

(1) Cl_2 dissociation energy : 2.48 eV

NaCl_2 dissociation energy : 4.27 eV

$\text{Cl}_2 \rightarrow \text{Cl} + \text{Cl}$ (large separation)
takes 2.48 eV

$\text{Na} + \text{Cl}$ (large separation) $\rightarrow \text{NaCl}$
yields 4.27 eV

$$2.48 \text{ eV} - 4.27 \text{ eV} = -1.79 \text{ eV}$$

exothermic reaction

1.79 eV given off per molecule

(2)

HF

$$r_0 = 0.0917 \text{ nm}$$

$$P = 6.40 \times 10^{-30} \text{ C}\cdot\text{m}$$

percentage ionic

$$\frac{P}{e r_0} =$$

$$\frac{6.40 \times 10^{-30} \text{ C}\cdot\text{m}}{(1.60 \times 10^{-19} \text{ C})(9.17 \times 10^{-11} \text{ m})}$$

$$= 0.436$$

$$= 43.6 \% \text{ ionic}$$

(3)

$$Ne: \quad \alpha = 1.1 \times 10^{-37} \text{ C}^2/\text{N}$$

a.) at $T = 300 \text{ K}$

$$\langle E_{kz} \rangle = \frac{3}{2} kT$$

Dipole - Dipole energy is

$$U = -\vec{p}_2 \cdot \vec{E}_d, \quad E_d = \frac{k p_1}{r^3}$$

for an induced dipole, (Ne) $\vec{p}_2 = \alpha \vec{E}_d$

and

$$U = - \frac{2 \alpha k^2 p_1^2}{r^6}$$

to survive collision

$$\frac{3}{2} kT = \frac{2 \alpha k^2 p_1^2}{r^6}$$

p_1 is H_2O dipole moment, not given in Tipler

from wikipedia

$$p_1 = 1.85 \text{ D}$$

$$1 \text{ D} = 3.34 \times 10^{-30} \text{ C}\cdot\text{m}$$

$$r = \left[\frac{2 \alpha k^2 p_1^2}{3 kT} \right]^{1/6} = \left[\frac{2 (1.1 \times 10^{-37} \text{ C}^2/\text{N}) (8.99 \times 10^9 \text{ N}\cdot\text{m}^2/\text{C}^2)^2 (1.85 \times 3.34 \times 10^{-30} \text{ C}\cdot\text{m})^2}{3 (1.38 \times 10^{-23} \text{ J/K}) (300 \text{ K})} \right]^{1/6}$$

$$= 0.62 \text{ nm}$$

b.)

$$\frac{3}{2} kT \sim 0.0375 \text{ eV}$$

I'll define "typical bonded molecule"

to be an ionic bond like

NaCl

at this low energy, there is
little contribution from E_{ex} (large distance)

$$U(r) = \frac{-ke^2}{r} + 1.53 \text{ eV}$$

$$-0.0375 \text{ eV} = \frac{-1.44 \text{ eV} \cdot \text{nm}}{r} + 1.53 \text{ eV}$$

$$r \sim 1 \text{ nm}$$

c.) Neon needs to be closer than a typical molecule to form a stable bond. But we are neglecting Exclusion energy, so this bond is probably not energetically favorable. In fact, Neon forms no chemical bonds with any other atoms or molecules at $T=300 \text{ K}$,

4.

a.) LiH $r_0 = 0.160 \text{ nm}$

$$f = 4.22 \times 10^{13} \text{ s}^{-1}$$

In lowest vibrational state

$$E_f = \frac{1}{2} hf = 87.3 \text{ meV}$$

b.) Li, $Z = 3$
H, $Z = 1$

$$m = 6.94 \text{ amu}$$

$$m = 1.01 \text{ amu}$$

(atomic mass unit)
A.K.A "unified mass unit"

$$\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{(6.94)(1.01)}{(6.94) + (1.01)} \text{ amu}$$

$$= 0.882 \text{ amu} = 1.46 \times 10^{-27} \text{ kg}$$

c.) $f = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}$

$$k = (2\pi f)^2 \mu = 4\pi^2 (4.22 \times 10^{13} \text{ s}^{-1})^2 (1.46 \times 10^{-27} \text{ kg})$$

$$= 103 \text{ kg s}^{-2} = 103 \text{ N/m}$$

d.) Estimate using infinite well with width r_0

$$E \approx \frac{\hbar^2 \pi^2}{2\mu r_0^2} = \frac{\hbar^2}{8\mu r_0^2} \approx \frac{1}{2} hf$$

$$r_0 \approx \left[\frac{\hbar}{4\mu f} \right]^{\frac{1}{2}} = \left[\frac{6.626 \times 10^{-34} \text{ J}\cdot\text{s}}{4(1.46 \times 10^{-27} \text{ kg})(4.22 \times 10^{13} \text{ s}^{-1})} \right]^{\frac{1}{2}} = 0.052 \text{ nm}$$

table: $r_0 = 0.160 \text{ nm} \approx 3 \times$, expected for crude estimate.

5.

H ionization energy: 13.6 eV

H electron affinity: 0.75 eV (Table 9-2)

$$u(r) = -\frac{Ke^2}{r} + E_{ex} + E_{ion}$$

$$E_{ion} = 13.6 \text{ eV} - 0.75 \text{ eV} = 12.85 \text{ eV}$$

Is bonded if $U(r)$ has a negative minimum

$$Ke^2 = 1,440 \text{ eV} \cdot \text{nm}$$

There is no E_{ex} since H^+ has no electrons

In H^- ion, electrons are in the 1s state

Calculate screening of nuclear charge from the 2 1s electrons

$$\psi(\vec{r}) = \frac{1}{\sqrt{4\pi}} \frac{2}{\sqrt{a_0^3}} e^{-r/a_0}$$

electron charge distribution is

$$2 |\psi(r)|^2 = \frac{2}{\pi} \frac{1}{a_0^3} e^{-2r/a_0}$$

if second proton is at r , it is affected by charge at distance less than r_e

(5) cont

$$Q_{\text{eff}} = \underbrace{e}_{\text{proton}} - e \int_0^{r_p} (4\pi r^2) \left(\frac{2}{\pi} \frac{1}{a_0^3} e^{-2r/a_0} \right) dr$$

↑
electron charge inside r_p

$$= e - 2e \left(1 - \frac{1}{a_0^2} e^{-2r_p/a_0} (a_0^2 + 2a_0 r_p + 2r_p^2) \right)$$

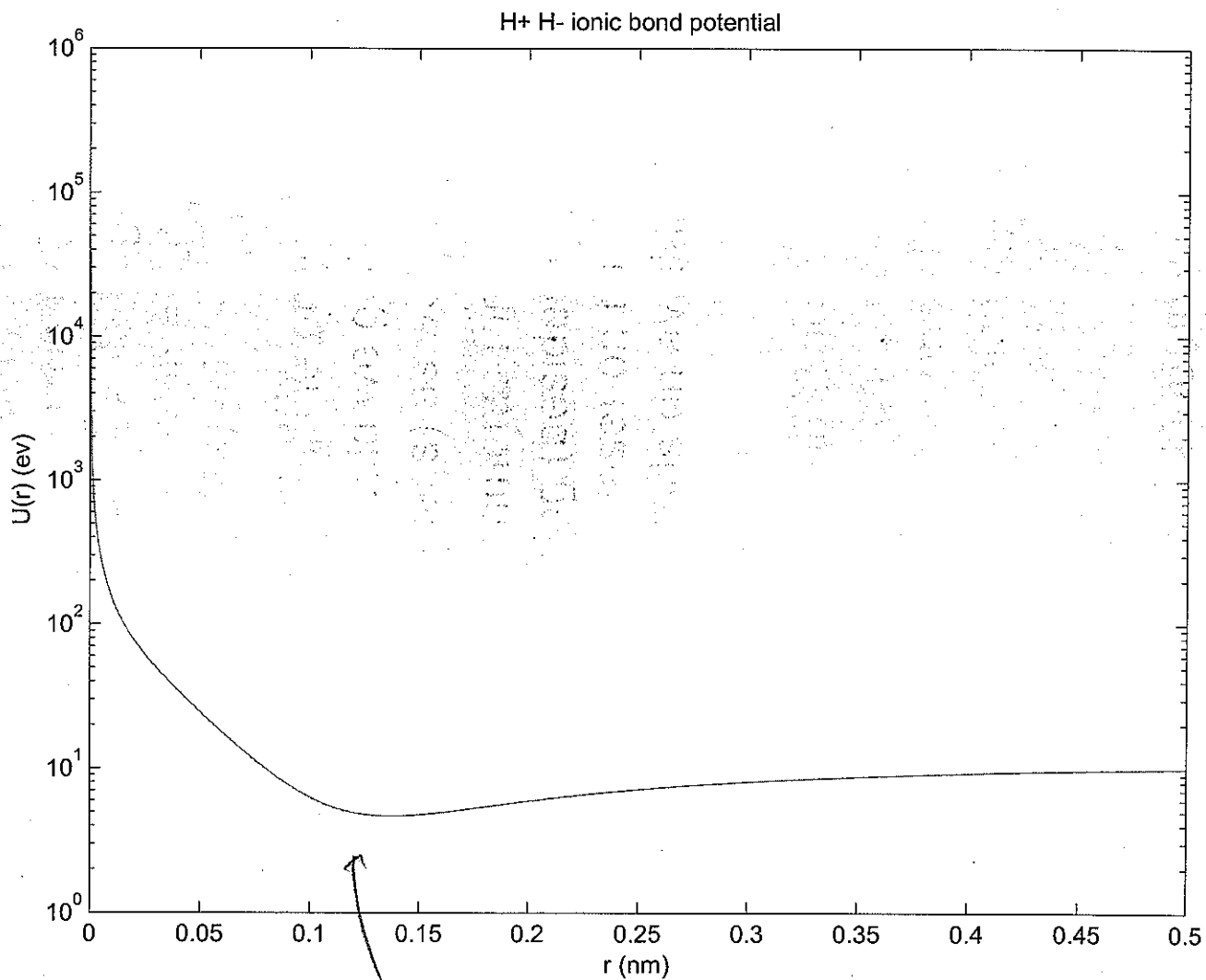
this gives the coulomb contribution to $V(r)$

$$\frac{K e Q_{\text{eff}}}{r}$$

$$V(r) = 12.85 \text{ eV} + \frac{K e^2}{r} \left[\frac{2e}{a_0^2} e^{-r_p/a_0} (a_0 + 2a_0 r_p + 2r_p^2) - \frac{2e}{a_0^2} \right]$$

I'm just going to plot this ...

5 cont,



a minimum, but $U(r)$ is
positive, so not a stable
bond.

(6.)

a.)

for $H^{35}Cl$

using $m = 35 \text{ amu}$ for ^{35}Cl
 $m = 37 \text{ amu}$ for ^{37}Cl

$$\mu_{35} = \frac{35}{36} \text{ amu}$$

$$\mu_{37} = \frac{37}{38} \text{ amu}$$

$$\mu_{ave} = \frac{\mu_{35} + \mu_{37}}{2} = .9730 \text{ amu}$$

$$\Delta \mu_{\mu} = \frac{\mu_{37} - \mu_{35}}{\mu_{ave}} = .0015$$

b.)

$$E_{or} = \frac{\hbar^2}{2I} \quad I = \mu r_0^2$$

$$E_{or} = \frac{\hbar^2}{2\mu r_0^2}$$

In changing rotational states, Energy changes by E_{or} , frequency changes

by $\frac{E_{or}}{h}$

$$f_{35} = \frac{\hbar^2}{h 2\mu_{35} r_0^2} = A \frac{1}{\mu_{35}} \quad A \equiv \frac{\hbar^2}{h 2 r_0^2}$$

$$f_{37} = A \frac{1}{\mu_{37}}$$

(c) cont.

$$\frac{\Delta f}{f} = \frac{f_{37} - f_{35}}{\frac{1}{2}(f_{35} + f_{37})} = \frac{\frac{1}{\mu_{37}} - \frac{1}{\mu_{35}}}{\frac{1}{2}\left(\frac{1}{\mu_{37}} + \frac{1}{\mu_{35}}\right)}$$

$$= \frac{\left(\frac{\mu_{35} - \mu_{37}}{\mu_{35} \mu_{37}}\right)}{\frac{1}{2}\left(\frac{\mu_{37} + \mu_{35}}{\mu_{35} + \mu_{37}}\right)} = \frac{\mu_{35} - \mu_{37}}{\frac{1}{2}(\mu_{35} + \mu_{37})} = -\frac{\Delta \mu}{\mu}$$

c.) $\frac{\Delta f}{f} = -0.0015$

This is less than 1%, the peaks in 9-29 look like they are spaced further apart than that.

We didn't consider any changes to r_0 , which might explain extra deviation.