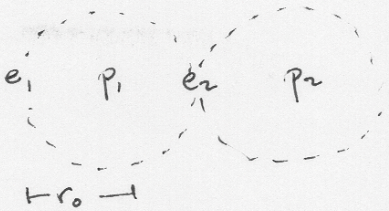
Kasap problem 1.3

$r_0 = 0.0529\,nm$

$k = 9.0\times10^9\ Nm^2/C^2$

$e = 1.602\times10^{-19}\,C$



a)

$$PE = -\underbrace{\frac{ke^2}{r_0}}_{e_1\leftrightarrow p_1} + \underbrace{\frac{ke^2}{2r_0}}_{e_1\leftrightarrow e_2} - \underbrace{\frac{ke^2}{3r_0}}_{e_1\leftrightarrow p_2} - \underbrace{\frac{ke^2}{r_0}}_{p_1\leftrightarrow e_2} - \underbrace{\frac{ke^2}{r_0}}_{e_2\leftrightarrow p_2} + \underbrace{\frac{ke^2}{2r_0}}_{p_1\leftrightarrow p_2} =$$

$$= \frac{ke^2}{r_0}\left(-1+\frac{1}{2}-\frac{1}{3}-1-1+\frac{1}{2}\right) = -\frac{7}{3}\frac{ke^2}{r_0} =$$

$$= -1.02\times10^{-17}\,J = -63.6\,eV < 0 \Rightarrow \text{energetically favorable}$$

b) for an isolated H atom,

$$\bar{E}_H = \frac{1}{2}\bar{PE} = -13.6\,eV$$

for the molecule,

$$\bar{E}_{H_2} = \bar{KE} + \bar{PE} = \frac{1}{2}\bar{PE} = \frac{1}{2}(-63.6\,eV) = -31.8\,eV$$

so the difference,

$$\bar{E}_{H_2} - 2\bar{E}_H = -31.8\,eV - 2(-13.6\,eV) = -4.6\,eV$$

The H_2 molecule has a lower energy than two H atoms by 4.6 eV, which is the covalent bond energy. This is very close to the experimental value.