

12.16 This problem asks that we compute the theoretical density of ZnS given that the Zn—S distance and bond angle are 0.234 nm and 109.5°, respectively. The first thing we need do is to determine the unit cell volume from the given Zn—S distance. From the previous problem, the unit cell volume V_C is just a^3 , a being the unit cell edge length, and

$$\begin{aligned} V_C &= (4y \sin \theta)^3 = [(4)(0.234 \text{ nm})(\sin 35.25^\circ)]^3 \\ &= 0.1576 \text{ nm}^3 = 1.576 \times 10^{-22} \text{ cm}^3 \end{aligned}$$

Now we must utilize Equation 12.1 with $n' = 4$ formula units, and A_{Zn} and A_{S} being 65.39 and 32.06 g/mol, respectively. Thus

$$\begin{aligned} \rho &= \frac{n'(A_{\text{Zn}} + A_{\text{S}})}{V_C N_A} \\ &= \frac{(4 \text{ formula units/unit cell})(65.39 \text{ g/mol} + 32.06 \text{ g/mol})}{(1.576 \times 10^{-22} \text{ cm}^3/\text{unit cell})(6.023 \times 10^{23} \text{ formula units/mol})} \\ &= 4.11 \text{ g/cm}^3 \end{aligned}$$

The measured value of the density is 4.10 g/cm³.