## Practice Exercise 12.3

Draw the condensed structural formula for 4,5-diethyl-3,4,5-trimethyloctane.

Answer:

The following example, which involves determining the structural formulas for and naming of alkane constitutional isomers, serves as a good review of the structural and naming concepts for alkanes considered so far in this chapter.



Determining Structural Formulas for and Naming Alkane Constitutional Isomers Draw skeletal structural formulas for, and assign IUPAC names to, all C<sub>6</sub>H<sub>14</sub> alkane constitutional isomers.

## Solution

Table 12.1 indicates that there are five constitutional isomers with the chemical formula  $C_6H_{14}$ . Part of the purpose of this example is to consider the "thinking pattern" needed to identify these five isomers. There are two concepts embedded in the thinking pattern.

- 1. Carbon chains of varying length are examined for isomerism possibilities, starting with the chain of maximum length and then examining increasingly shorter chain lengths.
- 2. Substituents are added to the various carbon chains, with the number of added carbons determined by the chain length. Various location possibilities for the substituents are examined.

Step 1: A  $C_6$  carbon chain is the longest chain possible; it contains all available carbon atoms.

This is the molecule hexane, the first of the five constitutional isomers. No substituents are added to this chain, as that would increase the carbon count beyond six.

**Step 2:** Decreasing the carbon-chain length by one gives a  $C_5$  chain.

A methyl group must be added to the chain to bring the carbon count back up to six.

Theoretically, there are five possible positions for the methyl group:

These five structures do not represent five new isomers. The first and last structures represent two alternate ways of drawing the molecule hexane, the first isomer. A methyl group (or any alkyl group) added to the end carbons of a carbon chain will always increase the chain length.

The second and third structures do represent new isomers:

$$\begin{array}{cccc} C-C-C-C-C & C-C-C-C-C \\ \downarrow & \downarrow & \\ C & C \\ 2\text{-methylpentane} & 3\text{-methylpentane} \end{array}$$