

12.18 (a) We are asked to compute the density of CsCl. Modifying the result of Problem 3.3, we get

$$a = \frac{2r_{\text{Cs}^+} + 2r_{\text{Cl}^-}}{\sqrt{3}} = \frac{2(0.170 \text{ nm}) + 2(0.181 \text{ nm})}{\sqrt{3}}$$

$$= 0.405 \text{ nm} = 4.05 \times 10^{-8} \text{ cm}$$

From Equation 12.1

$$\rho = \frac{n'(A_{\text{Cs}} + A_{\text{Cl}})}{V_C N_A} = \frac{n'(A_{\text{Cs}} + A_{\text{Cl}})}{a^3 N_A}$$

For the CsCl crystal structure, $n' = 1$ formula unit/unit cell, and thus

$$\rho = \frac{(1 \text{ formula unit/unit cell})(132.91 \text{ g/mol} + 35.45 \text{ g/mol})}{(4.05 \times 10^{-8} \text{ cm})^3/\text{unit cell} (6.023 \times 10^{23} \text{ formula units/mol})}$$

$$= 4.20 \text{ g/cm}^3$$

(b) This value of the density is greater than the measured density (3.99 g/cm^3). The reason for this discrepancy is that the ionic radii in Table 12.3, used for this computation, were for a coordination number of six, when, in fact, the coordination number of both Cs^+ and Cl^- is eight. The ionic radii should be slightly greater, leading to a larger V_C value, and a lower density.