ATOMS, MOLECULES & RESEARCH

QUANTUM MECHANICS - SPRING - WEEK 1

Chapter 11

① $$V_{NN} = \frac{(Ze)(Ze)}{(4\pi\varepsilon_0) R_e} = \frac{Z^2 e^2}{(4\pi\varepsilon_0) R_e}$$

For H_2^+, $Z = 1$ $\quad R_e = 106\ pm = 106 \times 10^{-12}\ m$

$$V_{NN} = \frac{e^2}{(4\pi\varepsilon_0) R_e} = \frac{(1.602 \times 10^{-19} C)^2}{(4\pi \times 8.854 \times 10^{-12} C^2 N^{-1} m^{-2})(106 \times 10^{-12} m)}$$

$$= 2.176 \times 10^{-18}\ N m^{+1} \times \frac{eV}{1.602 \times 10^{-19} J}$$

$$= \underline{13.583\ eV}$$

For H_2; $Z = 1$ $\quad R_e = 74.1\ pm = 74.1 \times 10^{-12}\ m$

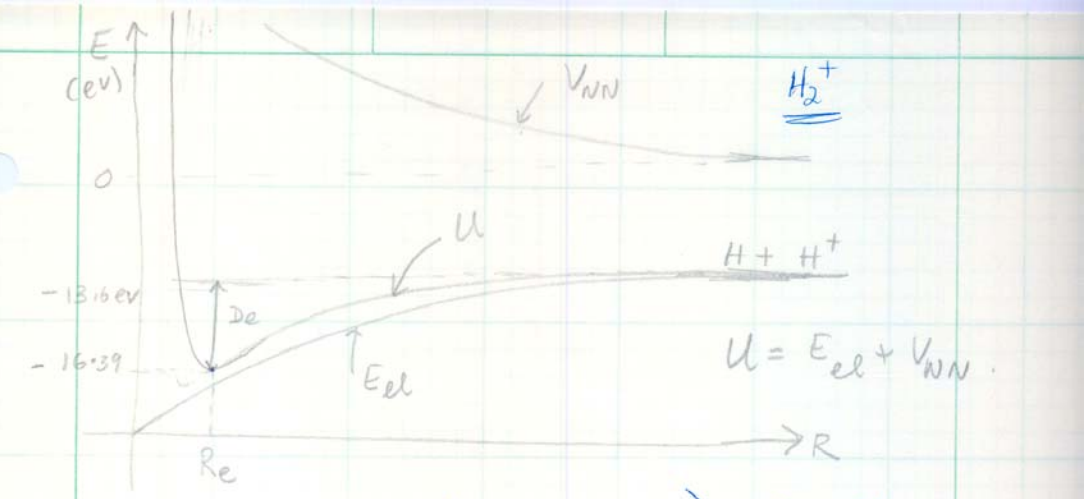
$$V_{NN} = \frac{e^2}{(4\pi\varepsilon_0) R_e} = \frac{(1.602 \times 10^{-19} C)^2}{(4\pi \times 8.854 \times 10^{-12} C^2 N^{-1} m^{-2})(74.1 \times 10^{-12} m)}$$

$$= 3.113 \times 10^{-18}\ Nm \times \frac{eV}{1.602 \times 10^{-19} J} = \underline{19.431\ eV}$$

$$U = V_{NN} + E_{el}$$

~~at R_e, $U = D_e$; at R_e $D_e = V_{NN} + E_{el}$~~

~~$E_{el} = D_e - V_{NN}(at\ R_e)$~~

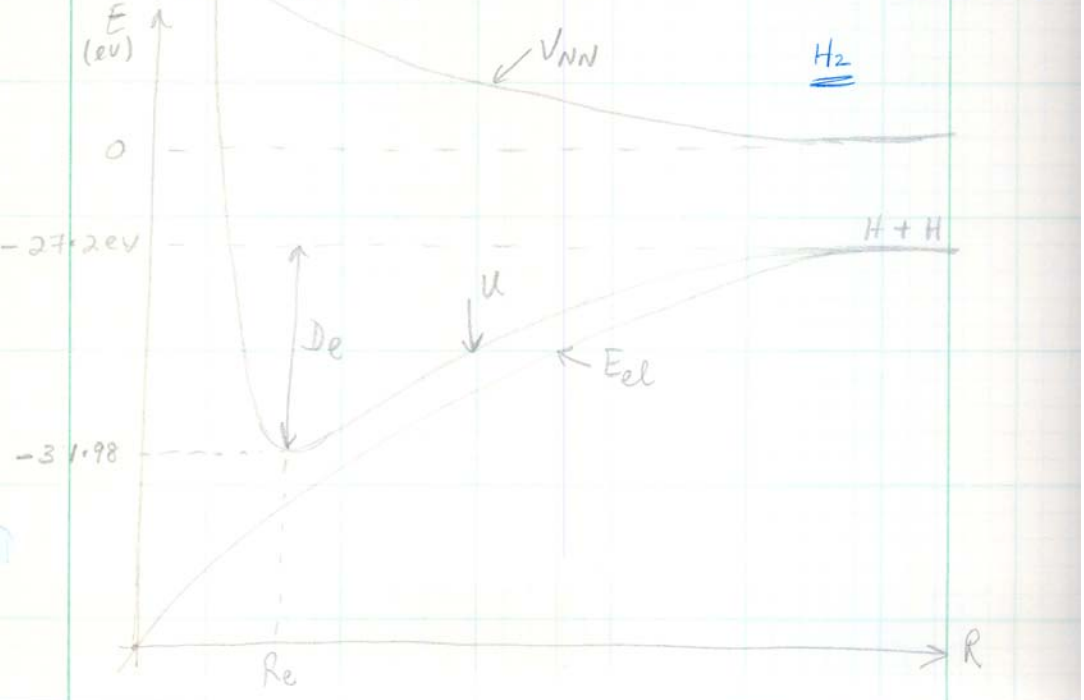


at R_e $U = -(D_e + 13.6\,eV)$ for H_2^+

$U = (-2.79 - 13.6)\,eV = -16.39\,eV$

$U = E_{el} + V_{NN} \Rightarrow E_{el} = U - V_{NN}$

$E_{el} = (-16.39\,eV - 13.583\,eV) = -29.97\,eV$



at R_e $U = (-27.2 - 4.78)\ eV = -31.98\ eV$

$U = E_{el} + V_{NN} \Rightarrow E_{el} = U - V_{NN}$

$E_{el} = (-31.98\ eV - 19.431)\ eV = \underline{\underline{-51.41\ eV}}$

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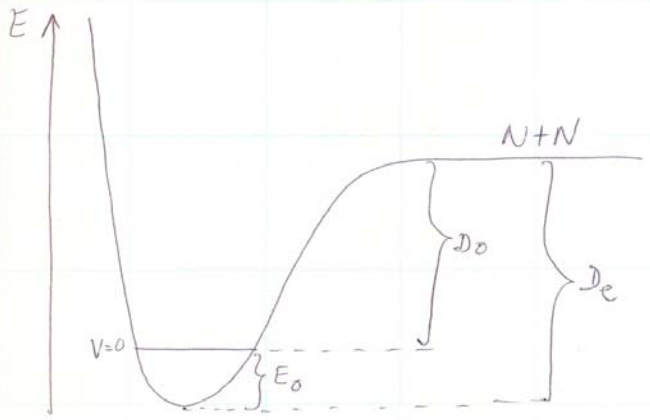

$D_E = D_0 + E_0$

E_0 = zero point energy $= \frac{1}{2} h\bar{\nu} = \frac{1}{2}\frac{hc}{\lambda} = \frac{1}{2} hc\left(\frac{1}{\lambda}\right)$

where $\frac{1}{\lambda} = 2331\ cm^{-1}$

$\therefore E_0 = \frac{1}{2}(6.626\times10^{-34}\ Js)(2.99\times10^{10}\ cm\,s^{-1})(2331\ cm^{-1})$

$= 2.309\times10^{-20}\ J \times \frac{1\ eV}{1.602\times10^{-19}\ J} = 0.144\ eV$

$D_0 = D_E - E_0 = 9.902\ eV - 0.144\ eV = 9.758\ eV$

$= 9.758\ eV \times \frac{1.602\times10^{-19}\ J}{1\ eV} \times \frac{kJ}{10^3\ J} \times 6.02\times10^{23}\ mol^{-1}$

$= \underline{\underline{941.07\ kJ\ mol^{-1}}}$