Answers to HW 10#

21.12 The formula for the volume of a general parallelepiped is in the text. It is

$$V = abc\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}$$

The crystal is monoclinic, so $\alpha = \gamma = 90°$. The cosine of 90° is zero, hence, using the trigonometric identity $\sin^2\beta + \cos^2\beta = 1$:

$$V = abc\sqrt{1-\cos^2\beta} = abc\sin\beta$$

Substitution gives $V = 589$ Å^3 for the unit cell of potassium hexacyanoferrate(III).

21.22 **a)** Metallic aluminum has four atoms per unit cell (n in the following).
b)

$$V_m = N_A\, a^3 = \frac{n\,\mathcal{M}}{\rho} = \frac{4\times 26.98\text{ g mol}^{-1}}{2.70\text{ g cm}^{-3}}$$

$$a = \sqrt[3]{\frac{4\times 26.98\text{ g mol}^{-1}}{6.022\times 10^{23}\text{ mol}^{-1}\times 2.70\text{ g cm}^{-3}}} = 4.05\times 10^{-8}\text{ cm}$$

$$d = \frac{a\sqrt{2}}{2} = 2.86\times 10^{-8}\text{ cm}^3$$

21.28 **a)** Rb is metallic. **b)** C_5H_{12} is molecular. **c)** B is covalent. **d)** Na_2HPO_4 is ionic.

21.34 The nearest neighbors of a Na^+ ion are 6 Cl^- ions. The second nearest neighbors are a set of 12 Na^+ ions. The third nearest neighbors are a set of 8 Cl^- ions.

21.40

The lattice energy in this problem is the energy required to separate 1.00 mol of RbCl(s) into its component ions. Use text equation 21.3 to compute the negative of the electrostatic potential energy among the ions in their equilibrium positions

$$-V = 1.00\text{ mol}\frac{1.7627\times(1.602\times10^{-19}\text{ C})^2\times 6.022\times10^{23}\text{ mol}^{-1}}{4\pi\times 8.854\times10^{-12}\text{ C}^2\text{ J}^{-1}\text{ m}^{-1}\times 3.48\times10^{-10}\text{ m}}$$
$$= 7.04\times10^5\text{ J} = 704\text{ kJ}$$

This result only approximates the lattice energy. A 10% reduction to account for the short-range repulsive interactions and zero-point energy gives a better estimate

$$\text{lattice energy} = 633\text{ kJ}$$

21.45 **a)** The unit-cell volume V_{cell} of NaCl is the cell edge cubed or $\boxed{179.43\text{ Å}^3}$.

b) The volume V_p of the primitive unit cell of NaCl equals one-fourth of the volume of the conventional unit cell or $\boxed{44.856\text{ Å}^3}$.

c)

$$N_{\text{beams}} = \frac{4}{3}\pi\left(\frac{2}{\lambda}\right)^3 V_p = \frac{4}{3}\pi\left(\frac{2}{2.2896\text{ Å}}\right)^3(44.856\text{ Å}^3) = \boxed{125}$$

d) For this shorter wavelength (0.7093 Å) there are far more diffracted beams:

$$N_{\text{beams}} = \frac{4}{3}\pi\left(\frac{2}{\lambda}\right)^3 V_p = \frac{4}{3}\pi\left(\frac{2}{0.7093\text{ Å}}\right)^3(44.856\text{ Å}^3) = \boxed{4212}$$