * = 10^{19-21} \text{ cm}^{-2}$$