

12.21 This problem asks us to compute the atomic packing factor for  $\text{Fe}_3\text{O}_4$  given its density and unit cell edge length. It is first necessary to determine the number of formula units in the unit cell in order to calculate the sphere volume. Solving for  $n'$  from Equation 12.1 leads to

$$n' = \frac{\rho V_C N_A}{\sum A_C + \sum A_A}$$

$$= \frac{(5.24 \text{ g/cm}^3) [(8.39 \times 10^{-8} \text{ cm})^3/\text{unit cell}] (6.023 \times 10^{23} \text{ formula units/mol})}{(3)(55.85 \text{ g/mol}) + (4)(16.00 \text{ g/mol})}$$

$$= 8.0 \text{ formula units/unit cell}$$

Thus, in each unit cell there are 8  $\text{Fe}^{2+}$ , 16  $\text{Fe}^{3+}$ , and 32  $\text{O}^{2-}$  ions. From Table 12.3,  $r_{\text{Fe}^{2+}} = 0.077 \text{ nm}$ ,  $r_{\text{Fe}^{3+}} = 0.069 \text{ nm}$ , and  $r_{\text{O}^{2-}} = 0.140 \text{ nm}$ . Thus, the total sphere volume in Equation 3.2 (which we denote as  $V_S$ ), is just

$$V_S = (8) \left( \frac{4}{3} \pi \right) (7.7 \times 10^{-9} \text{ cm})^3 + (16) \left( \frac{4}{3} \pi \right) (6.9 \times 10^{-9} \text{ cm})^3$$

$$+ (32) \left( \frac{4}{3} \pi \right) (1.40 \times 10^{-8} \text{ cm})^3$$

$$= 4.05 \times 10^{-22} \text{ cm}^3$$

Now, the unit cell volume ( $V_C$ ) is just

$$V_C = a^3 = (8.39 \times 10^{-8} \text{ cm})^3 = 5.90 \times 10^{-22} \text{ cm}^3$$

Finally, the atomic packing factor (APF) from Equation 3.2 is just

$$\text{APF} = \frac{V_S}{V_C} = \frac{4.05 \times 10^{-22} \text{ cm}^3}{5.90 \times 10^{-22} \text{ cm}^3} = 0.686$$