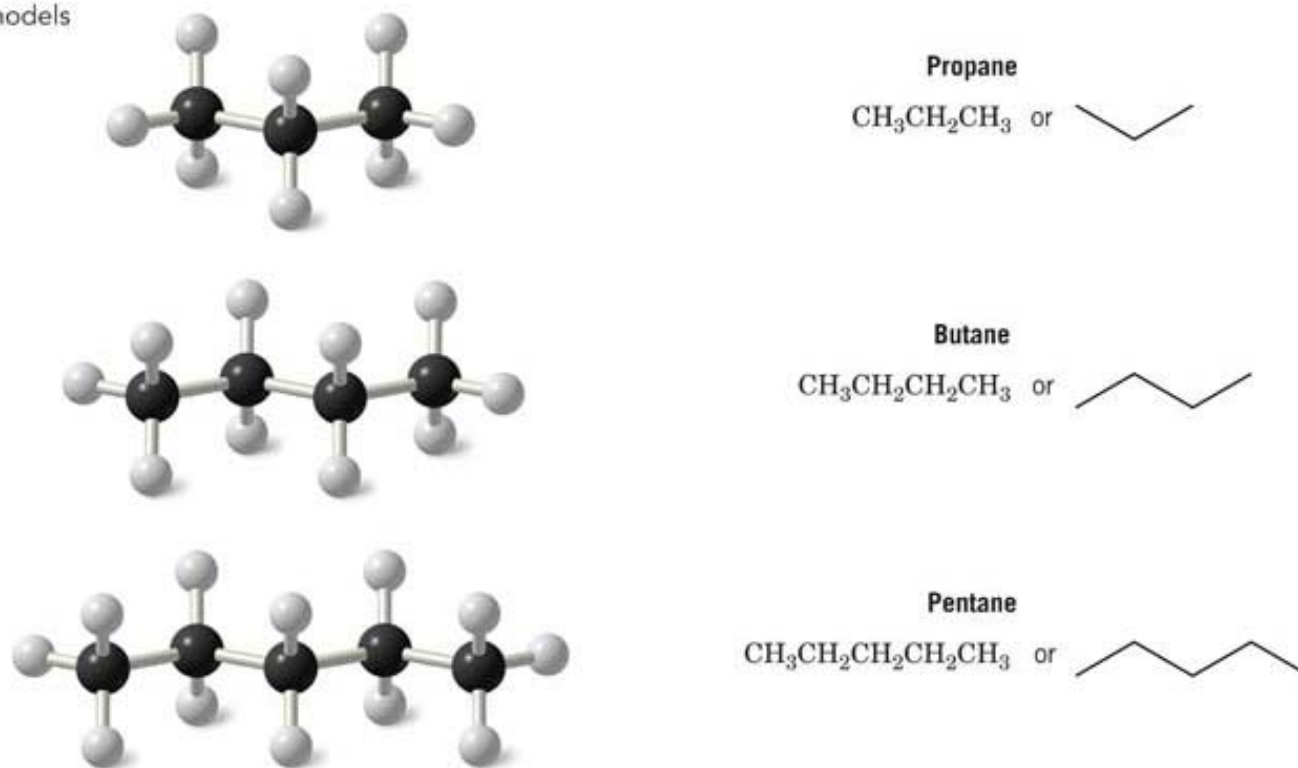


Section 2--Shapes of Alkanes

Shapes of Alkanes

Alkanes assume shapes imposed by the tetrahedral geometry at each carbon atom. Even "straight-chain" alkanes are not straight. The alkane chains take on a zigzag geometry.

FIGURE 4.1 Ball-and-stick models for three simple alkanes.



Constitutional Isomers

Butane and isobutane have the same molecular formula, C_4H_{10} , but different **bond connectivities**. Such compounds are called **constitutional isomers**.

From C_4 and higher, alkanes exist as constitutional isomers. The number of constitutional isomers goes up rapidly with the carbon number, as shown in the table below.

Constitutional Isomers	
Molecular Formula	Number of Isomers
C_4H_{10}	2
C_5H_{12}	3
C_6H_{14}	5
C_7H_{16}	9
C_8H_{18}	18
C_9H_{20}	35
$C_{10}H_{22}$	75
.	.
.	.
$C_{20}H_{42}$	366,319

**Section 3--IUPAC Nomenclature of Alkanes, Alkyl Halides
and Alcohols**

A Systematic Naming System

Because of the dramatic increase in C-C connectivity possibilities with increasing carbon number, it is necessary to have a systematic naming system that unambiguously identifies the carbon structure. The **IUPAC Nomenclature System** (described below) serves this need.

Common Names

Simpler organic compounds (C_4 or smaller) are often named by common or trivial names that go back hundreds of years. Because these names specifically refer to widely used compounds, there is no ambiguity. Larger structures require a systematic name.

IUPAC Names

In 1892, the International Union of Pure and Applied Chemistry proposed the systematic nomenclature system still in use today. Over the years, it has been revised. The IUPAC naming method is closely linked to structure, and is able to give a unique name to each of the known 7 million or more organic compounds.

IUPAC Core Names

The core of IUPAC names are the names of unbranched alkanes. It is important to know these names through $C_{10}H_{22}$. The first four alkane names are not systematic and must be memorized. Beginning with pentane (C_5H_{12}), the names are systematic.

Alkyl Groups and their Names

The removal of **one terminal hydrogen** from an **unbranched alkane** produces an **alkyl group**. The name of the alkyl group is derived from the alkane name by dropping the "ane" and adding "yl." Examples are shown in the table below.

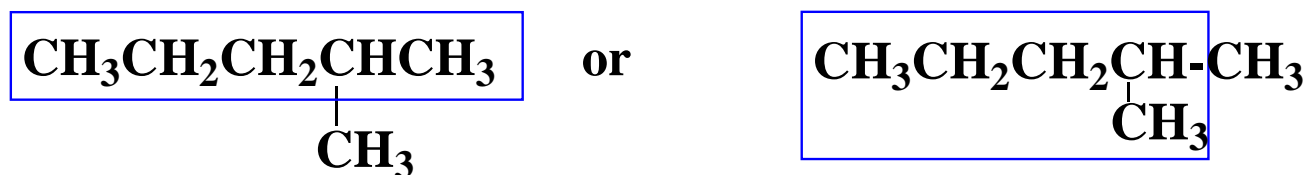
alkane	alkyl group	abbreviation
CH_3-H methane	CH_3^- methyl	Me ⁻
CH_3CH_2-H ethane	$CH_3CH_2^-$ ethyl	Et ⁻
$CH_3CH_2CH_2-H$ propane	$CH_3CH_2CH_2^-$ propyl	Pr ⁻
$CH_3CH_2CH_2CH_2-H$ butane	$CH_3CH_2CH_2CH_2^-$ butyl	Bu ⁻

Alkyl Group Names

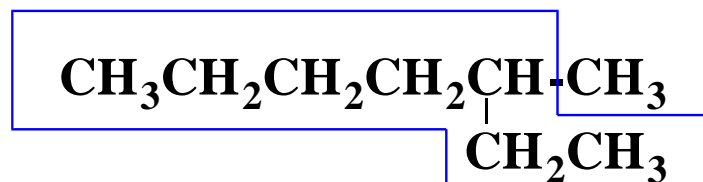
The alkyl group names are used in **common names** and when the alkyl groups are substituents along a "parent" carbon chain in the IUPAC naming system.

IUPAC Names of Alkanes

(1) Select the **longest continuous carbon chain** as the **parent name** of the alkane.

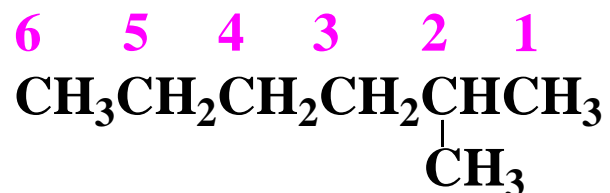


a pentane either way

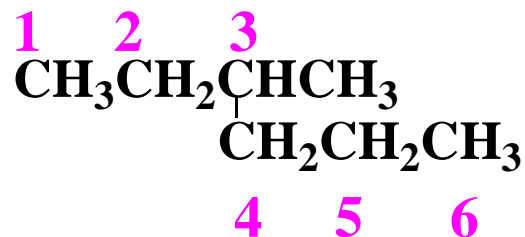


a heptane

- (2) Number the carbons of the longest chain beginning at the end that gives **lower numbers** to positions of substituents.

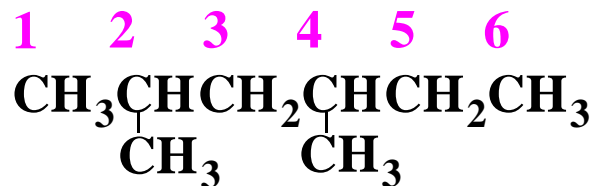


2-methylhexane



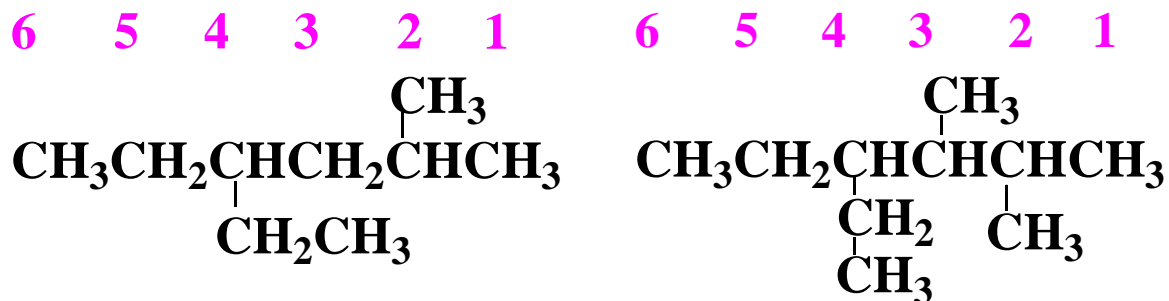
3-methylhexane

- (3) If the same substituent appears more than once, use the **prefixes di, tri, tetra....**



2,4-dimethylhexane

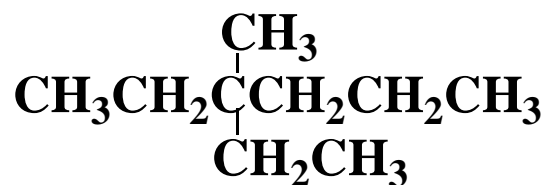
- (4) When two or more different substituents are present, give each a positional number and list them **alphabetically**. Disregard prefixes in determining alphabetical order.



4-ethyl-2-methylhexane

4-ethyl-2,3-dimethylhexane

- (5) When two substituents are on the same carbon, use the positional number twice.

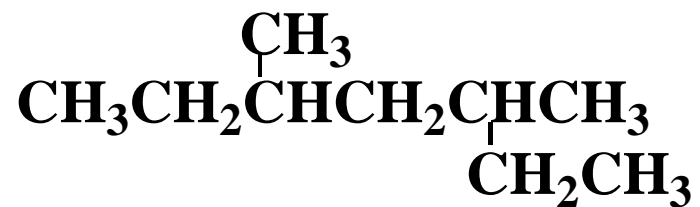


3-ethyl-3-methylhexane

These rules lead to unambiguous names for the alkanes and solve the problem of numerous constitutional isomers.

Quiz Chapter 4 Section 3

Provide the IUPAC names of the alkanes below.



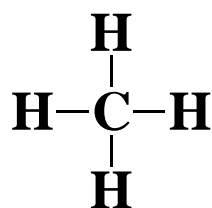
3,5-dimethylheptane



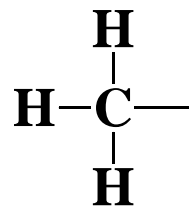
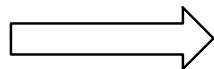
2,4-dimethylpentane

Nomenclature of Branched Alkyl Groups

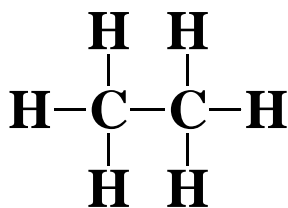
In methane and ethane, all the H are equivalent.
Therefore, only one alkyl group is possible for each.



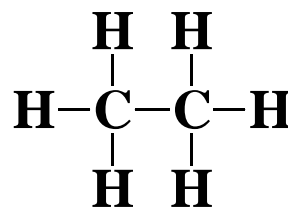
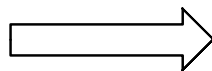
methane



methyl



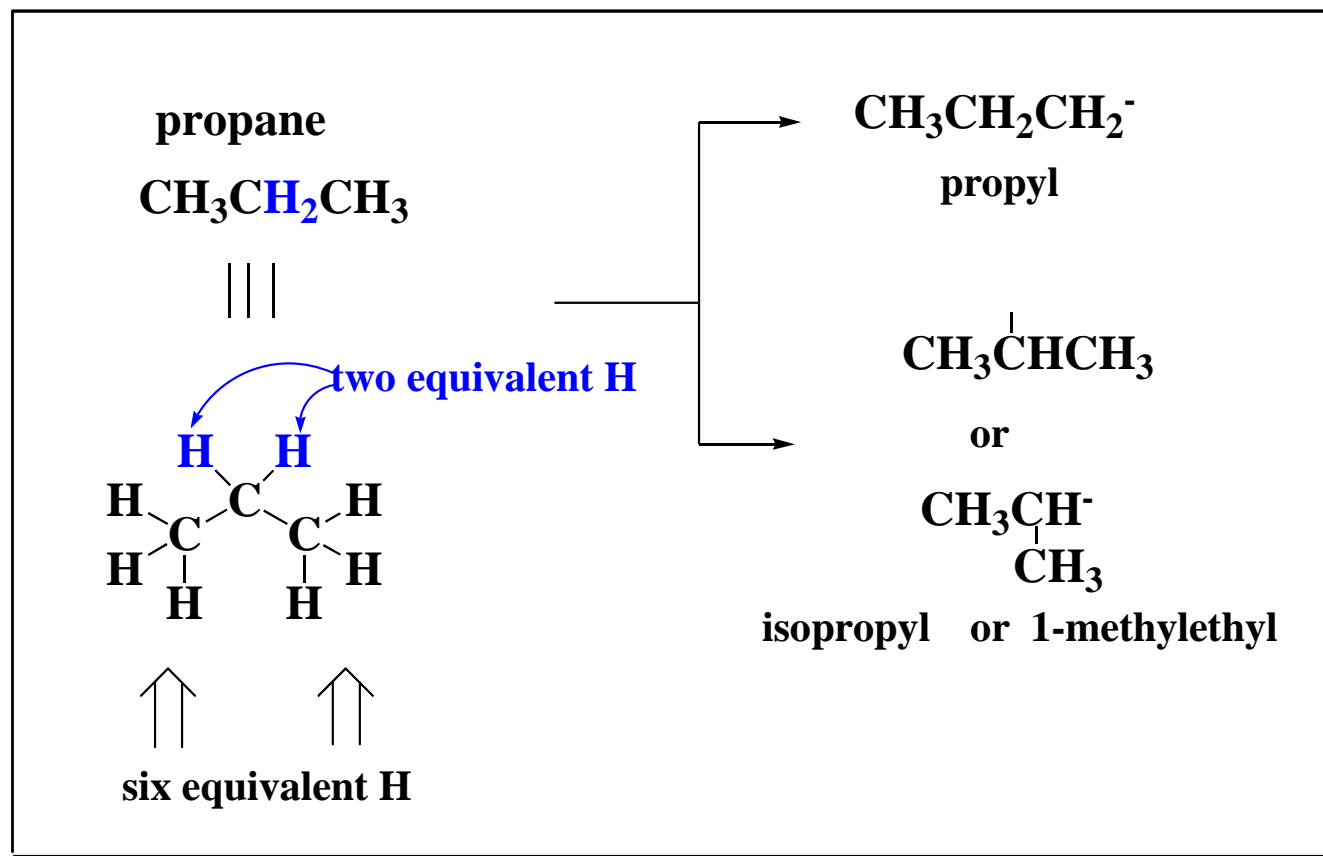
ethane



ethyl

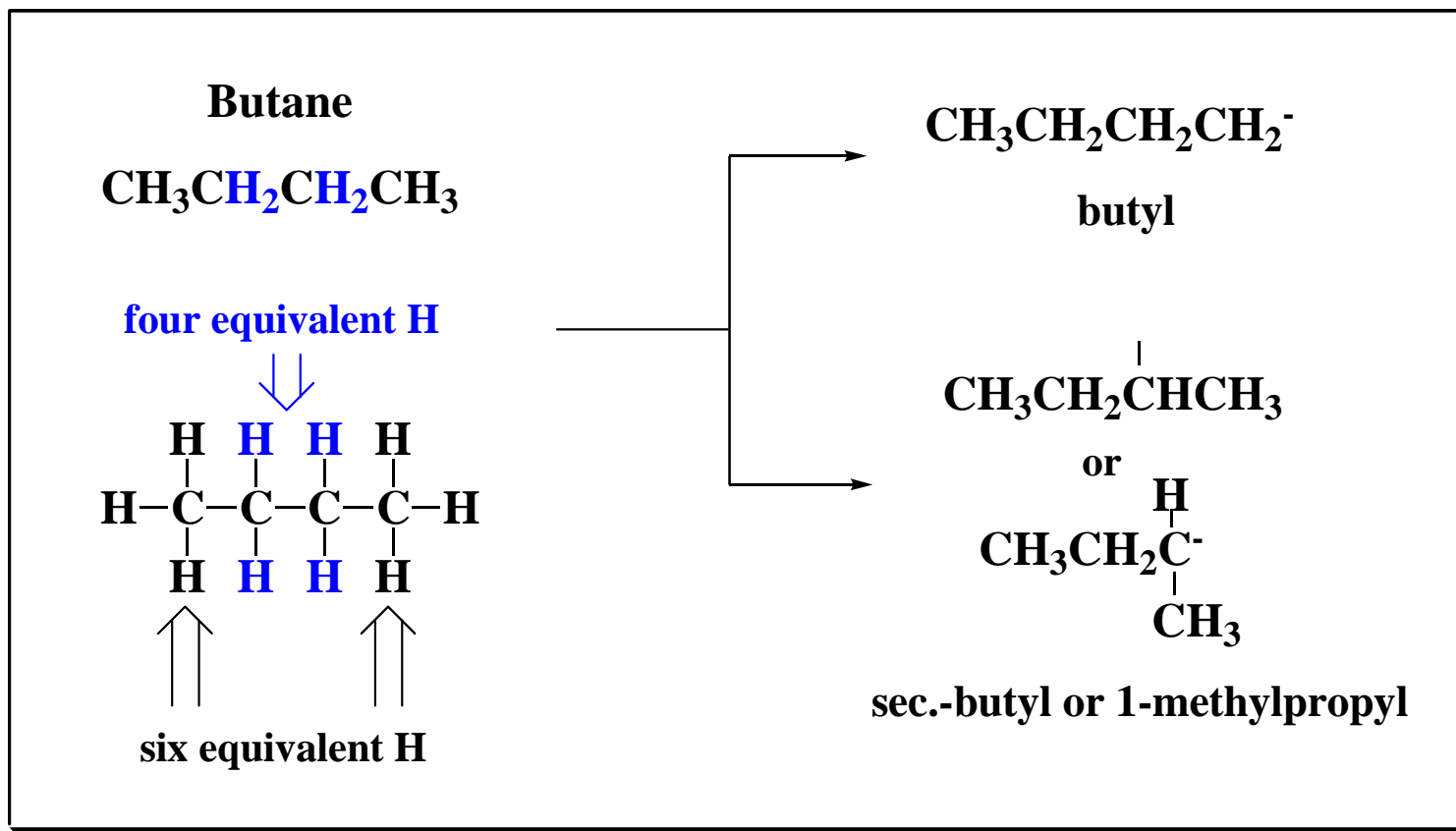
Branched Alkyl Groups from the Higher Alkanes

Beginning with C₃, more than one type of H is present. Different alkyl groups are formed depending on which H is removed.

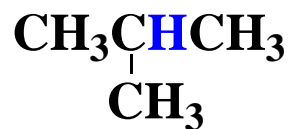


Alkyl Groups Derived from the Butanes

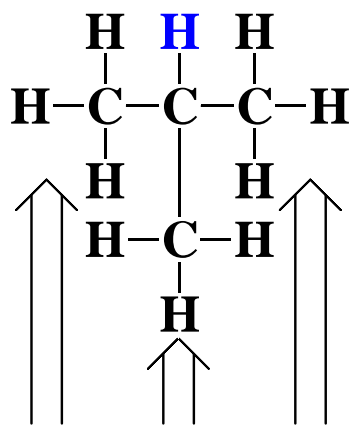
Each constitutional isomer of the butanes yields two alkyl groups.



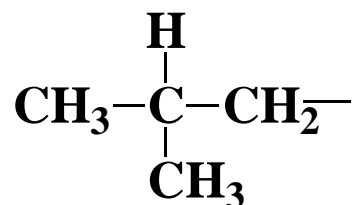
Isobutane



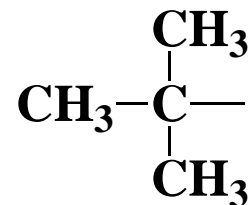
one H



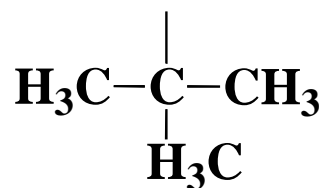
nine equivalent H



isobutyl or 2-methylpropyl

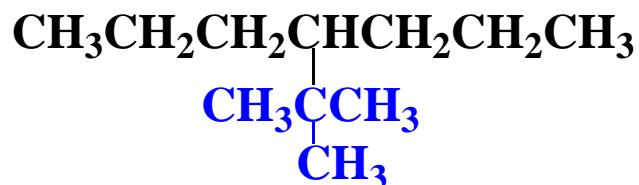


or



tert-butyl or 1,1-dimethylethyl

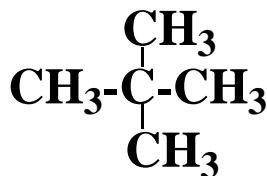
Branched Alkyl Groups as Substituents



4-**tert-butyl**heptane or 4-(1,1-dimethylethyl)heptane

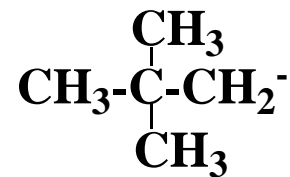
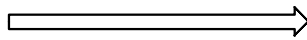
The common names **isopropyl**, **isobutyl**, **sec-butyl**, and **tert-butyl** are approved by the IUPAC for the unsubstituted alkyl groups.

Neopentane and the Neopentyl Group



neopentane

(a constitutional isomer of C₅H₁₂)



neopentyl

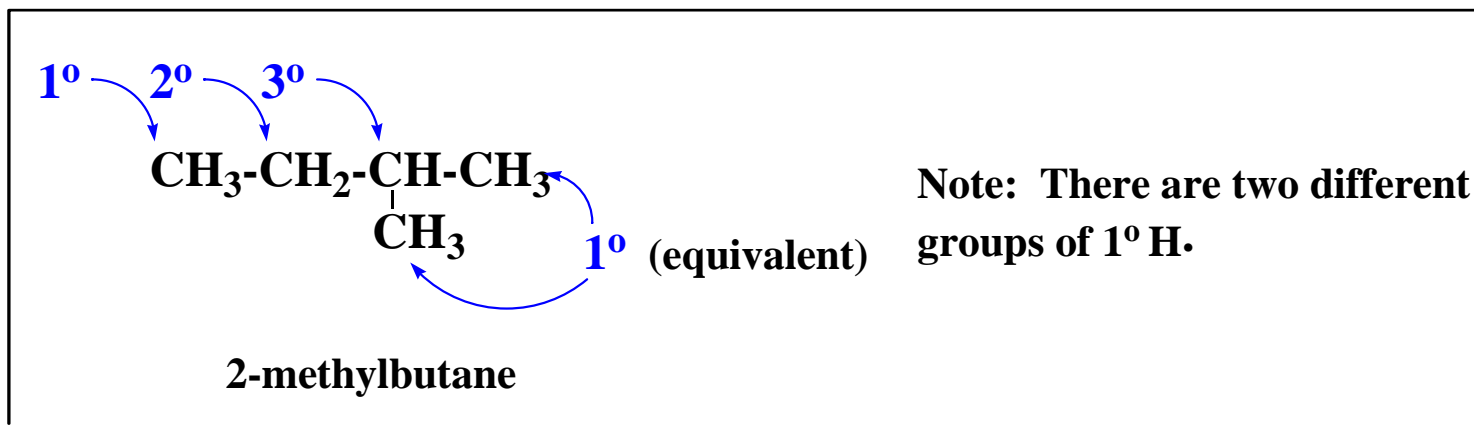
or

2,2-dimethylpropyl

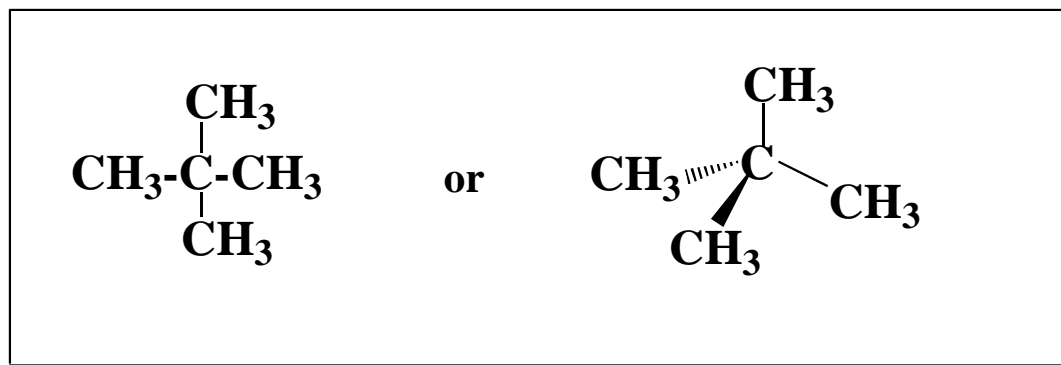
An additional IUPAC approved common name is the C₅ alkyl group derived from **neopentane**.

Classification of Hydrogen Atoms

The hydrogen in an alkane is classified as **primary (1°)**, **secondary (2°)**, or **tertiary (3°)** according to the type of carbon it is attached to.

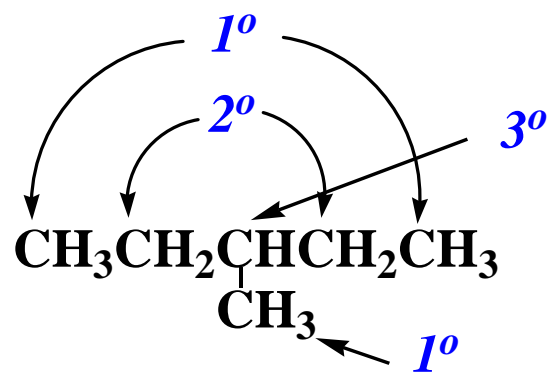


In neopentane (2,2-dimethylpropane),
all 12 primary-H are equivalent.



Quiz Chapter 4 Section 3D

Name the alkane below and identify as 1° , 2° and 3° , all groups of equivalent H.



3-methylpentane

Nomenclature of Alkyl Halides

The halogen substituted alkanes are named as **haloalkanes** in the IUPAC system. All the rules presented earlier apply.

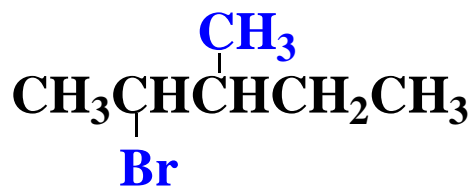


2-chloropropane



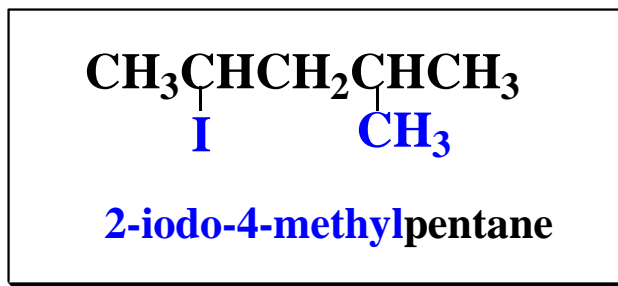
1-bromobutane

When both halo and alkyl substituents are present, number from the end nearer the first substituent, whether halo or alkyl, and list the substituents in alphabetical order.



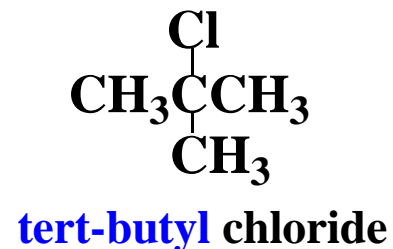
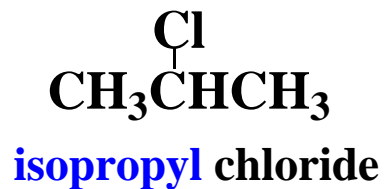
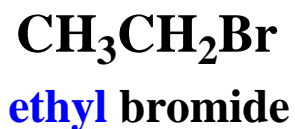
2-bromo-3-methylpentane

If the two substituents are equal distance from an end of the chain, number from the end that gives alphabetical preference.



Common Names: Alkyl Halides

Common names of alkyl halides are based on the **alkyl group name** and the name of the halide.



Nomenclature of Alcohols

In the IUPAC naming system, there may be as many as **four components** to the name:

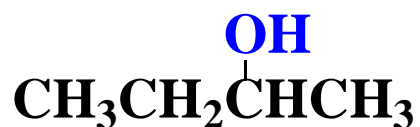
Locant indicates the position of a substituent.

Prefix names the substituent group.

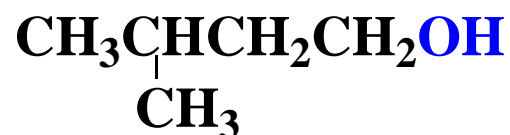
Parent is the parent alkane.

Suffix names a key function.

Examples



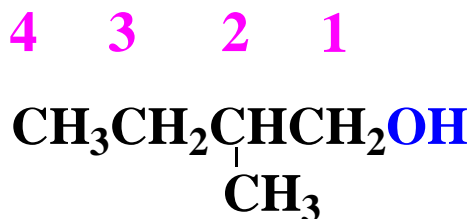
2-butanol
locant → 2 → parent → -butanol → suffix



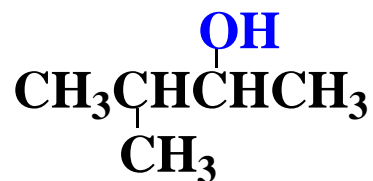
3-methyl-1-butanol
locant → 3 → prefix → methyl → parent → 1-butanol → suffix

IUPAC Rules for Naming Alcohols

- (1) Select the longest continuous chain containing the hydroxyl group as the parent. Drop the "e" in the alkane name and add the suffix "ol."
- (2) Number the chain from the end that gives a lower number to the position of the hydroxyl group.



2-methyl-1-butanol



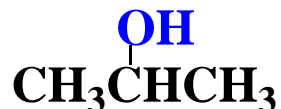
3-methyl-2-butanol

Common Names of Alcohols

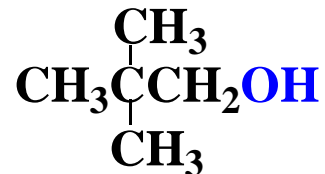
Alkyl group names are approved by IUPAC for naming alcohols:
"alkyl group + alcohol."



ethyl alcohol



isopropyl alcohol



neopentyl alcohol

"Glycol" is a common name for compounds containing two hydroxyl groups. In the IUPAC system, they are diols.



ethylene glycol
(1,2-ethanediol)



propylene glycol
(1,2-propanediol)

Note: The glycol name uses the common name of the alkene that yields the diol upon hydroxylation.

Quiz Chapter 4 Section 3F

Name the following compound.

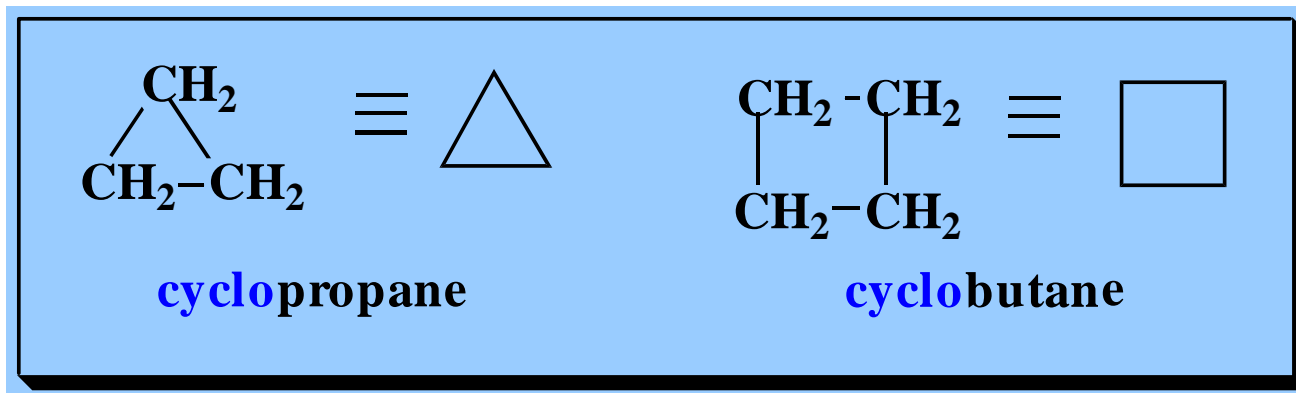


4-chloro-2-pentanol

Section 4--Nomenclature of Cycloalkanes

Nomenclature of Cycloalkanes

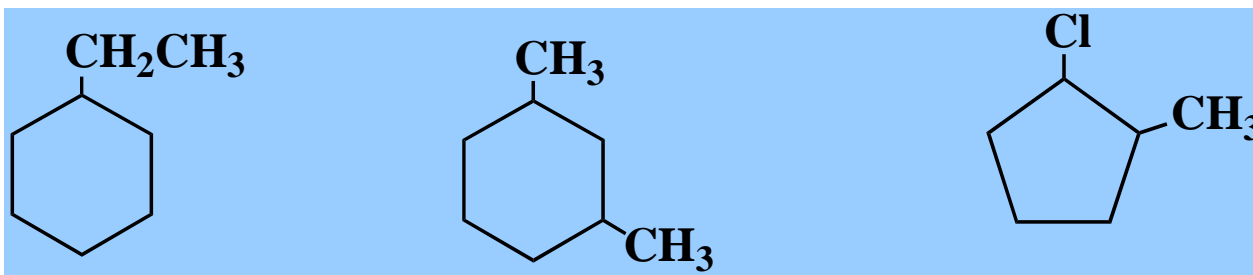
Cyclic alkanes are named with the "**cyclo**" prefix followed by the alkane name indicating the number of carbon atoms in the ring.



Substituted Cycloalkanes

The name of a substituent is added as a **prefix to the cycloalkane name**. Alkyl group names are used for simple alkyl group substituents.

When there are **two or more substituents**, the positions around the ring are **numbered** beginning with the substituent first in the alphabet.

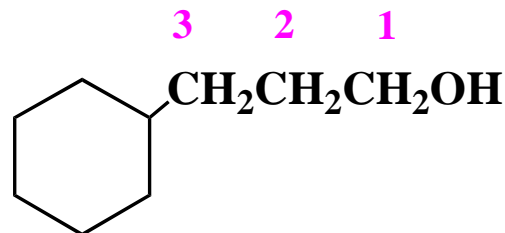


ethylcyclohexane

1,3-dimethylcyclohexane

1-chloro-2-methylcyclopentane

The cycloalkane also can be named as a **substituent** on a long chain, which is sometimes more convenient.

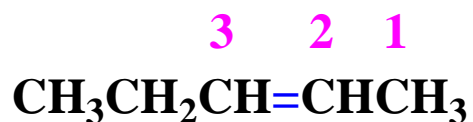


3-cyclohexyl-1-propanol

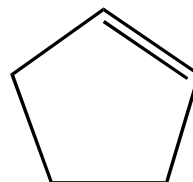
Section 5--Nomenclature of Alkenes and Cycloalkenes

IUPAC Names of Alkenes and Cycloalkenes

- (1) Select the longest continuous carbon chain that **contains the double bond as the parent**. Drop the "ane" in the alkane name and add "ene." Similarly, cycloalkanes become **cycloalkenes**.
- (2) Number the chain from the end to give lower numbers to the alkene carbons. The location of the double bond is given by **the number of the first carbon** of the alkene function.

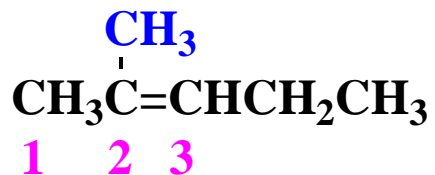


2-pentene

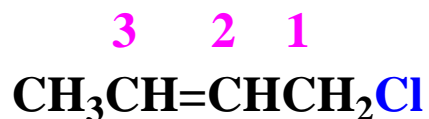


cyclopentene

- (3) **Substituents** are indicated by **positional numbers**.

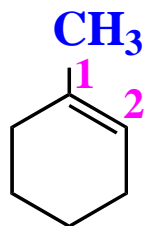


2-methyl-2-pentene

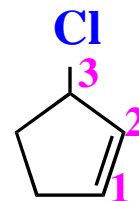


1-chloro-2-butene

- (4) Number substituted cycloalkenes so that the alkene carbons are positions 1 and 2 and in the direction that gives the lower positional numbers to substituents.

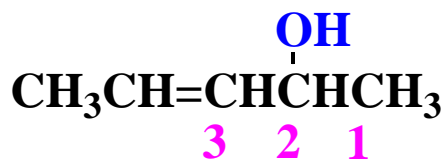


1-methylcyclohexene



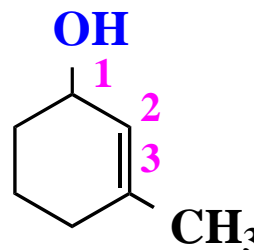
3-chlorocyclopentene

- (5) When an alcohol function is present, the substitutive naming system is used. Alkenol and cycloalkenol names are assigned such that the alcohol always has the lower possible number.



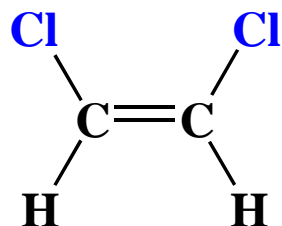
3-penten-2-ol

(not **2-penten-4-ol**)

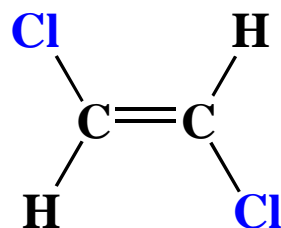


3-methyl-2-cyclohexen-1-ol

(6) "*Cis*" and "*trans*" can be used to designate **isomers** when there are **two identical substituents** on the alkene.



cis-1,2-dichloroethene



trans-1,2-dichloroethene

Two important
common names
involving alkenes are

$\text{CH}_2=\text{CH}-$
vinyl group

$\text{CH}_2=\text{CH}-\text{Cl}$

"vinyl chloride"

(chloroethene)

$\text{CH}_2=\text{CH}-\text{CH}_2-$
allyl group

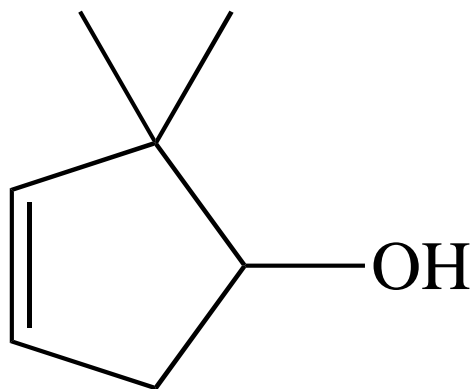
$\text{CH}_2=\text{CH}-\text{CH}_2-\text{Cl}$

"allyl chloride"

(3-chloropropene)

Quiz Chapter 4, Section 5

Name the compound below.



2,2-dimethylcyclopent-3-en-ol

or

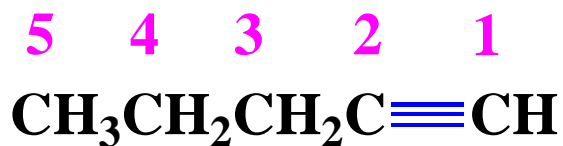
2,2-dimethyl-3-cyclopenten-1-ol

Section 6--Nomenclature of Alkynes

IUPAC Names of Alkynes

Alkynes are named in a similar way as alkenes.

- (1) The name of the parent alkane is modified by dropping the "ane" ending and adding "yne."
- (2) The parent chain is numbered to give the carbons of the alkyne **lower numbers**.
- (3) The **location** of the triple bond is given by the lower positional number of the alkynyl carbons.

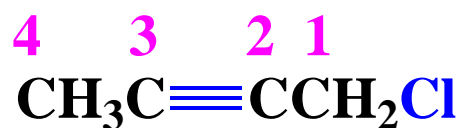


1-pentyne

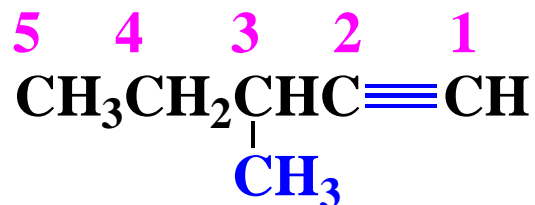


2-butyne

(4) Positions of substituents are determined by the usual rules.



1-chloro-**2**-butyne



3-methyl-**1**-pentyne

(5) In an **alkynol**, the alcohol has priority in numbering.



3-butyn-**1**-ol

1-Alkynes are also called **terminal alkynes**.

