Molecular Shape

14.9 This problem first of all asks for us to calculate, using Equation 14.11, the average total chain length, L, for a linear polyethylene polymer having a number-average molecular weight of 300,000 g/mol. It is necessary to calculate the number-average degree of polymerization, DP, using Equation 14.6. For polyethylene, from Table 14.3, each repeat unit has two carbons and four hydrogens. Thus,

$$m = 2(A_{\mathrm{C}}) + 4(A_{\mathrm{H}})$$

$$= (2)(12.01 \text{ g/mol}) + (4)(1.008 \text{ g/mol}) = 28.05 \text{ g/mol}$$

and

$$DP = \frac{\overline{M}_n}{m} = \frac{300{,}000 \text{ g/mol}}{28.05 \text{ g/mol}} = 10{,}695$$

which is the number of repeat units along an average chain. Since there are two carbon atoms per repeat unit, there are two C—C chain bonds per repeat unit, which means that the total number of chain bonds in the molecule, N, is just (2)(10,695) = 21,390 bonds. Furthermore, assume that for single carbon-carbon bonds, d = 0.154 nm and θ = 109° (Section 14.4); therefore, from Equation 14.11

$$L = Nd \sin\left(\frac{\theta}{2}\right)$$

$$= (21{,}390)(0.154 \text{ nm})\left[\sin\left(\frac{109°}{2}\right)\right] = 2682 \text{ nm}$$

It is now possible to calculate the average chain end-to-end distance, r, using Equation 14.12 as

$$r = d\sqrt{N} = (0.154 \text{ nm})\sqrt{21{,}390} = 22.5 \text{ nm}$$