

# The Bohr's Molecule

## 1 H<sub>2</sub> molecule in equilibrium

### 1.1 $r/R$ and $\rho/R$

Let  $\theta$  be the angle subtended by the proton-electron line from the proton-proton line, i.e. the angle between the lines with length  $R$  and  $r$  respectively. Then, balancing the repulsive and attractive forces,

$$\frac{ke^2}{R^2} = 2 \frac{ke^2}{r^2} \cos \theta$$

noting that  $\cos \theta = \frac{r}{2R}$ ,

$$\begin{aligned} \frac{1}{R^2} &= \frac{r/R}{r^2} \\ \frac{1}{R^2} &= \frac{r}{R} \\ R &= r \end{aligned}$$

hence the two protons and one electron form the vertices of an equilateral triangle. This makes sense as now the forces are of equal magnitude and all are  $120^\circ$  from each other. Hence  $\theta = \frac{\pi}{3}$  and

$$\frac{r}{R} = 1$$

$$\begin{aligned} \frac{\rho}{R} &= \sin \frac{\pi}{3} \\ &= \frac{\sqrt{3}}{2} \end{aligned}$$

### 1.2 $E_p$

Let  $E_{pp}$  be the electric potential energy between a pair of protons in the configuration,  $E_{pe}$  be the electric potential energy between a proton and an electron, and  $E_{ee}$  be that between two electrons. Then

$$\begin{aligned} E_{pp} &= \frac{ke^2}{R} \\ E_{pe} &= -\frac{ke^2}{r} \\ &= -\frac{ke^2}{R} \\ E_{ee} &= \frac{ke^2}{2\rho} \\ &= \frac{ke^2}{2R} \frac{2}{\sqrt{3}} \\ &= \frac{ke^2}{R} \frac{\sqrt{3}}{3} \end{aligned}$$

since there is one pair of protons, one of electrons and 4 proton-electron pairs,

$$\begin{aligned} E_p &= E_{pp} + E_{ee} + 4E_{pe} \\ &= \frac{ke^2}{R} \left( \frac{\sqrt{3}}{3} - 3 \right) \end{aligned}$$

### 1.3 $E_k/E_p$

Let  $F_c$  be the centripetal force pulling the electron in. Then

$$\begin{aligned} F_c &= 2 \frac{ke^2}{R^2} \cos \frac{\pi}{6} - \frac{ke^2}{(2\rho)^2} \\ &= \frac{ke^2}{R^2} \left( \sqrt{3} - \frac{1}{3} \right) \end{aligned}$$

Also,

$$\begin{aligned} F_c &= \frac{m_e v^2}{\rho} \\ &= \frac{m_e v^2}{R} \frac{2\sqrt{3}}{3} \end{aligned}$$

So

$$\begin{aligned} \frac{m_e v^2}{R} \frac{2\sqrt{3}}{3} &= \frac{ke^2}{R^2} \left( \sqrt{3} - \frac{1}{3} \right) \\ m_e v^2 &= \frac{ke^2}{R} \left( \sqrt{3} - \frac{1}{3} \right) \frac{\sqrt{3}}{2} \\ &= \frac{ke^2}{R} \left( \frac{9 - \sqrt{3}}{6} \right) \end{aligned}$$

Since there are two electrons,  $E_k = 2(\frac{1}{2}m_e v^2) = m_e v^2$

$$E_k = \frac{ke^2}{R} \left( \frac{9 - \sqrt{3}}{6} \right)$$

So

$$\begin{aligned} \frac{E_k}{E_p} &= \frac{\frac{ke^2}{R} \left( \frac{9 - \sqrt{3}}{6} \right)}{\frac{ke^2}{R} \left( \frac{\sqrt{3}}{3} - 3 \right)} \\ &= -\frac{1}{2} \end{aligned}$$

### 1.4 $R_0$

Now

$$m_e v^2 = \frac{ke^2}{R} \left( \frac{9 - \sqrt{3}}{6} \right)$$

and so

$$v = \sqrt{\frac{ke^2}{m_e R} \left( \frac{9 - \sqrt{3}}{6} \right)}$$

the momentum  $p$  is

$$\begin{aligned} p &= m_e v \\ &= \sqrt{\frac{m_e k e^2}{R} \left( \frac{9 - \sqrt{3}}{6} \right)} \end{aligned}$$

since the momentum of the electron about the center of the molecule is perpendicular to the radial vector to the electron,  $L = \rho p = R p \frac{\sqrt{3}}{2}$  and

$$\begin{aligned} L &= \frac{\sqrt{3}}{2} R p \\ &= \frac{\sqrt{3}}{2} \sqrt{\frac{m_e k e^2}{R} \left( \frac{9 - \sqrt{3}}{6} \right)} \\ &= \sqrt{\frac{m_e R k e^2}{8} \left( \frac{9 - \sqrt{3}}{8} \right)} \\ &= n \hbar \end{aligned}$$

$R$  will be minimized when  $n$  is the smallest, which occurs when  $n = 1$

$$\begin{aligned} \sqrt{\frac{m_e R_0 k e^2}{8} \left( \frac{9 - \sqrt{3}}{8} \right)} &= \hbar \\ R_0 &= \frac{\hbar^2}{k m_e e^2} \left( \frac{8}{9 - \sqrt{3}} \right) \\ &= 5.82478 \times 10^{-11} \text{ m} \end{aligned}$$

## 1.5 $E_b$

The total energy of the molecule is

$$\begin{aligned} E &= E_k + E_p \\ &= \frac{k e^2}{R_0} \left( \frac{3}{2} - \frac{\sqrt{3}}{6} + \frac{\sqrt{3}}{3} - 3 \right) \\ &= -29.946 \text{ eV} \end{aligned}$$

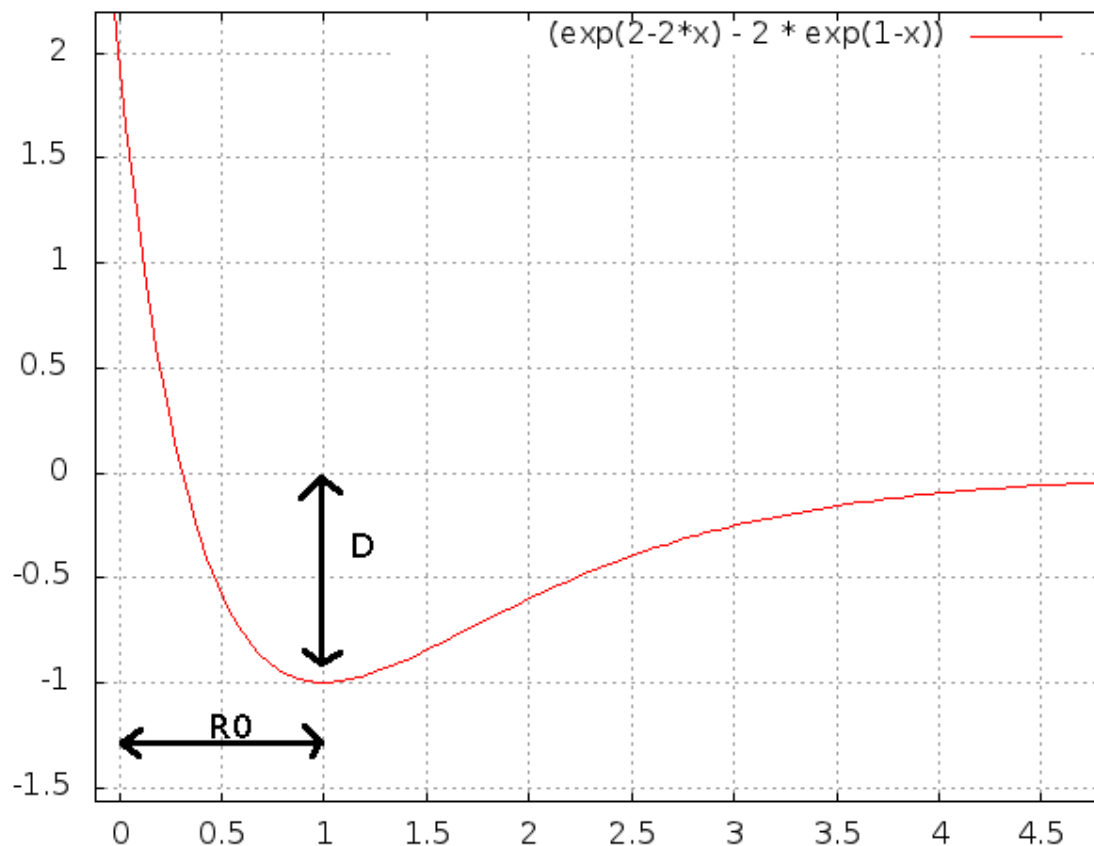
whereas the energy of the hydrogen atom is  $E_I$ . Hence the binding energy, which is the difference between the energy of a  $\text{H}_2$  molecule and two H atoms, is

$$\begin{aligned} E_b &= -2E_I - E \\ &= 29.946 \text{ eV} - 2(13.606 \text{ eV}) \\ &= 2.73 \text{ eV} \end{aligned}$$

## 2 Vibrating H<sub>2</sub> molecule

### 2.1 Morse potential

We sketch the morse potential with  $D = R_0 = \alpha = 1$ .



Clearly the potential reaches a minimum at  $R = R_0$  where it has the minimum value of  $-D$ . We can see this more clearly by writing  $E(R) = (1 - e^{1-x})^2 - 1$ . There is a horizontal asymptote at  $E = 0$ .  $\alpha$  seems to control the ‘width’ of the dip.

### 2.2 $D$ and $E_b$

When  $R = R_0, E = -D$

As  $R \rightarrow \infty, E \rightarrow 0$

Hence the bonding energy  $E_b = D$ .

### 2.3 Linear frequency of vibration

Let  $F(R)$  be the force exerted on the electron. Then

$$\begin{aligned} F(R) &= -\frac{dE}{dR} \\ &= \frac{2\alpha D}{R_0} \left( e^{2\alpha(1-R/R_0)} - e^{\alpha(1-R/R_0)} \right) \end{aligned}$$

as expected,  $F(R_0) = 0$ , so  $R_0$  is an equilibrium position and the system will oscillate around it. Let  $r$  be a small increase in  $R$ ; then

$$F(R_0 + r) \approx \left. \frac{dF}{dR} \right|_{R_0} r$$

and

$$\begin{aligned}\left.\frac{dF}{dR}\right|_{R_0} &= -\frac{2\alpha^2 D}{R_0^2} \left(2e^{2\alpha(1-R/R_0)} - e^{\alpha(1-R/R_0)}\right) \Big|_{R_0} \\ &= -\frac{2\alpha^2 D}{R_0^2}\end{aligned}$$

Let the acceleration be  $\ddot{r}$ . Since there are 2 protons,

$$\ddot{r} = \frac{F}{2m_p} = -\frac{\alpha^2 D}{m_p R_0^2} r$$

Let  $\omega$  be the angular frequency; then

$$\begin{aligned}\omega &= \sqrt{\frac{\alpha^2 D}{m_p R_0^2}} \\ &= \frac{\alpha}{R_0} \sqrt{\frac{E_b}{m_p}}\end{aligned}$$

$$\begin{aligned}v_{vib} &= \frac{\omega}{2\pi} \\ &= \frac{\alpha}{2\pi R_0} \sqrt{\frac{E_b}{m_p}}\end{aligned}$$

## 2.4 $\alpha$

The energy of a photon is  $hc/\lambda$ ; hence the photon lost in the Raman process is

$$\frac{hc}{\lambda_i} - \frac{hc}{\lambda_s} = hv_{vib}$$

so

$$\begin{aligned}v_{vib} &= c \left( \frac{1}{514 \text{ nm}} - \frac{1}{664 \text{ nm}} \right) \\ &= 1.32 \times 10^{14} \text{ s}^{-1}\end{aligned}$$

and the energy lost was 0.54 eV.

$$\begin{aligned}\alpha &= 2\pi R_0 v_{vib} \sqrt{\frac{m_p}{E_b}} \\ &= 2.98\end{aligned}$$

## 2.5 Minimum amplitude

We approximate  $E$  by a Taylor series

$$E(R_0 + r) \approx E(R_0) + \frac{1}{2} \left. \frac{d^2 E}{dR^2} \right|_{R_0} r^2$$

and

$$\begin{aligned}\frac{1}{2} \frac{d^2 E}{dR^2} \Big|_{R_0} &= \frac{\alpha^2 D}{R_0^2} \\ &= 7.15 \times 10^{21} \text{ eV m}^{-2}\end{aligned}$$

We know that  $E(R_0 + A_{min}) = E(R_0) + 0.54 \text{ eV}$ ; hence

$$\begin{aligned}A_{min} &= \sqrt{\frac{0.54 \text{ eV}}{7.15 \times 10^{21} \text{ eV m}^{-2}}} \\ &= 8.69 \times 10^{-12} \text{ m}\end{aligned}$$

or about  $0.1 \text{ \AA}$ .