

Chapter 10 - Introduction to Organic Chemistry: The Alkanes

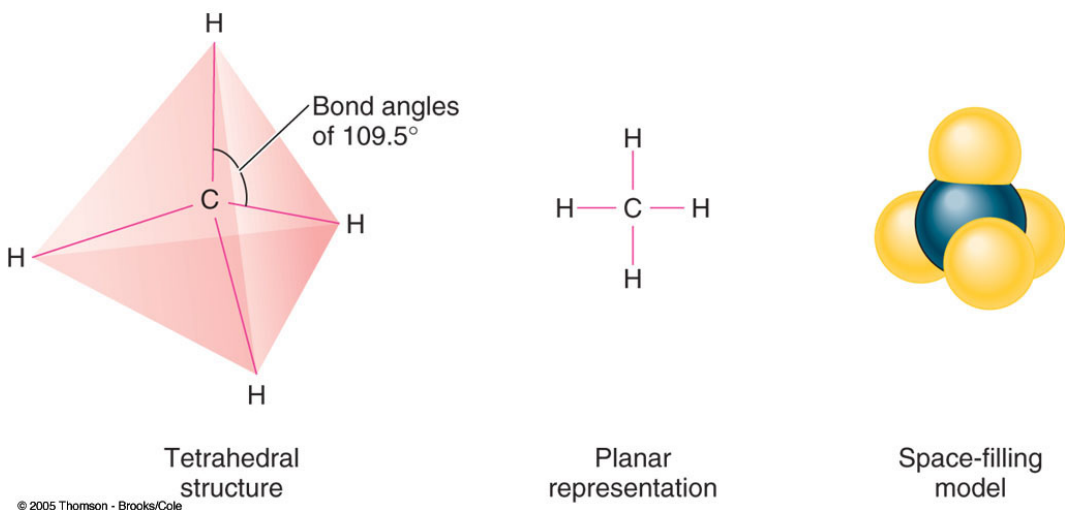
The study of carbon-containing compounds and their properties is called organic chemistry (“organic” originally meant it came from an organism). Organic compounds are the basis of life; **90% of the compounds in the world are organic.**

Organic compounds contain **carbon and hydrogen atoms**, or carbon and hydrogen atoms in combination with a few other types of atoms such as oxygen, nitrogen, and sulfur.

Carbon is singled out for special study because of the ability of C atoms to form strong covalent bonds with one another, as well as many other atoms. This property allows them to join together into straight chains, branched chains, and rings. Nearly infinite numbers of combinations are possible.

The simplest organic compounds are those composed of carbon and hydrogen, and the simplest of these are the alkanes. The simplest alkane is methane, CH_4 , the principle component of natural gas. It consists of a carbon atom with four hydrogen atoms bound to it.

VSEPR theory (Chapter 4) predicts this molecule will have a tetrahedral arrangement of the atoms to minimize repulsive forces of the hydrogen atoms.

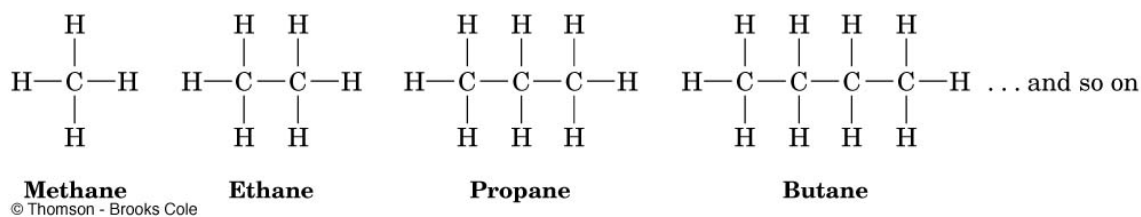


Alkanes are referred to as “saturated” hydrocarbons, because each carbon atom is bound to four other atoms. Hydrocarbons containing multiple bonds are called “unsaturated” hydrocarbons (see chapter 11).

Alkanes have the general formula: $\text{C}_n\text{H}_{2n+2}$.

The next alkane, containing two carbon atoms, is ethane: C_2H_6 .

The next two alkanes after ethane are the straight chain alkanes propane (C₃H₈) and butane (C₄H₁₀). All are represented by complete structural formulas showing all the bonds as shown below.



The first four single chain alkanes employ the common names given above.

Starting with the five-carbon alkane, the IUPAC naming system employing Greek numerical prefixes is used to name subsequent alkanes.

<u># of Carbons</u>	<u>Root Name</u>
1	meth-
2	eth-
3	prop-
4	but-
5	pent-
6	hex-
7	hept-
8	oct-
9	non-
10	dec-

Note that in addition to writing the complete structural formula, these compounds can be written in two other ways:

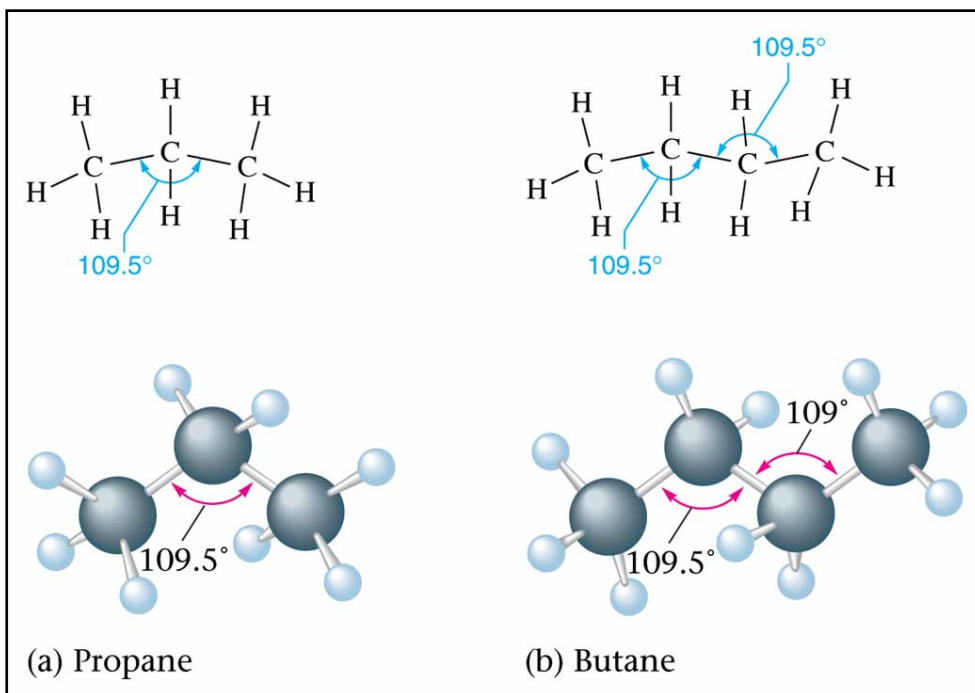
- A **condensed** structural formula list all the atoms in order implying how they are bound together: CH₃-(CH₂)_n-CH₃. For example, the single chain hydrocarbon hexane can be written as CH₃-(CH₂)₄-CH₃.
- A **molecular** formula: C_nH_{2n+2}. Thus, hexane can be written as C₆H₁₄.

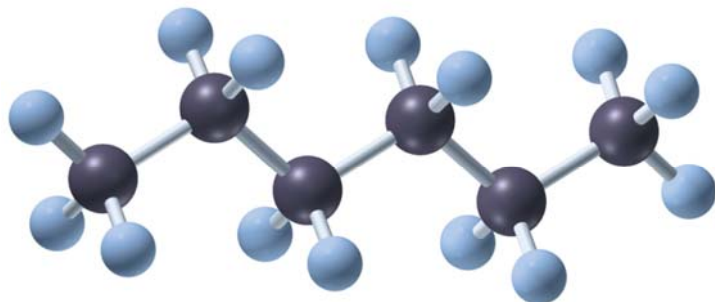
TABLE 10.2 IUPAC Names for the First Ten Alkanes

Number of Carbon Atoms	Prefix	Name	Molecular Formula	Condensed Structural Formula
1	Meth	Methane	CH ₄	CH ₄
2	Eth	Ethane	C ₂ H ₆	CH ₃ —CH ₃
3	Prop	Propane	C ₃ H ₈	CH ₃ —CH ₂ —CH ₃
4	But	Butane	C ₄ H ₁₀	CH ₃ —CH ₂ —CH ₂ —CH ₃
5	Pent	Pentane	C ₅ H ₁₂	CH ₃ —CH ₂ —CH ₂ —CH ₂ —CH ₃
6	Hex	Hexane	C ₆ H ₁₄	CH ₃ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₃
7	Hept	Heptane	C ₇ H ₁₆	CH ₃ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₃
8	Oct	Octane	C ₈ H ₁₈	CH ₃ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₃
9	Non	Nonane	C ₉ H ₂₀	CH ₃ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₃
10	Dec	Decane	C ₁₀ H ₂₂	CH ₃ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —CH ₃

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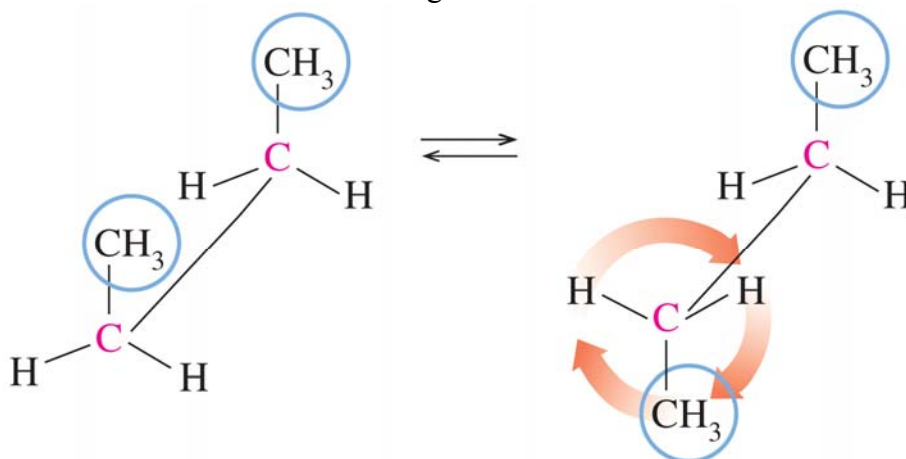
Note that when there are three or more carbons, the molecule does not maintain a straight-line arrangement, despite writing the condensed formulas that way above. That's because the tetrahedral C-C-C bond angle is 109.5°, so these single chain molecules must take a zig-zag three dimensional shape to maintain this bond angle:





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Because the carbon-carbon bonds are single bonds, they can freely rotate, so the attached groups are not in fixed positions. Thus, for butane, one can easily envision two very different three-dimensional arrangements to this molecule:



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Indeed, an infinite number of positional variations are possible, all with the same molecular / structural formula. However, steric interference (interaction) between various parts of the molecule limit the positional variations to favor only a very few.







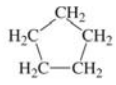
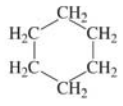




Cycloalkanes

Cycloalkanes are alkanes that have carbon atoms that form a ring. Simple cycloalkanes are rings of CH_2 units, $(\text{CH}_2)_n$, or C_nH_{2n} , so they have two fewer hydrogen atoms.

In addition to ball and stick models, and condensed structural formulas, these molecules can also be represented by simple geometric shapes or formulas.

Naming these compounds begins with the prefix cyclo-, followed by the name of the corresponding alkane.

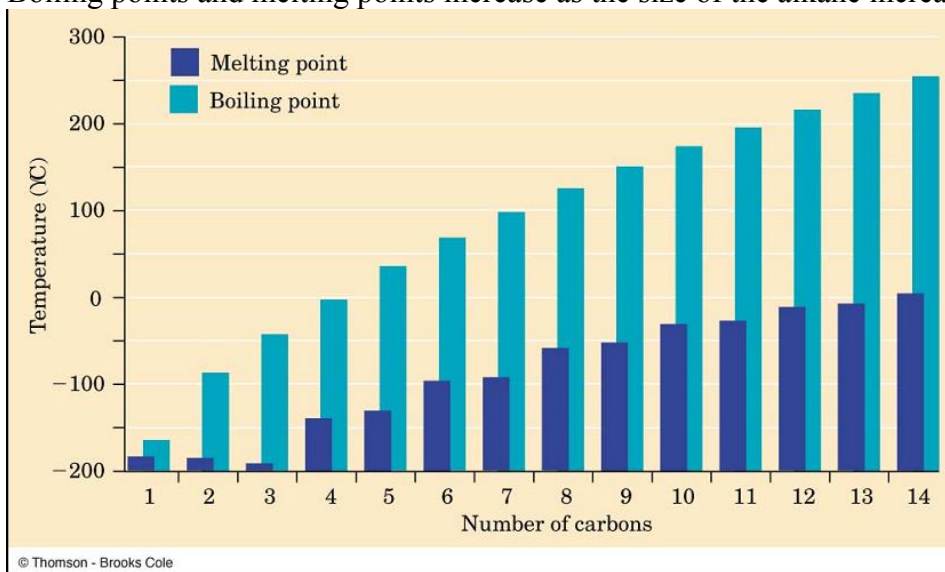
TABLE 10.5 Formulas of Some Common Cycloalkanes

Ball-and-Stick Models			
			
Condensed Structural Formula			
			
Geometric Formula			
			
Name			
Cyclopropane	Cyclobutane	Cyclopentane	Cyclohexane

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Properties as a Function of Size

Boiling points and melting points increase as the size of the alkane increases



Alkanes: Number of Carbons	Properties
1-4 carbon atoms	<ul style="list-style-type: none"> • methane, ethane, propane, and butane. • Gases at room temperature. • Used for heating

5-8 carbon atoms	<ul style="list-style-type: none"> Liquids at room temperature. pentane, hexane, heptane, and octane. Very volatile. Used to make gasoline
9-17 carbon atoms	<ul style="list-style-type: none"> Liquids at room temperature Higher boiling points. Found in kerosene, diesel, and jet fuels
18 or more carbon atoms	<ul style="list-style-type: none"> High molar masses. Waxy solids at room temperature. Used in waxy coatings of fruits and vegetables.

Properties: Organic and Inorganic Compounds Compared

TABLE 10.1 Some Properties of Organic and Inorganic Compounds

Property	Organic	Example: C ₃ H ₈	Inorganic	Example: NaCl
Elements	C and H, sometimes O, S, N, or Cl	C and H	Most metals and nonmetals	Na and Cl
Particles	Molecules	C ₃ H ₈	Mostly ions	Na ⁺ and Cl ⁻
Bonding	Mostly covalent	Covalent (4 bonds to each C)	Many are ionic, some covalent	Ionic
Polarity of bonds	Nonpolar, unless a more electronegative atom is present	Nonpolar	Most are ionic or polar covalent, a few are nonpolar covalent	Ionic
Melting point	Usually low	-188 °C	Usually high	801 °C
Boiling point	Usually low	-42 °C	Usually high	1413 °C
Flammability	High	Burns in air	Low	Does not burn
Solubility in water	Not soluble, unless a polar group is present	No	Most are soluble, unless nonpolar	Yes

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10.3 Alkanes with Substituents

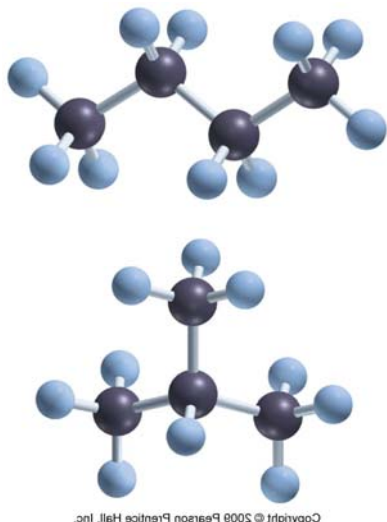
Skeletal Isomerism

For an alkane with four or more carbons, is possible for **more than one structural formula** to correspond to the identical molecular formula. We refer to such structural variations as skeletal isomers.

Skeletal isomerism occurs when two molecules have the same number of atoms, but a different arrangement of the bonds.

For example, here are the two possible condensed structural formulas for C₄H₁₀ (butane):

- CH₃CH₂CH₂CH₃
- (CH₃)₂CHCH₃



These two **isomers** have identical chemical formulas (C_4H_{10}), but major differences in the three-dimensional molecular structure.

The isomeric alkane can be viewed as having a side group or **substituent** attached to a carbon chain. A naming convention must be devised to accurately indicate which C_4H_{10} molecule is being referred to.

- The linear or “straight chain” molecule is referred to as “normal” butane, or **n-butane**
- The butane isomer or “branched chain” molecule above has a common name: **iso-butane**
- IUPAC name: The butane isomer could also be viewed as propane with a methyl group substituent attached. The IUPAC name for iso-butane is **2-methylpropane** (see naming convention below).

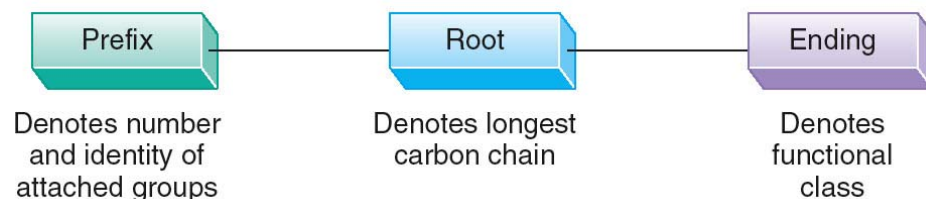
Note that the molecule methane (CH_4) with one hydrogen group removed has the **–ane** ending of the name changed to **–yl** to indicate that it is a substituent group covalently bound and not a separate molecule. Other examples of constituent groups are given in table 10.6 below.

TABLE 10.6 Names and Formulas of Some Common Substituents

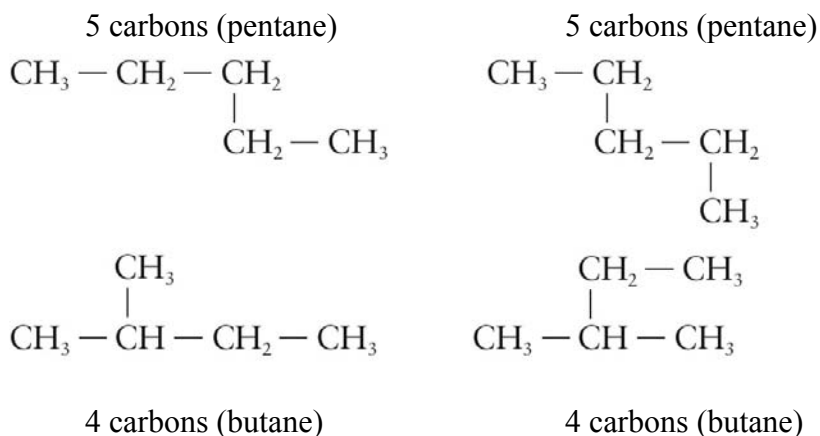
Substituent	Name
CH ₃ —	Methyl
CH ₃ —CH ₂ —	Ethyl
CH ₃ —CH ₂ —CH ₂ —	Propyl
$\begin{array}{c} \\ \text{CH}_3\text{—CH—CH}_3 \end{array}$	Isopropyl
F—, Cl—, Br—, I—	Fluoro, chloro, bromo, iodo

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Rules for Naming Alkanes with Substituents



Step 1. Identify the longest chain of carbon atoms and determine its alkane name, e.g.



Step 2. Number the carbon atoms of the longest chain beginning from the end closest to the substituent group, in order to identify the number of the carbon atom with the substituent attached.

Step 3. Give the location and name of each alkyl or other substituent in alphabetical order as a prefix to the name of the main alkane chain.

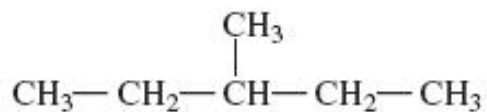
Common alkyl groups

Parent alkane	Structure of parent alkane	Structure of alkyl group	Name of alkyl group
methane	CH ₄	CH ₃ —	methyl
ethane	CH ₃ CH ₃	CH ₃ CH ₂ —	ethyl
propane	CH ₃ CH ₂ CH ₃	CH ₃ CH ₂ CH ₂ —	propyl
		$\begin{array}{c} \\ \text{CH}_3\text{CHCH}_3 \end{array}$	isopropyl
<i>n</i> -butane	CH ₃ CH ₂ CH ₂ CH ₃	CH ₃ CH ₂ CH ₂ CH ₂ —	butyl
		$\begin{array}{c} \\ \text{CH}_3\text{CH}_2\text{CHCH}_3 \end{array}$	<i>sec</i> -butyl (secondary-butyl)
isobutane	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3\text{CHCH}_3 \end{array}$	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3\text{CHCH}_2\text{—} \end{array}$	isobutyl
		$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3\text{CCH}_3 \\ \end{array}$	<i>t</i> -butyl (tertiary-butyl)

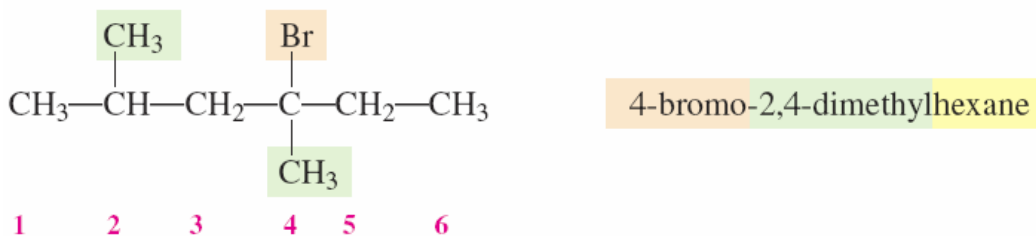
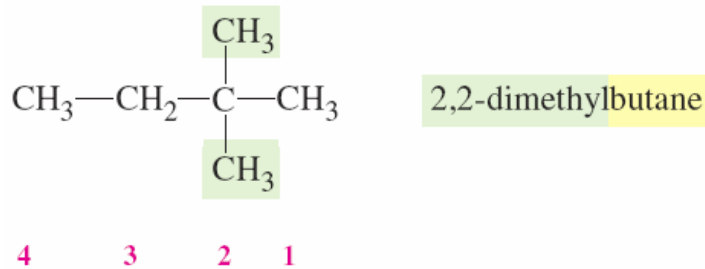
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Step 4. If the same alkyl group, or other species, appears more than once, indicate the number of appearances by di-, tri-, tetra-, etc., and show the location of each branch by number

Examples



3 – methyl pentane



Positional Isomers

n – pentane with a bromine substituent can have three possible isomers, all with the same chemical formula, $\text{C}_5\text{H}_{11}\text{Br}$, depending on which carbon in the chain the substituent is attached to:

- 1-bromopentane
- 2-bromopentane
- 3-bromopentane

10.4 Properties of Alkanes

A review of the electronegativity values for carbon and hydrogen reveals that these bonds – and therefore alkane hydrocarbons – are very **non-polar**. Since “like dissolves like”, alkanes are not soluble in polar substances, e.g. water.

Only the weakly attractive intermolecular forces (IMF) are in effect, therefore, small alkanes such as methane (CH_4), ethane (C_2H_6), propane (C_3H_8) and butane (C_4H_{10}) are gases at room temperature.

Alkanes with 5 – 8 carbons are liquids at room temperature, but with very low boiling points making them very volatile. With additional carbons, the alkane molecules are less volatile and these liquids become more dense and flow sluggishly.

Alkanes with 18 or more carbons are waxy solids at room temperature.

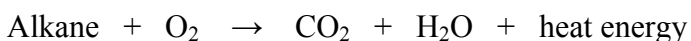
TABLE 10.7 Typical Alkane Mixtures Obtained by Distillation of Crude Oil

Distillation Temperatures (°C)	Number of Carbon Atoms	Product
Below 30	1–4	Natural gas
30–200	5–12	Gasoline
200–250	12–16	Kerosene, jet fuel
250–350	15–18	Diesel fuel, heating oil
350–450	18–25	Lubricating oil
Nonvolatile residue	Over 25	Asphalt, tar

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Chemical Reactivity:

The C – C and C – H chemical bonds are relatively strong. That makes alkanes fairly unreactive at room temperature. This makes them good lubricants such as motor oils, where they operate in a high temperature environment. However, at sufficiently high temperatures, alkanes react vigorously and completely with oxygen in a combustion reaction:



Problem: Write the balanced equation for the complete combustion of

