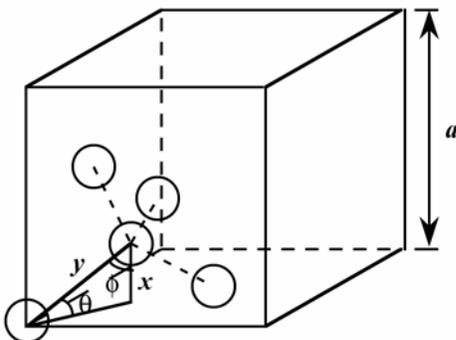


12.15 This problem asks that we compute the theoretical density of diamond given that the C—C distance and bond angle are 0.154 nm and 109.5° , respectively. The first thing we need do is to determine the unit cell edge length from the given C—C distance. The drawing below shows the cubic unit cell with those carbon atoms that bond to one another in one-quarter of the unit cell.



From this figure, ϕ is one-half of the bond angle or $\phi = 109.5^\circ/2 = 54.75^\circ$, which means that

$$\theta = 90^\circ - 54.75^\circ = 35.25^\circ$$

since the triangle shown is a right triangle. Also, $y = 0.154$ nm, the carbon-carbon bond distance.

Furthermore, $x = a/4$, and therefore,

$$x = \frac{a}{4} = y \sin \theta$$

Or

$$a = 4y \sin \theta = (4)(0.154 \text{ nm})(\sin 35.25^\circ) = 0.356 \text{ nm}$$

$$= 3.56 \times 10^{-8} \text{ cm}$$

The unit cell volume, V_C is just a^3 , that is

$$V_C = a^3 = (3.56 \times 10^{-8} \text{ cm})^3 = 4.51 \times 10^{-23} \text{ cm}^3$$

We must now utilize a modified Equation 12.1 since there is only one atom type. There are 8 equivalent atoms per unit cell, and therefore