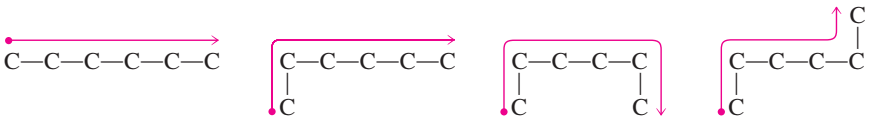
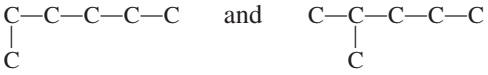


Note that the structures



are not two conformations of the same alkane but, rather, represent two different alkanes. The first structure involves a continuous chain of six carbon atoms, and the second structure involves a continuous chain of five carbon atoms to which a branch is attached. There is no way that you can get a continuous chain of six carbon atoms out of the second structure without "back-tracking," and "back-tracking" is not allowed.

You should learn to recognize molecules drawn in several different ways (conformations). Like friends, they can be recognized whether they are sitting, reclining, or standing.

EXAMPLE 12.1
Recognizing Different Conformations of a Molecule and Constitutional Isomers

Determine whether the members of each of the following pairs of structural formulas represent (1) different conformations of the same molecule, (2) different compounds that are constitutional isomers, or (3) different compounds that are not constitutional isomers.

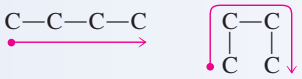
a. $CH_3—CH_2—CH_2—CH_3$ and $\begin{matrix} CH_2—CH_2 \\ | \quad\quad | \\ CH_3 \quad CH_3 \end{matrix}$

b. $\begin{matrix} CH_2—CH_2—CH_3 \\ | \\ CH_3 \end{matrix}$ and $\begin{matrix} CH_2—CH_2—CH_2—CH_3 \\ | \\ CH_3 \end{matrix}$

c. $\begin{matrix} CH_3—CH—CH_3 \\ \quad\quad | \\ \quad\quad CH_3 \end{matrix}$ and $\begin{matrix} CH_3—CH_2—CH_2 \\ \quad\quad\quad\quad | \\ \quad\quad\quad\quad CH_3 \end{matrix}$

Solution

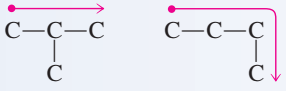
a. Both molecules have the molecular formula C_4H_{10}. The connectivity of carbon atoms is the same for both molecules: a continuous chain of four carbon atoms. For the second structural formula, we need to go around two corners to get a four-carbon-atom chain, which is fine because of the free rotation associated with single bonds in alkanes.



With the same molecular formula and the same connectivity of atoms, these two structural formulas are conformations of the same molecule.

b. The molecular formula of the first compound is C_4H_{10}, and that of the second compound is C_5H_{12}. Thus the two structural formulas represent different compounds that are not constitutional isomers. Constitutional isomers must have the same molecular formula.

c. Both molecules have the same molecular formula, C_4H_{10}. The connectivity of atoms is different. In the first case, we have a chain of three carbon atoms with a branch off the chain. In the second case, a continuous chain of four carbon atoms is present.



These two structural formulas are those of constitutional isomers.