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Tutorial 8

Q.1 a.) Ionization Energy :- Minimum amount of energy required to remove the most loosely bound electron, or the valence electron of an isolated neutral gaseous atom or molecule.

b.) Electron Affinity :- Amount of energy released when an electron is attached to a neutral atom or molecule in the gaseous state to form a negative ion.

c.) Lattice Energy :- Energy released when ions are combined to make a compound

d.) Cohesive Energy :- The energy corresponding to the equilibrium position ($r = r_0$) is called energy of cohesion.

Q.2 a.) Hydrogen

b.) Electronegativity

Q.3 a) A covalent bond is formed by the overlap of half-filled atomic orbitals which have definite directions. Hence covalent bond is directional. It is saturated because each atom is bonded to as many atoms as possible.

b) Ionic bonds are non-directional because it is the electrostatic force between two opposite charges. Hence bonding direction does not matter.

Q.4
$$u(r) = \frac{-\alpha}{r^4} + \frac{\beta}{r^{12}}$$

for equilibrium position

For ~~u'~~
$$F = \left(-\frac{du(r)}{dr}\right)_{r=r_0} = 0.$$

$$r_0 = \left(\frac{3\beta}{\alpha}\right)^{1/8}.$$

To have stable bonding between atoms the energy released is

$$U(r_0) = \left(\frac{4\alpha^3}{27\beta}\right)^{1/2}.$$

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Q.5 $U(r) = \frac{-A}{r^2} + \frac{B}{r^{10}}$

for equilibrium position

$$F = \left(-\frac{dU(r)}{dr}\right)_{r=r_0} = 0.$$

$$A = 5B\, r_0^{-8}. \quad \text{—— (i)}$$

Dissociation energy is given by

$$U(r_0) = \frac{-A}{r_0^2} + \frac{B}{r_0^{10}}$$

from eq. (i)

$$U(r_0) = \frac{-4}{5}\frac{A}{r_0^2} \quad \text{—— (ii)}$$

According to ques. $U(r_0) = -8.0$ eV.

From eq. (i) & (ii)

$$A = 7.84 \times 10^{-19} \text{ eV}\cdot\text{m}^2$$
$$B = 5.92 \times 10^{-96} \text{ eV}\cdot\text{m}^{10}.$$

Now

$$F = -\frac{dU(r)}{dr} = -\frac{2A}{r^3} + \frac{10B}{r^{11}}$$

In order to dissociate this molecule into atoms

$$\left[\frac{dF}{dr}\right]_{r=r_c} = 0$$

$$\Rightarrow r_c = \left(\frac{100B}{6A}\right)^{1/8}$$

$$\Rightarrow r_c = 3.25 \text{ Å}$$

$$F(r=r_c) = 9.53 \text{ nN}$$

Q.6 Energy required for transferring an electron = Ionization energy − Electron affinity − Coulombic Energy.

Coulomb energy between cation and anion

$$= \frac{1}{4\pi\epsilon_0} \frac{(e)(e)}{r_0} = 2.821 \text{ eV}$$

$$E_{required} = (13.595 - 0.754 - 2.821) \text{ eV}$$

$$= 10.020 \text{ eV}$$

Q.7 $Z_1 = Z_2 = 1$

$$e = 1.6 \times 10^{-19} \text{ C}$$

$$r_0 = 1.67 + 1.95 = 3.62 \text{ Å}$$

$$F = \frac{1\, Z_1 Z_2\, e^2}{4\pi\epsilon_0\, r_0^2}$$

$$= \frac{1\times(1.6\times10^{-19})^2}{4\pi\epsilon_0\times 10^{6}\,(3.62)^2}$$

$$F = 1.76\, nN.$$

8 (a). $U(r) = -\frac{a}{r^m} + \frac{b}{r^n}.$

$U(r)$ is minimum at $r = r_0$

Thus, $\left[\frac{dU}{dr}\right]_{r=r_0} = 0.$

$\Rightarrow \quad U(r) = -\frac{a}{r_0^m} + \frac{b}{r_0^n}.$

$\Rightarrow \quad \left[\frac{dU}{dr}\right]_{r=r_0} = \frac{ma}{r_0^{m+1}} - \frac{nb}{r_0^{n+1}} = 0$

$\Rightarrow \quad r_0^n = r_0^m \left[\left(\frac{b}{a}\right)\left(\frac{n}{m}\right)\right].$

$\Rightarrow \quad \frac{r_0^n}{r_0^m} = \left[\left(\frac{b}{a}\right)\left(\frac{n}{m}\right)\right]$

$\Rightarrow \quad \boxed{r_0 = \left[\left(\frac{b}{a}\right)\left(\frac{n}{m}\right)\right]^{1/(n-m)}}$

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$$\left[\frac{d^2u}{dr^2}\right]_{r=r_0} = -\frac{am(m+1)}{r_0^{m+2}} + \frac{bn(n+1)}{r_0^{n+2}} > 0$$

$$bn(n+1) > am(m+1)\, r_0^{n-m}$$

$$bn(n+1) > am(m+1)\left(\frac{b}{a}\right)\left(\frac{n}{m}\right).$$

$$(n+1) > (m+1)$$

$$\Rightarrow \quad n > m.$$

(b) $$U_{min} = -\frac{a}{r_0^m} + \frac{b}{r_0^n}$$

$$= -\frac{a}{r_0^m} + b\left(\frac{a}{b}\right)\left(\frac{m}{n}\right)\frac{1}{r_0^m}$$

$$U_{min} = \frac{a}{r_0^m}\left(\frac{m}{n} - 1\right).$$

(c). $$U(r) = -\frac{a}{r^m} + \frac{b}{r^n}$$

$$m = 1, \quad n = 8.$$

$$\Rightarrow \quad U(r) = -\frac{a}{r} + \frac{b}{r^8}.$$

molecule will break at a critical distance r_c.

$$\left[\frac{dF}{dr}\right]_{r=r_c} = 0$$

$$F = \frac{-\partial U}{\partial r}$$

$$= \frac{-a}{r^2} + \frac{8b}{r^9}$$

$$\therefore \left(\frac{\partial F}{\partial r}\right)_{r_c} = \frac{2a}{r^3} - \frac{72b}{r^{10}} = 0.$$

$$\Rightarrow \frac{2a}{r_c^3} - \frac{72b}{r_c^{10}} = 0.$$

$$\Rightarrow r_c = \left[\frac{36b}{a}\right]^{1/7}.$$

At $r = r_c$, $F = F_{min}$

$$\Rightarrow F_{min} = \frac{-a}{r_c^2} + \frac{8b}{r_c^9}$$

$$= -a \times \left(\frac{a}{36b}\right)^{2/7} + 8b \times \left(\frac{a}{36b}\right)^{9/7}$$

$$= \frac{-a^{9/7}}{(36b)^{2/7}} + \frac{8b(a)^{9/7}}{(36b)^{2/7}(36b)}$$

$$= \frac{-a^{9/7}}{(36b)^{2/7}}\left(1 - \frac{8b}{36b}\right).$$

$$= \frac{-a^{9/7}}{(36b)^{2/7}} \times \frac{7}{9}$$