

12.13 We are asked to calculate the theoretical density of NiO. This density may be computed using Equation (12.1) as

$$\rho = \frac{n'(A_{\text{Ni}} + A_{\text{O}})}{V_C N_A}$$

Since the crystal structure is rock salt, $n' = 4$ formula units per unit cell. Using the ionic radii for Ni^{2+} and O^{2-} from Table 12.3, the unit cell volume is computed as follows:

$$\begin{aligned} V_C = a^3 &= \left(2r_{\text{Ni}^{2+}} + 2r_{\text{O}^{2-}} \right)^3 = [2(0.069 \text{ nm}) + 2(0.140 \text{ nm})]^3 \\ &= 0.0730 \frac{\text{nm}^3}{\text{unit cell}} = 7.30 \times 10^{-23} \frac{\text{cm}^3}{\text{unit cell}} \end{aligned}$$

Thus,

$$\begin{aligned} \rho &= \frac{(4 \text{ formula units/unit cell})(58.69 \text{ g/mol} + 16.00 \text{ g/mol})}{\left(7.30 \times 10^{-23} \text{ cm}^3/\text{unit cell} \right) \left(6.023 \times 10^{23} \text{ formula units/mol} \right)} \\ &= 6.79 \text{ g/cm}^3 \end{aligned}$$