HW-3

1)

$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$ $\quad 2d\sin\theta = \lambda \Rightarrow \theta = \sin^{-1}\left(\frac{\lambda}{2d}\right)$

for $h^2+k^2+l^2 = 3$; $\quad d_{111} = \frac{6}{\sqrt{3}} \Rightarrow \theta = \sin^{-1}\left(\frac{1.54 \times \sqrt{3}}{2\times 6}\right) =$

Similarly for $" = 4$: $d_{200} = \frac{6}{\sqrt{4}} \Rightarrow \theta = \sin^{-1}(\quad) =$

$" = 8$; $d_{220} = \frac{6}{\sqrt{8}} \Rightarrow \theta = \sin^{-1}(\quad) =$

2) $\lambda_e = \sqrt{\frac{150}{80}}\,\text{Å} = \sqrt{\frac{15}{8}}\,\text{Å} \cdot \ell \quad d_{111} = \frac{a}{\sqrt{3}} = \frac{3.5}{\sqrt{3}}$

$\theta = \sin^{-1}\left(\frac{\lambda}{2d}\right) = \sin^{-1}\left(\frac{\sqrt{15}/2\sqrt{2}}{2\times 3.5/\sqrt{3}}\right) = \sin^{-1}\left(\frac{3\sqrt{5}}{14\sqrt{2}}\right)$

3) Types of bonds

i) Metallic → unlocalised valance electrons.

ii) Covalent → sharing of electrons. → directional

iii) Ionic → Exchange of $e^{\ominus}$ due to difference in electronegativity leading to electrostatic interaction.

iv) Van der Waals → Instantaneous attraction due to polarization of charge. → London force via dipole moment.

v) Hydrogen bond → Oxygen $^{\delta-}$ draws $e^{\ominus}$ leading to partially positive $H^{\delta+}$ atom which form hydrogen bond with nearing $O^{\delta-}$ atom

4) $U(r) = \frac{\phi_a}{r^8} + \frac{\phi_r}{r^9}$

a) $\left.\frac{dU}{dR}\right|_{R=R_e} = 0 \Rightarrow R_e = \left(9B/A\right)^{1/8}$

b) At $R = R_e$: $\left(\frac{9B}{A}\right)^{1/8}$; $\frac{\phi_a}{\phi_r} = \frac{A/R_e^8}{B/R_e^9} = \frac{A}{B} \times R_e^8 = 9$

c) $U_{min} = -\frac{A}{R_e^8} + \frac{B}{R_e^9} = -\frac{8A}{9R_e}$

5) $U = -\frac{e^2}{4\pi\epsilon_0 R_e}$ in $J = \frac{-e}{4\pi\epsilon_0 R_e}$ in eV

Substituting values:

$$U = \frac{-1.6 \times 10^{-19} \times 9 \times 10^{9}}{2 \times 10^{-18}} = -7.2\,eV.$$

$\times e\,(1.6 \times 10^{-19})$ in Joules.

$= -1.15 \times 10^{-18}\,J$ Ans.