Organic Chemistry I

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Organic Chemistry, (9th edition)

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2. Organic Compounds: Alkanes

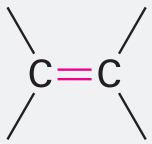
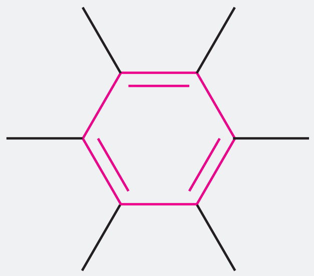
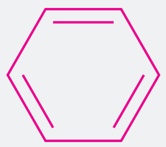
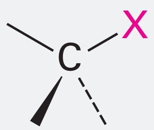
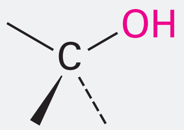
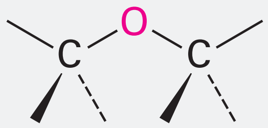
The structural features that make it possible to **classify compounds into families** are called ***functional groups***.

A **functional group** is a group of atoms within a molecule that has a characteristic chemical behavior.

Chemically, a given functional group behaves in nearly the same way in every molecule it's a part of.

The chemistry of every organic molecule, regardless of size and complexity, is determined by the functional groups it contains.

TABLE 3-1 Structures of Some Common Functional Groups

Name	Structure*	Name ending	Example
Alkene (double bond)		*-ene*	$H_2C{=}CH_2$ Ethene
Alkyne (triple bond)	$—C{\equiv}C—$	*-yne*	$HC{\equiv}CH$ Ethyne
Arene (aromatic ring)		None	 Benzene
Halide	 (X = F, Cl, Br, I)	None	CH_3Cl Chloromethane
Alcohol		*-ol*	CH_3OH Methanol
Ether		*ether*	CH_3OCH_3 Dimethyl ether

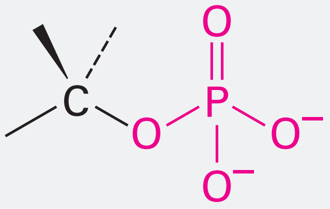
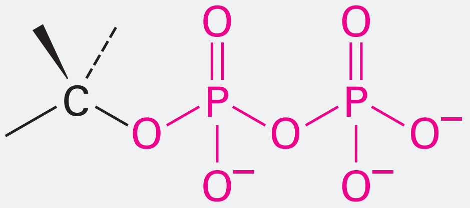
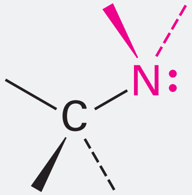
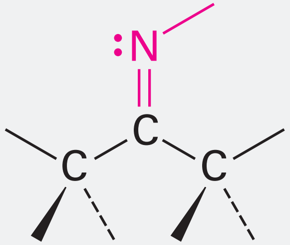
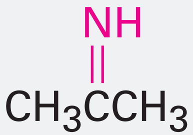
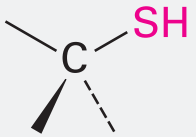
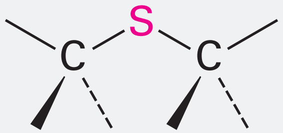
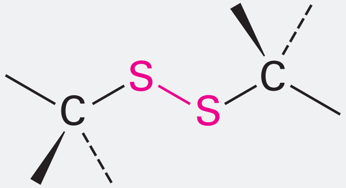
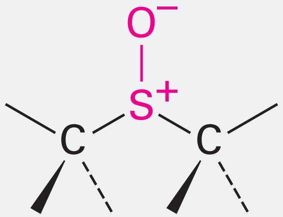
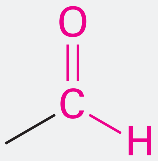
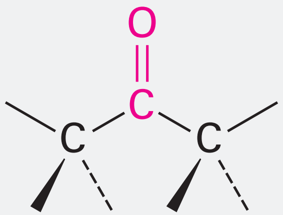
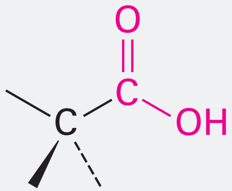
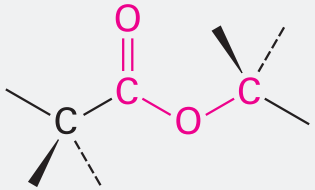
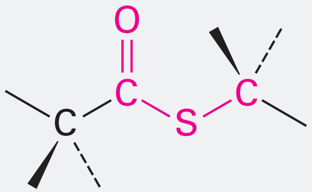
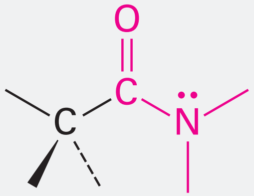
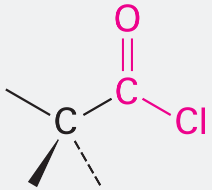
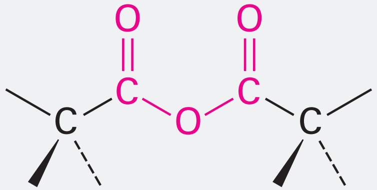
Monophosphate		*phosphate*	$CH_3OPO_3^{2-}$ Methyl phosphate
Diphosphate		*diphosphate*	$CH_3OP_2O_6^{3-}$ Methyl diphosphate
Amine		*-amine*	CH_3NH_2 Methylamine
Imine (Schiff base)		None	 Acetone imine
Nitrile	—C≡N	*-nitrile*	$CH_3C{\equiv}N$ Ethanenitrile
Thiol		*-thiol*	CH_3SH Methanethiol

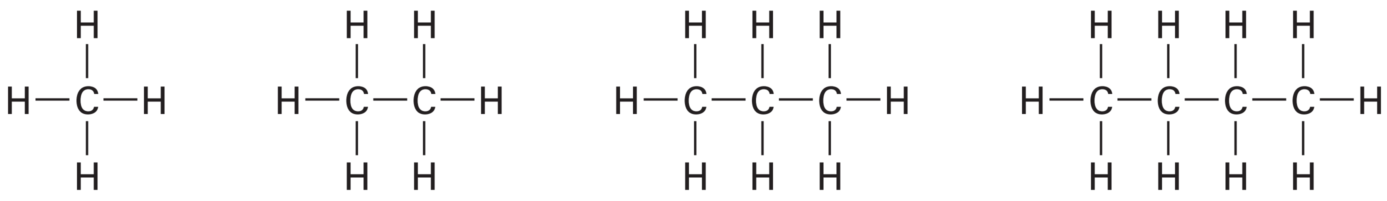
TABLE 3-1 Structures of Some Common Functional Groups *(continued)*

Name	Structure*	Name ending	Example
Sulfide		*sulfide*	CH_3SCH_3 Dimethyl sulfide
Disulfide		*disulfide*	CH_3SSCH_3 Dimethyl disulfide
Sulfoxide		*sulfoxide*	$CH_3\overset{\overset{O^-}{\vert}}{S^+}CH_3$ Dimethyl sulfoxide
Aldehyde		*-al*	$CH_3\overset{\overset{O}{\Vert}}{C}H$ Ethanal
Ketone		*-one*	$CH_3\overset{\overset{O}{\Vert}}{C}CH_3$ Propanone

Carboxylic acid		*-oic acid*	$CH_3\overset{O}{\overset{\|}{C}}OH$ Ethanoic acid
Ester		*-oate*	$CH_3\overset{O}{\overset{\|}{C}}OCH_3$ Methyl ethanoate
Thioester		*-thioate*	$CH_3\overset{O}{\overset{\|}{C}}SCH_3$ Methyl ethanethioate
Amide		*-amide*	$CH_3\overset{O}{\overset{\|}{C}}NH_2$ Ethanamide
Acid chloride		*-oyl chloride*	$CH_3\overset{O}{\overset{\|}{C}}Cl$ Ethanoyl chloride
Carboxylic acid anhydride		*-oic anhydride*	$CH_3\overset{O}{\overset{\|}{C}}O\overset{O}{\overset{\|}{C}}CH_3$ Ethanoic anhydride

Alkanes and Alkane Isomers

The carbon–carbon single bond in alkanes results from σ (head-on) overlap of carbon sp^3 hybrid orbitals. If we imagine joining three, four, five, or even more carbon atoms by C–C single bonds, we can generate the large family of molecules called **alkanes**.



. . . and so on

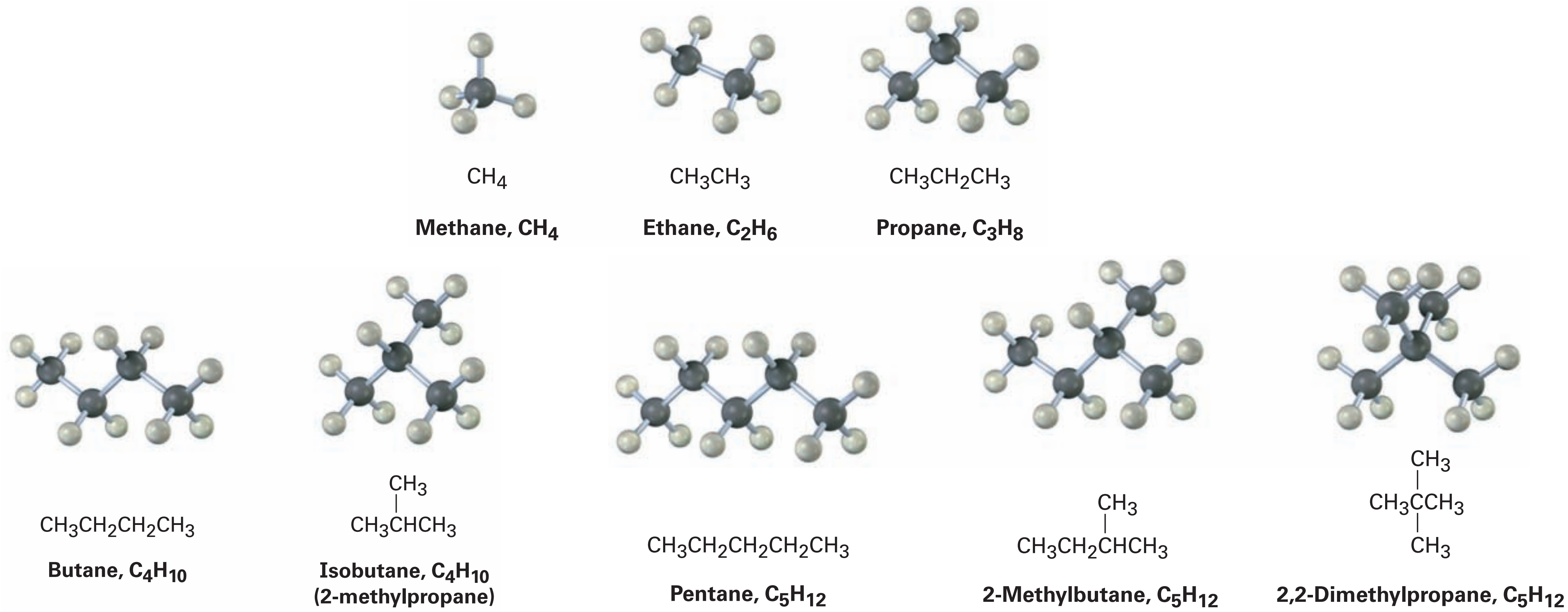
Methane **Ethane** **Propane** **Butane**

Alkanes are often described as *saturated hydrocarbons:* **hydrocarbons** because they contain only carbon and hydrogen; **saturated** because they have only C–C and C–H single bonds and thus contain the maximum possible number of hydrogens per carbon.

They have the general formula C_nH_{2n+2}, where n is an integer. Alkanes are also occasionally called **aliphatic** compounds, a name derived from the Greek *aleiphas,* meaning “fat.”

With one carbon and four hydrogens, only one structure is possible: methane, CH_4. Similarly, there is only one combination of two carbons with six hydrogens (ethane, CH_3CH_3) and only one combination of three carbons with eight hydrogens (propane, $CH_3CH_2CH_3$).

When larger numbers of carbons and hydrogens combine, more than one structure is possible. There are *two* substances with the formula C_4H_{10}: four carbons in a row (butane), or they can branch (isobutane). There are three C_5H_{12} molecules, and so on for larger alkanes.



Compounds like butane and pentane, whose carbons are all connected in a row, are called **straight-chain alkanes**, or *normal alkanes.*

Compounds like 2-methylpropane (isobutane), 2-methylbutane, and 2,2-dimethylpropane, whose carbon chains branch, are called **branched-chain alkanes**.

Isomers: compounds like the two C_4H_{10} molecules and the three C_5H_{12} molecules, which have the same formula but different structures. They are called from the Greek *isos* + *meros,* meaning "made of the same parts."

Isomers are compounds that have the same numbers and kinds of atoms but differ in the way the atoms are arranged.

Compounds like butane and isobutane, whose atoms are connected differently, are called **constitutional isomers**.

The number of possible alkane isomers increases dramatically with the number of carbon atoms.

Constitutional isomerism is not limited to alkanes. Different functional groups (as in ethanol and dimethyl ether), or different locations of a functional group along the chain (as in isopropylamine and propylamine).

Different carbon skeletons **C_4H_{10}**	$CH_3\overset{\overset{CH_3}{\vert}}{C}HCH_3$ **2-Methylpropane (isobutane)**	and	$CH_3CH_2CH_2CH_3$ **Butane**
Different functional groups **C_2H_6O**	CH_3CH_2OH **Ethanol**	and	CH_3OCH_3 **Dimethyl ether**
Different position of functional groups **C_3H_9N**	$CH_3\overset{\overset{NH_2}{\vert}}{C}HCH_3$ **Isopropylamine**	and	$CH_3CH_2CH_2NH_2$ **Propylamine**

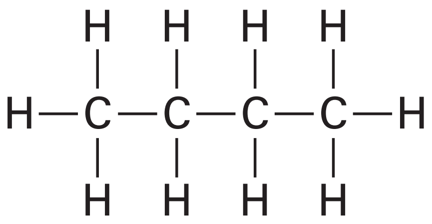
TABLE 3-2 Number of Alkane Isomers

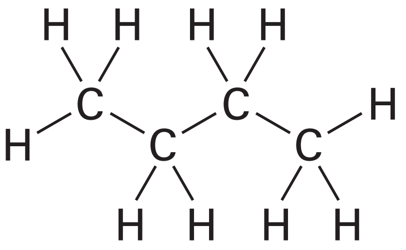
Formula	Number of isomers
C_6H_{14}	5
C_7H_{16}	9
C_8H_{18}	18
C_9H_{20}	35
$C_{10}H_{22}$	75
$C_{15}H_{32}$	4347
$C_{20}H_{42}$	366,319
$C_{30}H_{62}$	4,111,846,763

Regardless of the reason for the isomerism, constitutional isomers are always different compounds with different properties but with the same formula.

A given alkane can be drawn in many ways. For example, the straight-chain, four-carbon alkane called butane can be represented by any of the structures shown in below.

Still more simply, butane can be represented as *n*-C_4H_{10}, where *n* denotes *normal* (straight-chain) butane.





$CH_3—CH_2—CH_2—CH_3$ $CH_3CH_2CH_2CH_3$ $CH_3(CH_2)_2CH_3$

Straight-chain alkanes are named according to the number of carbon atoms they contain.

With the exception of the first four compounds—methane, ethane, propane, and butane—whose names have historical roots, the alkanes are named based on Greek numbers.

The suffix ***-ane*** is added to the end of each name to indicate that the molecule identified is an alkane.

TABLE 3-3 Names of Straight-Chain Alkanes

Number of carbons (n)	Name	Formula (C_nH_{2n+2})	Number of carbons (n)	Name	Formula (C_nH_{2n+2})
1	Methane	CH_4	9	Nonane	C_9H_{20}
2	Ethane	C_2H_6	10	Decane	$C_{10}H_{22}$
3	Propane	C_3H_8	11	Undecane	$C_{11}H_{24}$
4	Butane	C_4H_{10}	12	Dodecane	$C_{12}H_{26}$
5	Pentane	C_5H_{12}	13	Tridecane	$C_{13}H_{28}$
6	Hexane	C_6H_{14}	20	Icosane	$C_{20}H_{42}$
7	Heptane	C_7H_{16}	30	Triacontane	$C_{30}H_{62}$
8	Octane	C_8H_{18}			