The Bohr's Molecule

1 H_2 molecule in equillibrium

1.1 r/R and ρ/R

Let θ 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° 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_p/E_k

Let F_c be the centripetal force pulling the electron down. Then

$$\begin{aligned} F_c &= 2\cos\frac{\pi}{6}\frac{ke^2}{\rho^2} \\ &= m_e\frac{v^2}{\rho} \end{aligned}$$

Hence

$$\begin{aligned} E_k &= \frac{1}{2}m_e v^2 \\ &= \cos\frac{\pi}{6}\frac{ke^2}{\rho} \\ &= \frac{ke^2}{R} \end{aligned}$$

So

$$\begin{aligned} \frac{E_k}{E_p} &= \frac{\frac{ke^2}{R}}{\frac{ke^2}{R}\left(\frac{\sqrt{3}}{3} - 3\right)} \\ &= -\frac{\sqrt{3}+3}{26} \end{aligned}$$

1.4 R_0

Now

$$\frac{1}{2}m_e v^2 = \frac{ke^2}{R}$$

and so

$$v = e\sqrt{\frac{2k}{m_e R}}$$

the momentum p is

$$\begin{aligned} p &= m_e v \\ &= e\sqrt{\frac{2km_e}{R}} \end{aligned}$$

since the momentum of the electron about the center of the molecule is perpendual to the radial vector to the electron, $L = rp$ and

$$
\begin{aligned}
L &= Rp \\
&= e\sqrt{2km_e R} \\
&= n\hbar
\end{aligned}
$$

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

$$
\begin{aligned}
e\sqrt{2km_e R_0} = \hbar \\
R_0 = \frac{\hbar^2}{2km_e e^2}
\end{aligned}
$$

1.5 E_b

The total energy of the molecule is

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

wheares the energy of the hydrogen atom is E_I. Hence the binding energy, which is the difference between the energy of a H_2 molecule and two H atoms, is

$$
\begin{aligned}
E_b &= E - 2E_I \\
&= \frac{ke^2}{R}\left(\frac{\sqrt{3}}{3} - 2\right) - 2E_I
\end{aligned}
$$

2 Vibrating H_2 molecule

2.1 Morse potential

2.2 D and E_b

$$
\begin{gathered}
\text{When } R = R_0, E = -D \\
\text{As } R \to \infty, E \to 0
\end{gathered}
$$

Hence the bonding energy $E_b = D$.

2.3 Linear frequency of vibration