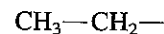


TABLE 2-4		Branched Alkyl Groups		
Structure	Common name	Example of common name in use	Systematic name	Designation
$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3-\text{C}- \\ \\ \text{H} \end{array}$	Isopropyl	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3-\text{C}-\text{Cl} \text{ (Isopropyl chloride)} \\ \\ \text{H} \end{array}$	1-Methylethyl	Secondary
$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3-\text{C}-\text{CH}_2- \\ \\ \text{H} \end{array}$	Isobutyl	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3-\text{C}-\text{CH}_3 \text{ (Isobutane)} \\ \\ \text{H} \end{array}$	2-Methylpropyl	Primary
$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3-\text{CH}_2-\text{C}- \\ \\ \text{H} \end{array}$	<i>sec</i> -Butyl	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3-\text{CH}_2-\text{C}-\text{NH}_2 \text{ (} \textit{sec}\text{-Butyl amine)} \\ \\ \text{H} \end{array}$	1-Methylpropyl	Secondary
$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3-\text{C}- \\ \\ \text{CH}_3 \end{array}$	<i>tert</i> -Butyl	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3-\text{C}-\text{Br} \text{ (} \textit{tert}\text{-Butyl bromide)} \\ \\ \text{CH}_3 \end{array}$	1,1-Dimethylethyl	Tertiary
$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3-\text{C}-\text{CH}_2- \\ \\ \text{CH}_3 \end{array}$	Neopentyl	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3-\text{C}-\text{CH}_2-\text{OH} \text{ (Neopentyl alcohol)} \\ \\ \text{CH}_3 \end{array}$	2,2-Dimethylpropyl	Primary

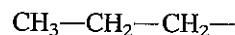
Alkyl groups



Methyl



Ethyl



Propyl

As mentioned in Section 2-2, an **alkyl** group is formed by the removal of a hydrogen from an alkane. It is named by replacing the ending -ane in the corresponding alkane by -yl, as in methyl, ethyl, and propyl. Table 2-4 shows a few branched alkyl groups having common names. Note that some use the prefixes *sec*- (or *s*-), which stands for secondary, and *tert*- (or *t*-), for tertiary. To apply these prefixes, we must first see how to classify carbon atoms in organic molecules. A **primary** carbon is one attached to only one other carbon atom. For example, all carbon atoms at the ends of alkane chains are primary. The hydrogens attached to such carbons are designated primary hydrogens, and an alkyl group created by removing a primary hydrogen also is called primary. A **secondary** carbon is attached to two other carbon atoms, and a **tertiary** carbon to three others. Their hydrogens are labeled similarly. As shown in Table 2-4, removal of a secondary hydrogen results in a secondary alkyl group, and removal of a tertiary hydrogen in a tertiary alkyl group. Finally, a carbon bearing four alkyl groups is called **quaternary**.

Primary, Secondary, and Tertiary Carbons and Hydrogens

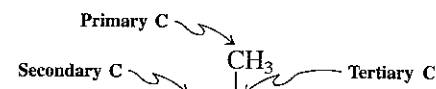


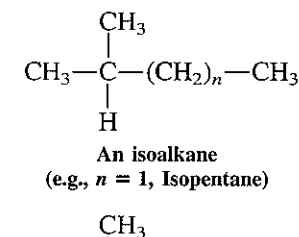
TABLE 2-3 Names and Physical Properties of Straight-Chain Alkanes, C_nH_{2n+2}

n	Name	Formula	Boiling point (°C)	Melting point (°C)	Density at 20°C (g ml ⁻¹)
1	Methane	CH ₄	-161.7	-182.5	0.466 (at -164°C)
2	Ethane	CH ₃ CH ₃	-88.6	-183.3	0.572 (at -100°C)
3	Propane	CH ₃ CH ₂ CH ₃	-42.1	-187.7	0.5853 (at -45°C)
4	Butane	CH ₃ CH ₂ CH ₂ CH ₃	-0.5	-138.3	0.5787
5	Pentane	CH ₃ (CH ₂) ₃ CH ₃	36.1	-129.8	0.6262
6	Hexane	CH ₃ (CH ₂) ₄ CH ₃	68.7	-95.3	0.6603
7	Heptane	CH ₃ (CH ₂) ₅ CH ₃	98.4	-90.6	0.6837
8	Octane	CH ₃ (CH ₂) ₆ CH ₃	125.7	-56.8	0.7026
9	Nonane	CH ₃ (CH ₂) ₇ CH ₃	150.8	-53.5	0.7177
10	Decane	CH ₃ (CH ₂) ₈ CH ₃	174.0	-29.7	0.7299
11	Undecane	CH ₃ (CH ₂) ₉ CH ₃	195.8	-25.6	0.7402
12	Dodecane	CH ₃ (CH ₂) ₁₀ CH ₃	216.3	-9.6	0.7487
13	Tridecane	CH ₃ (CH ₂) ₁₁ CH ₃	235.4	-5.5	0.7564
14	Tetradecane	CH ₃ (CH ₂) ₁₂ CH ₃	253.7	5.9	0.7628
15	Pentadecane	CH ₃ (CH ₂) ₁₃ CH ₃	270.6	10	0.7685
16	Hexadecane	CH ₃ (CH ₂) ₁₄ CH ₃	287	18.2	0.7733
17	Heptadecane	CH ₃ (CH ₂) ₁₅ CH ₃	301.8	22	0.7780
18	Octadecane	CH ₃ (CH ₂) ₁₆ CH ₃	316.1	28.2	0.7768
19	Nonadecane	CH ₃ (CH ₂) ₁₇ CH ₃	329.7	32.1	0.7855
20	Icosane	CH ₃ (CH ₂) ₁₈ CH ₃	343	36.8	0.7886



Propane, stored under pressure in liquefied form in canisters such as these, is a common fuel for torches, lanterns, and outdoor cooking stoves.

word *hepta*, seven, and the Latin word *decem*, ten. The first four alkanes have special names that have been accepted as part of the systematic nomenclature but also all end in **-ane**. It is important to know these names, because they serve as the basis for naming a large fraction of all organic molecules. A few smaller branched alkanes have common names that still have widespread use. They make use of the prefixes **iso-**



Typical Values of Proton NMR Chemical Shifts	
Type of proton	Approximate δ
alkane	($-\text{CH}_3$) 0.9
	($-\text{CH}_2-$) 1.3
	($-\text{CH}-$) 1.4
$\begin{array}{c} \text{O} \\ \parallel \\ -\text{C}-\text{CH}_3 \end{array}$	2.1
$-\text{C}\equiv\text{C}-\text{H}$	2.5
$\text{R}-\text{CH}_2-\text{X}$ (X = halogen, $-\text{O}-$)	3-4
$\begin{array}{c} & \\ -\text{C}=\text{C}-\text{H} \end{array}$	5-6
$\begin{array}{c} & \\ -\text{C}=\text{C}-\text{CH}_3 \end{array}$	1.7
Ph-H	7.2
Ph- CH_3	2.3
R-CHO	9-10
R-COOH	10-12
R-OH	variable, about 2-5
Ar-OH	variable, about 4-7
R-NH ₂	variable, about 1.5-4

These values are approximate, because all chemical shifts are affected by neighboring substituents. The numbers given here assume that alkyl groups are the only other substituents present. A more complete table of chemical shifts appears in Appendix 1.

Summary of Functional Group Nomenclature		
Functional Group	Name as Main Group	Name as Substituent
<i>Main groups in order of decreasing priority</i>		
carboxylic acids	-oic acid	carboxy ^a
esters	-oate	alkoxycarbonyl ^a
amides	-amide	amido ^a
nitriles	-nitrile	cyano
aldehydes	-al	formyl
ketones	-one	oxo
alcohols	-ol	hydroxy
amines	-amine	amino
alkenes	-ene	alkenyl
alkynes	-yne	alkynyl
alkanes	-ane	alkyl
ethers		alkoxy
halides		halo

^a Denotes rare usage.

Typical Values of IR Stretching Frequencies		
Frequency	Functional group	Comments
3300 cm^{-1}	alcohol O-H	Always broad.
	amine, amide N-H	May be broad, sharp, or broad with spikes.
	alkyne $\equiv\text{C}-\text{H}$	Always sharp.
3000 cm^{-1}	alkane C-H	Alkane $\begin{array}{c} \diagup \\ \text{C}-\text{H} \\ \diagdown \end{array}$ just below 3000 cm^{-1} .
	alkene C-H	Alkene $\begin{array}{c} \text{=C}-\text{H} \\ \end{array}$ just above 3000 cm^{-1} .
	acid O-H	Very broad, 2500-3500 cm^{-1} .
2200 cm^{-1}	alkyne $-\text{C}\equiv\text{C}-$	Alkyne $\text{C}\equiv\text{C}$ just below 2200 cm^{-1} .
	nitrile $-\text{C}\equiv\text{N}$	Nitrile $\text{C}\equiv\text{N}$ just above 2200 cm^{-1} .
1710 cm^{-1}	$\begin{array}{c} \diagup \\ \text{C}=\text{O} \\ \diagdown \end{array}$ (very strong)	Ketones, aldehydes, acids. Esters higher, about 1735 cm^{-1} . Conjugation lowers frequency. Amides lower, about 1650 cm^{-1} .