

12.19 This problem asks that we compute the density of CaF_2 . A unit cell of the fluorite structure is shown in Figure 12.5. It may be seen that there are four CaF_2 units per unit cell (i.e., $n' = 4$ formula units/unit cell). Assume that for each of the eight small cubes in the unit cell

$$a = \frac{2r_{\text{Ca}^{2+}} + 2r_{\text{F}^{-}}}{\sqrt{3}}$$

and, from Table 12.3

$$a = \frac{2(0.100 \text{ nm}) + 2(0.133 \text{ nm})}{\sqrt{3}} = 0.269 \text{ nm} = 2.69 \times 10^{-8} \text{ cm}$$

The volume of the unit cell is just

$$V_C = (2a)^3 = \left[(2)(2.69 \times 10^{-3} \text{ cm}) \right]^3 = 1.56 \times 10^{-22} \text{ cm}^3$$

Thus, from Equation 12.1

$$\begin{aligned} \rho &= \frac{n' A_{\text{Ca}} + 2 A_{\text{F}}}{V_C N_A} \\ &= \frac{(4 \text{ formula units/unit cell}) [40.08 \text{ g/mol} + (2)(19.00 \text{ g/mol})]}{(1.56 \times 10^{-22} \text{ cm}^3/\text{unit cell}) (6.023 \times 10^{23} \text{ formula units/mol})} \\ &= 3.33 \text{ g/cm}^3 \end{aligned}$$

The measured density is 3.18 g/cm^3 .