

MECH 221 Session #1

Chapter 2: Atomic Structure and Interatomic Bonding

1. Cesium bromide (CsBr) exhibits predominantly ionic bonding. The Cs^+ and Br^- ions have electron structures that are identical to which two inert gases?

Cs^+ is positively charged due to the loss of one electron.
 $Z = 55 \quad 55 - 1 = 54 \rightarrow \text{Xe}$

Br^- has negative charge from gaining one extra electron
 $Z = 35 \quad 35 + 1 = 36 \rightarrow \text{Kr}$

2. Calculate the force of attraction between a K^+ and an O^{2-} ion, the centers of which are separated by a distance of 1.5 nm.

$$E_A = -\frac{A}{r}$$

$$F_A = \frac{dE_A}{dr} = \frac{A}{r^2}$$

$$A = \frac{1}{4\pi\epsilon_0} (Z_1 e)(Z_2 e)$$

permittivity of a vacuum: $\epsilon_0 = 8.85 \times 10^{-12} \frac{\text{F}}{\text{m}}$

elementary charge: $e = 1.602 \times 10^{-19} \text{ C}$

valence: Z_n

$$Z_{\text{K}^+} = 1$$

$$Z_{\text{O}^{2-}} = 2$$

$$A = 4.615 \times 10^{-28}$$

$$F_A = \frac{4.615 \times 10^{-28}}{(1.5 \times 10^{-9})^2} = \underline{2.05 \times 10^{-10} \text{ N}}$$

Consider a hypothetical $X^+ Y^-$ ion pair for which the equilibrium interatomic spacing and bonding energy values are 0.35 nm and -6.13 eV respectively. If $n=10$, using the results from question 3, determine expressions for attractive and repulsive energies

$$r_0 = 0.35 \text{ nm} \quad E_0 = -6.13 \text{ eV} \quad n = 10$$

$$r_0 = \left(\frac{nB}{A} \right)^{\frac{1}{n-1}}$$

$$E_0 = -\frac{A}{\left(\frac{nB}{A} \right)^{\frac{n-1}{n}}} + \frac{B}{\left(\frac{nB}{A} \right)^{\frac{n}{n-1}}}$$

$$0.35 = \left(\frac{10B}{A} \right)^{\frac{1}{9}}$$

$$-6.13 = -\frac{A}{\left(\frac{10B}{A} \right)^{\frac{1}{9}}} + \frac{B}{\left(\frac{10B}{A} \right)^{\frac{10}{9}}}$$

t tedious to solve

$$A = 2.38$$

$$B = 1.88 \times 10^{-5}$$

$$E_A = -\frac{2.38}{r}$$

$$E_r = \frac{1.88 \times 10^{-5}}{r^{10}}$$

3. The net potential energy between two adjacent ions, E_N , may be represented by the sum of Equations 2.8 and 2.9, that is,

$$E_N = -\left(\frac{A}{r}\right) + \left(\frac{B}{r^n}\right)$$

Calculate the bonding energy E_0 in terms of the parameters A , B , and n .

The bonding energy E_0 corresponds to the interatomic separation r_0 at which both attractive and repulsive forces are equal.

$$E_N = \int F_N dr \quad \longrightarrow \quad F_N = \frac{dE_N}{dr} = \frac{A}{r^2} - \frac{nB}{r^{n+1}}$$

$$\text{at } r_0, \quad F_N = 0 = \frac{A}{r^2} - \frac{nB}{r^{n+1}}$$

$$\frac{A}{r^2} = \frac{nB}{r^{n+1}}$$

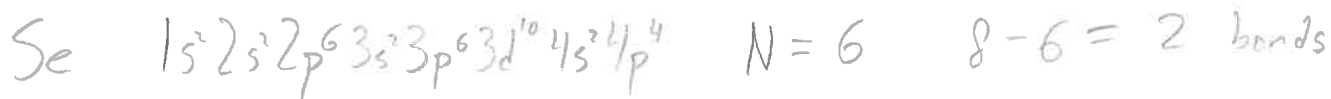
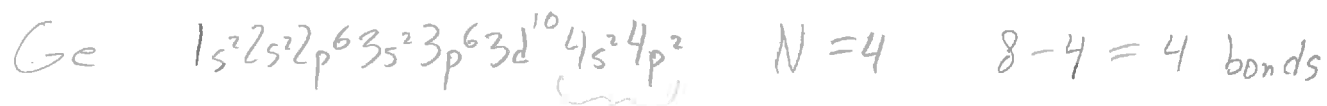
$$\frac{r^{n+1}}{r^2} = \frac{nB}{A}$$

$$r^{n-1} = \frac{nB}{A}$$

$$r_0 = \left(\frac{nB}{A}\right)^{\frac{1}{n-1}}$$

$$E_0 = \frac{-A}{\left(\frac{nB}{A}\right)^{\frac{1}{n-1}}} + \frac{B}{\left(\frac{nB}{A}\right)^{\frac{n}{n-1}}}$$

8.11 Determine the number of covalent bonds that are possible for atoms of the following elements: germanium, phosphorous, selenium and chlorine



4. For a $K^+ - Cl^-$ ion pair, attractive and repulsive energies E_A and E_R , respectively, depend on the distance between the ions r , according to:

$$E_A = -\frac{1.436}{r} \quad E_R = \frac{5.86 \times 10^{-6}}{r^9}$$

For these expressions, energies are expressed in electron volts per $K^+ - Cl^-$ pair, and r is the distance in nanometers. Mathematically determine the r_0 and E_0 values.

$$E_N = E_A + E_R$$

$$F_N = \frac{dE_N}{dr} = \frac{1.436}{r^2} - \frac{9(5.86 \times 10^{-6})}{r^{10}}$$

at r_0 , $F_N = 0$

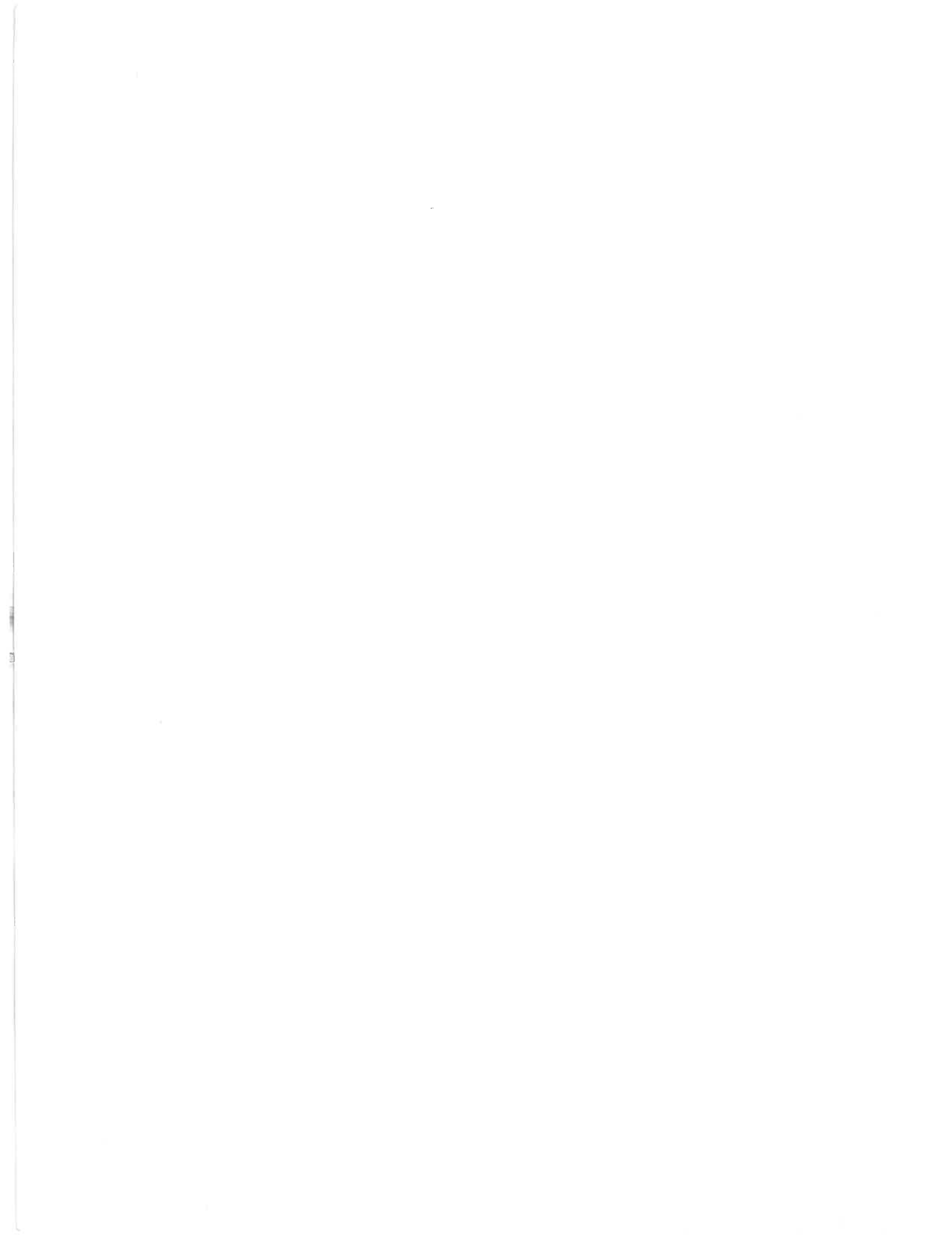
$$\frac{1.436}{r^2} = \frac{9(5.86 \times 10^{-6})}{r^{10}}$$

$$\frac{r^{10}}{r^2} = \frac{9(5.86 \times 10^{-6})}{1.436}$$

$$r^8 = 3.673 \times 10^{-5}$$

$$r_0 = (3.673 \times 10^{-5})^{\frac{1}{8}} = 0.279 \text{ nm}$$

$$E_0 = \frac{-1.436}{0.279} + \frac{5.86 \times 10^{-6}}{0.279^9} = -4.57 \text{ eV}$$



5. (a) Briefly cite the main differences between ionic, covalent, and metallic bonding.
 (b) State the Pauli exclusion principle.

Ionic bonds arise from an electrostatic attraction between oppositely charged atoms (ions).

Covalent bonds arise from atoms sharing valence electrons in order to have a stable configuration

Metallic bonding is due to valence electrons which are free to flow between nuclei that are shared by all atoms in the material

6. Explain the nature of secondary (Van der Waals) bonding and the special case of hydrogen bonding.

Van der Waals bonding exists between all atoms or molecules but are weak compared to primary bonds. They arise from dipoles either induced or permanent.

Permanent dipoles are due to the geometry of a molecule that results in an uneven distribution of charge.

Induced dipoles are caused by atomic vibration which in turn causes instantaneous non-uniform charge distribution.

Hydrogen bonding occurs when H is covalently bonded to F, O or N. The unshielded hydrogen atom creates a very strong permanent dipole.



7. Compute the percent ionic character of the interatomic bonds for the following compounds: TiO_2 , ZnTe , CsCl , InSb , and MgCl_2 .

$$\text{TiO}_2: \% \text{IC} = 100 \left(1 - e^{-0.25(1.5-3.5)^2} \right) = 63.2\%$$

$$\text{ZnTe}: \% \text{IC} = 100 \left[1 - e^{-0.25(2.1-1.6)^2} \right] = 6.1\%$$

$$\text{CsCl}: \% \text{IC} = 100 \left[1 - e^{-0.25(3.0-0.7)^2} \right] = 73.4\%$$

$$\text{InSb}: \% \text{IC} = 100 \left[1 - e^{-0.25(1.9-1.7)^2} \right] = 1.0\%$$

$$\text{MgCl}_2: \% \text{IC} = 100 \left[1 - e^{-0.25(3.0-1.2)^2} \right] = 55.5\%$$

What are the electron configurations for the following atoms/ions?

