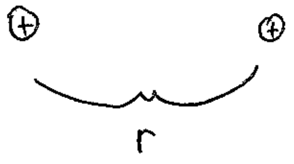
The H_2^+ Molecule

The simplist molecule: two protons, one electron

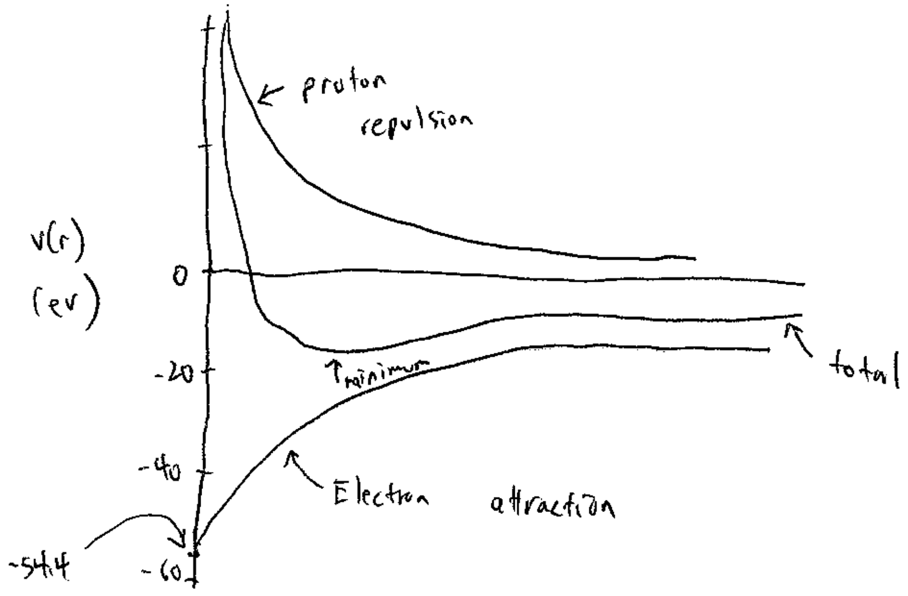


proton coulomb repulsion: $V(r) = \frac{Ke^2}{r}$

for large r $V = -13.6$ eV - electron is near one proton

for small r, this looks like $Z=2$ atom

$V = -54.4$ eV



$r_0 = 0.1$ nm

at minimum

$E_b = 2.6$ eV

The H_2 Molecule

two protons, two electrons

since electrons can have different spin, they can have the same spatial distribution

Spin- anti-symmetric

Spatial- Symmetric

total- anti-symmetric

r large: -27.2 eV - twice hydrogen

r small: -79 eV - doubly ionize helium

$r_0 = 0.075$ nm at Energy minimum

$E_b = 4.5$ eV

NaCl Molecule

$Na\ (Z=11)\quad 1s^2 2s^2 2p^6 3s^1$

$Cl\ (Z=17) = \quad 1s^2 2s^2 2p^6 3s^2 3p^5$

ionization of Na takes 5.1 eV

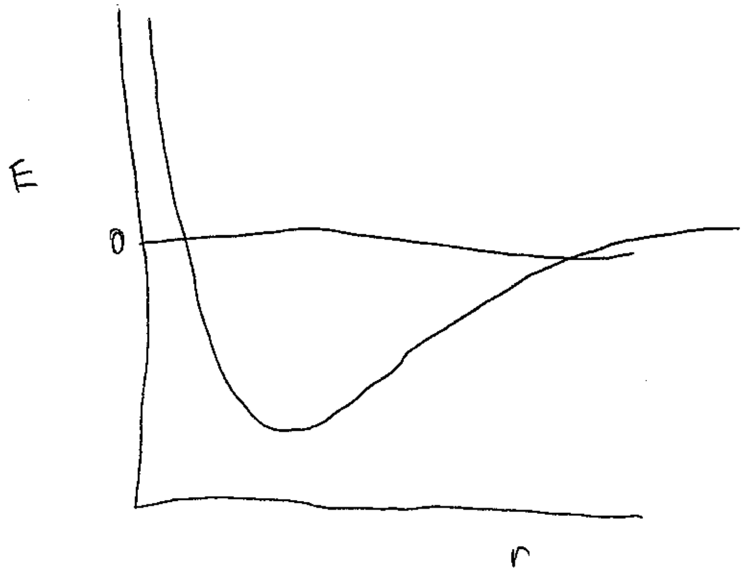
adding electron to Clorine gives 3.6 eV

$$E(r) = 5.1\text{ eV} - 3.6\text{ eV} \underset{\substack{\uparrow \\ \text{Coulomb} \\ \text{attraction}}}{- \frac{ke^2}{r}} + \underset{\substack{\nwarrow \\ \text{pauli exclusion} \\ \text{repulsion}}}{C\frac{e^{-ar}}{r}}$$

$E_b = 6.4$ eV

$r_0 = 0.28$ nm

vibrational levels



$$v(r) = V(r_0) + \frac{1}{2}(r-r_0)^2 \left[\frac{d^2V}{dr^2}\right]_{r=0}$$

$v(x) = \frac{1}{2} K x^2$ - Harmonic oscillator

$E_n \approx \left(n - \frac{1}{2}\right)\hbar w$ $n = 1, 2, 3 \ldots$

$w = \sqrt{\frac{K}{M}}$ $M = \frac{m_1 m_2}{m_1 + m_2}$. reduced mass

$E_v \approx \hbar w = \hbar \sqrt{\frac{K}{M}}$

$\hbar w \sim 0.1$ eV - IR light

for fixed electronic transitions,

$\Delta n = \pm 1$

Rotation levels

$$E_r = \frac{1}{2} I w^2$$

I : Moment of Inertia

$$I = M_1 r_1^2 + M_2 r_2^2$$

$$E_r = \frac{L^2}{2I}$$

$$L^2 = \ell(\ell+1)\hbar^2 \qquad \ell = 0, 1, 2 \ldots$$

$$E_r \approx \frac{\hbar^2}{4\pi M d_{atom}^2} \approx 10^{-3}\ eV$$

Vibration - Rotational spectra

$$E_{n,\ell} \approx E_e + \left(n + \frac{1}{2}\right)\hbar w + \frac{\ell(\ell+1)\hbar^2}{2I}$$

$$\Delta\ell = \pm 1$$

$$\Delta n = \pm 1$$