Principles of Organic Chemistry I
CHEM 244

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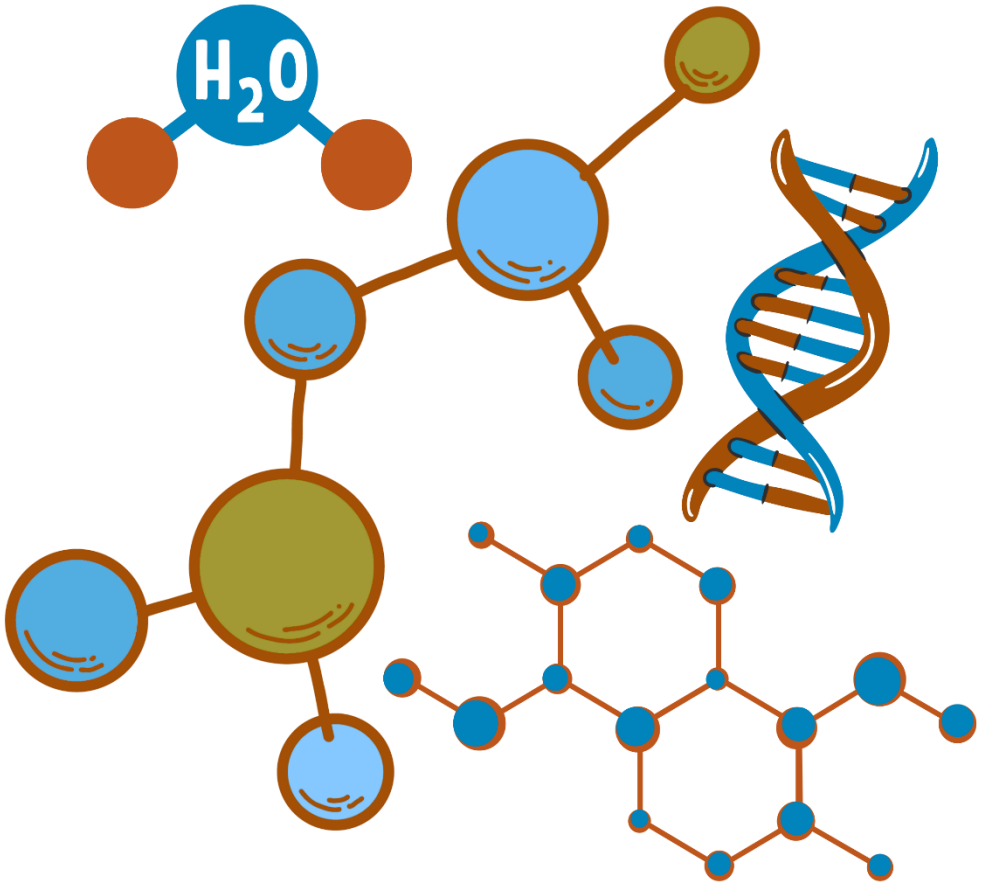
Chapter 3: Nomenclature of Organic Compounds



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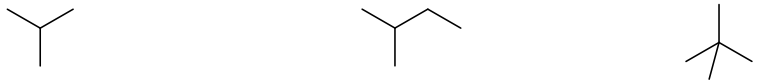
- The older unsystematic names, (*Common names*).
- Systematic nomenclature developed and updated by the *International Union of Pure and Applied Chemistry (IUPAC)*.



	Isobutane	Isopentane	Neopentane
Common name			
IUPAC name	2-Methylpropane	2-Methylbutane	2,2-Dimethylpropane

1. Nomenclature of Alkanes and Cycloalkanes

- The names for some unbranched alkanes are listed in Table 3.1.
- The ending for all of the names of alkanes is *-ane*.
- The stems of the names of most of the alkanes (above C4) are of Greek and Latin origin. Thus, one, two, three, four, and five become meth-, eth-, prop-, but-, and pent-.

Table 3-1 The Unbranched alkanes

Name	Number of Carbon Atoms	Structure	Name	Number of Carbon Atoms	Structure
Methane	1	CH_4	Hexane	6	$CH_3(CH_2)_4CH_3$
Ethane	2	CH_3CH_3	Heptane	7	$CH_3(CH_2)_5CH_3$
Propane	3	$CH_3CH_2CH_3$	Octane	8	$CH_3(CH_2)_6CH_3$
Butane	4	$CH_3(CH_2)_2CH_3$	Nonane	9	$CH_3(CH_2)_7CH_3$
Pentane	5	$CH_3(CH_2)_3CH_3$	Decane	10	$CH_3(CH_2)_8CH_3$

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1. Nomenclature of Alkanes and Cycloalkanes

1.1. How to Name Alkyl Groups

- **If we remove one terminal hydrogen atom from an alkane, we obtain what is called an alkyl group.**
- **These alkyl groups have names that end in *-yl*.**

Alkane ⟹ Alkyl

- **Example;**

$CH_3—H$

Methane

$CH_3—$

Methyl

Me-

$CH_3CH_2—H$

Ethane

$CH_3CH_2—$

Ethyl

Et-

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1. Nomenclature of Alkanes and Cycloalkanes

1.1. How to Name Alkyl Groups

- For alkanes with more than two carbon atoms, more than one derived group is possible.
- For example;

  Two groups can be derived from propane,

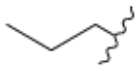
  the propyl group is derived by removal of a terminal hydrogen, and

  the isopropyl (common name) is derived by removal of a hydrogen from the central carbon.

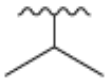
Three-Carbon Groups

$CH_3CH_2CH_3$
Propane

$CH_3CH_2CH_2$—
Propyl (or Pr)



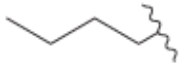
$CH_3CH(\text{—})CH_3$
Isopropyl (or *i*-Pr)



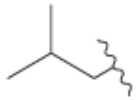
Four-Carbon Groups

$CH_3CH_2CH_2CH_3$
Butane

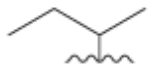
$CH_3CH_2CH_2CH_2$—
Butyl (or Bu)



$CH_3CH(CH_3)CH_2$—
Isobutyl



$CH_3CH_2CH(\text{—})CH_3$
***sec*-Butyl**



$(CH_3)_3C$ —
***tert*-Butyl (or *t*-Bu)**

- The common names isopropyl, isobutyl, *sec*-butyl, and *tert*-butyl are approved by IUPAC for the unsubstituted groups, and they are still very frequently used.

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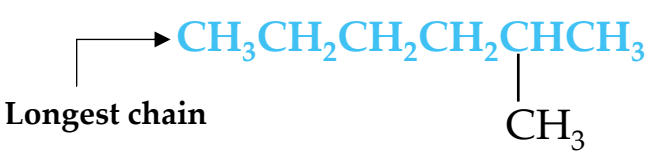
1. Nomenclature of Alkanes and Cycloalkanes

1.2. How to Name Alkanes

- **Branched-chain alkanes are named according to the following rules:**

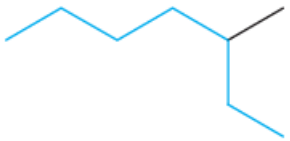
1. Locate the longest continuous chain of carbon atoms; this chain determines the parent's name for the alkane.

The longest continuous chain may not always be obvious from the way the formula is written.



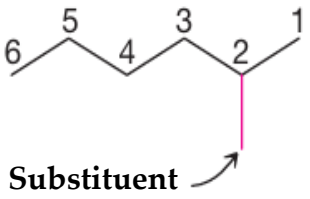
or

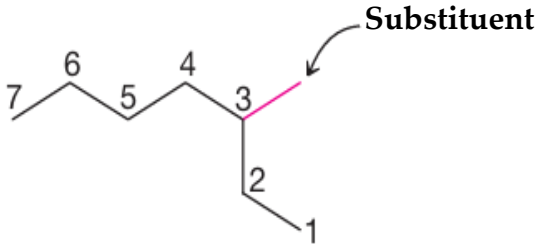
Hexane
Because the longest continuous chain contains six carbon atoms



Heptane
Because the longest chain contains seven carbon atoms

2. Number the longest chain beginning with the end of the chain nearer the substituent.





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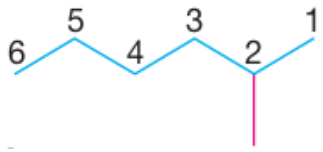
1. Nomenclature of Alkanes and Cycloalkanes

1.2. How to Name Alkanes

3. Use the numbers obtained by application of rule 2 to designate the location of the substituent group.

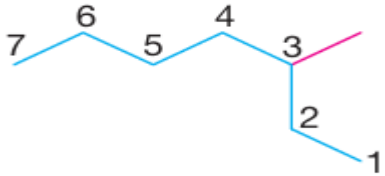
The parent's name is placed last, and the substituent group, preceded by the number designating its location on the chain, is placed first. Numbers are separated from words by a hyphen (-).



Substituent

Longest chain

Locant → **2-Methylhexane**

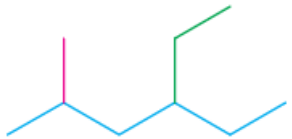


3-Methylheptane

4. When two or more substituents are present, give each substituent a number corresponding to its location on the longest chain.

The substituent groups should be listed alphabetically (i.e., ethyl before methyl).

In deciding on alphabetical order, disregard multiplying prefixes such as "di" and "tri".



4-Ethyl-2-methylhexane

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1. Nomenclature of Alkanes and Cycloalkanes

1.2. How to Name Alkanes

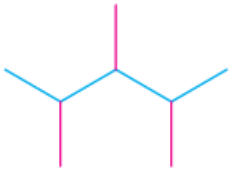
5. When two substituents are present on the same carbon atom, use that number repeated twice.

3-Ethyl-3-methylhexane

6. When two or more substituents are identical, indicate this by the use of the prefixes di-, tri-, tetra-, and so on.

Then, make sure that each substituent is assigned a number. Commas (,) are used to separate numbers from each other.

2,3-Dimthylbutane



2,3,4-Trimthylpentane

2,2,4,4-Tetramthylpentane

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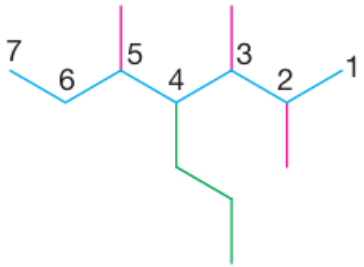
1. Nomenclature of Alkanes and Cycloalkanes

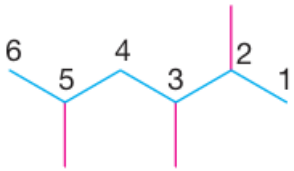
1.2. How to Name Alkanes

7. When two chains of equal length compete for selection as the parent chain, choose the chain with the greater number of substituents.



2,3,5-Trimthyl-4-propylheptane
(four substituent)

8. When branching first occurs at an equal distance from either end of the longest chain, choose the name that gives the lower number at the first point of difference.



2,3,5-Trimthylhexane
(*not* 2,4,5-Trimthylhexane)

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1. Nomenclature of Alkanes and Cycloalkanes

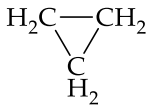
1.3. How to Name Monocyclic Cycloalkanes

- **Cycloalkanes are named by adding "*cyclo*" before the parent's name.**

1. Cycloalkanes with one ring and no substituents:

Count the number of carbon atoms in the ring, then add "*cyclo*" to the beginning of the name of the alkane with that number of carbons.

Example; cyclopropane has three carbons and cyclopentane has five carbons.



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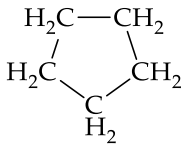
Cyclopropane



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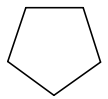
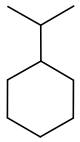


Cyclopentane

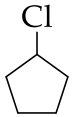
2. Cycloalkanes with one ring and one substituent:

Add the name of the substituent to the beginning of the parent's name.

For compounds with only one substituent, it is not necessary to specify a number (locant) for the carbon bearing the substituent.



Isopropylcyclohexane



Chlorocyclopentane

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1. Nomenclature of Alkanes and Cycloalkanes

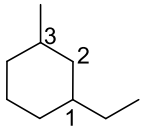
1.3. How to Name Monocyclic Cycloalkanes

3. Cycloalkanes with one ring and two or more substituents:

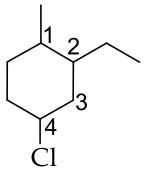
For a ring with two substituents, begin by numbering the carbons in the ring, starting at the carbon with the substituent that is first in the alphabet and number in the direction that gives the next substituent the lower number possible.

When there are three or more substituents, begin at the substituent that leads to the lowest set of numbers (locants).

The substituents are listed in alphabetical order, not according to the number of their carbon atom.

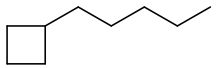


1-Ethyl-3-methylcyclohexane
(*not* 1-ethyl-5-methylcyclohexane)

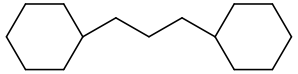


4-Chloro-2-ethyl-1-methylcyclohexane
(*not* 1-Chloro-3-ethyl-4-methylcyclohexane

4. When a single ring system is attached to a single chain with a greater number of carbon atoms, or when more than one ring system is attached to a single chain, then it is appropriate to name the compounds as cycloalkylalkanes.



1-Cyclobutylpentane



1,3-Dicyclohexylpropane

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2. Nomenclature of Alkenes and Cycloalkenes

2.1. How to Name Alkenes

- **The IUPAC rules for naming alkenes are similar in many respects to those for naming alkanes:**

1. **Determine the parent's name by selecting the longest chain that contains the double bond and change the ending of the name of the alkane of identical length from *-ane* to *-ene*.**

IUPAC name	**Ethene**	**Propene**	**2-Methylpropene**
Common name	**Ethylene**	**Propylene**	**Isobutylene**

2. **Number the chain from the end nearest the double bond, ensuring that both double-bonded carbon atoms are included in the parent chain.**
   - Designate the location of the double bond by using the number of the first atom of the double bond as a prefix. The locant for the alkene suffix may precede the parent's name or be placed immediately before the suffix.

3. **Indicate the locations of the substituent groups by the numbers of the carbon atoms to which they are attached.**

$\overset{1}{C}H_2{=}\overset{2}{C}H\overset{3}{C}H_2\overset{4}{C}H_3$

1-Butene
(*not* 3-butene)

$\overset{1}{C}H_3\overset{2}{C}H{=}\overset{3}{C}H\overset{4}{C}H_2\overset{5}{C}H_3$

2-Pentene
(*not* 3-Pentene)

2-Methyl-2-butene
or 2-Methylbut-2-ene

2,5-Dimethyl-2-hexene
or 2,5-Dimethylhex-2-ene

(*Z*)-1-Chloro-2-butene

(*E*)-2-Chloro-2-pentene

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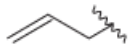
2. Nomenclature of Alkenes and Cycloalkenes

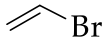
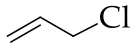
2.1. How to Name Alkenes

4. **Two frequently encountered alkenyl groups are the vinyl group and the allyl group.**

The vinyl group

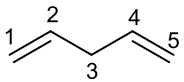


The allyl group

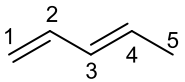
			
IUPAC name	**Bromoethene**	**Ethenylcyclopropane**	**3-Chloropropene**
Common name	**Vinyl bromide**	**Vinylcyclopropane**	**Allyl chloride**

2.2. How to Name Dienes

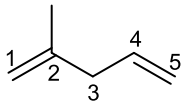
5. **Number the chain from the end nearest the first double bond, giving the substituents the lowest possible numbers.**



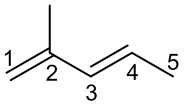
Penta-1,4-diene
or **1,4-Pentadiene**
(*not* Penta-2,5-diene)



Penta-1,3-diene
or **1,3-Pentadiene**
(*not* Penta-2,4-diene)



2-Methylpenta-1,4-diene
or **2-Methyl-1,4-pentadiene**
(*not* 4-Methylpenta-1,4-diene)



2-Methylpenta-1,3-diene
or **2-Methyl-1,3-pentadiene**
(*not* 4-Methylpenta-2,4-diene)

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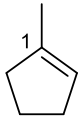
2. Nomenclature of Alkenes and Cycloalkenes

2.3. How to Name Cycloalkenes

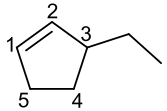
6. **Number substituted cycloalkenes in the way that gives the carbon atoms of the double bond the 1 and 2 positions and that also gives the substituent groups the lower numbers at the first point of difference.**

- *With substituted cycloalkenes it is not necessary to specify the position of the double bond since it will always begin with C1 and C2.*

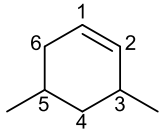
Cyclopentene
(*not* 1-Cyclopentene)



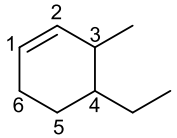
1-Methylcyclopentene
(*not* 2-Methylcyclopentene)



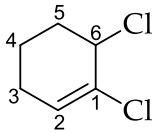
3-Ethylcyclopentene
(*not* 5-Ethylcyclopentene)



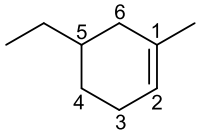
3,5-Dimethylcyclohexene
(*not* 4,6-Dimethylcyclohexene)



4-Ethyl-3-methylcyclohexene
(*not* 3-Methyl-4-ethylcyclohexene)
(*not* 5-Ethyl-6-methylcyclohexene)



1,6-Dichlorocyclohexene
(*not* 2,3-Dimethylcyclohexene)



5-Ethyl-1-methylcyclohexene
(*not* 4-Ethyl-2-methylcyclohexene)
(*not* 2-Methyl-4-Ethylcyclohexene)

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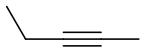
3. Nomenclature of Alkyne

3.1. How to Name Alkyne

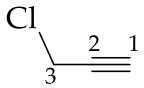
- **Alkynes are named in much the same way as alkenes.**
- **Alkynes, are named by replacing the *-ane* of the name of the corresponding alkane with the ending *-yne*.**

  The chain is numbered to give the carbon atoms of the triple bond the lower possible numbers. The lower number of the two carbon atoms of the triple bond is used to designate the location of the triple bond.
- **The locations of substituent groups of branched alkynes and substituted alkynes are also indicated with numbers.**

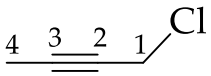
IUPAC name **Ethyne**
Common name **Acetylene**



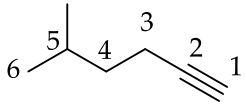
2-Pentyne



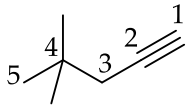
3-Chloropropyne



1-Chlorobut-2-yne
***or* 1-Chloro-2-butyne**



5-Methylhex-1-yne
***or* 5-Methyl-1-hexyne**



4,4-Dimethylpent-1-yne
***or* 4,4-Dimethyl-1-pentyne**

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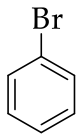
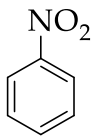
4. Nomenclature of Aromatic Compounds

4.1. How to Name Monosubstituted Benzene

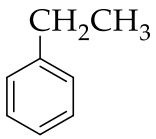
- **Benzene is the simplest aromatic compound, and the simple monosubstituted ring is named as derivative of benzene.**



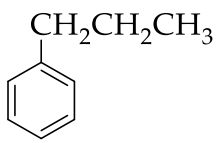
Bromobenzene



Nitrobenzene

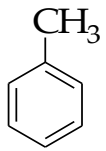


Ethylbenzene

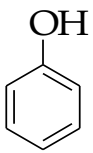


Propylbenzene

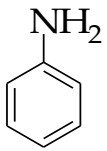
- **Common names are accepted by IUPAC as parent compounds.**



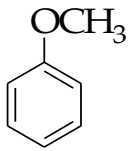
Toluene



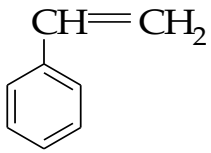
Phenol



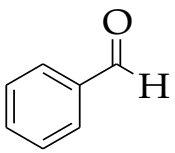
Aniline



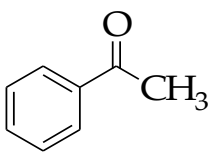
Anisole



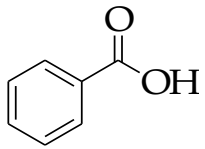
Styrene



Benzaldehyde



Acetophenone



Benzoic acid

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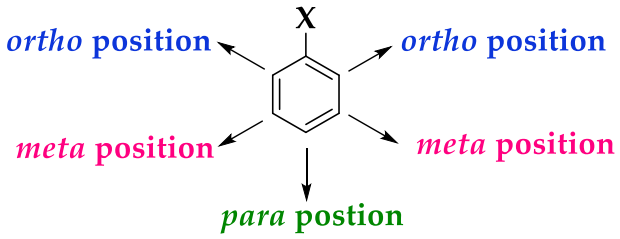
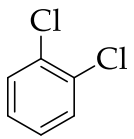
4. Nomenclature of Aromatic Compounds

4.2. How to Name Disubstituted Benzene

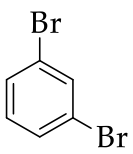
- **When two substituents are present, their relative positions are indicated by the prefixes *ortho-*, *meta-*, and *para-* (abbreviated *o-*, *m-*, and *p-*) or using numbers.**

- **If substituent X is attached to carbon 1;**
  o- groups are on carbons 2 and 6;
  m- groups are on carbons 3 and 5, and
  p- groups are on carbon 4.

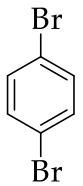




1,2-Dichlorobenzene
(*o*-Dichlorobenzene)



1,3-Dibromobenzene
(*m*-Dibromobenzene)



1,4-Dibromobenzene
(*p*-Dibromobenzene)

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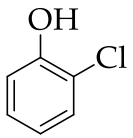
4. Nomenclature of Aromatic Compounds

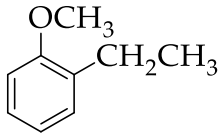
4.2. How to Name Disubstituted Benzene

- **If a substituent have a special name, it could be used as the parent's name with the possible lowest number .**
- **Some disubstituted benzene derivatives have a common names.**

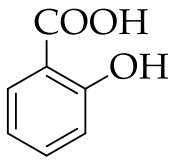


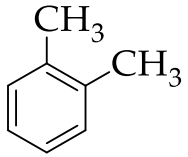
2-Chlorophenol
(*o*-Chlorophenol)

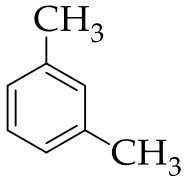
3-Bromobenzoic acid
(*m*-Bromobenzoic acid)

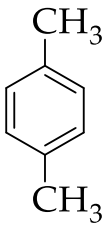


2-Ethylanisole
(*o*-Ethylanisole)









IUPAC name	**2-Hydroxybenzoic acid**	**1,2-Dimethylbenzene**	**1,3-Dimethylbenzene**	**1,4-Dimethylbenzene**
Common name	**Salicylic acid**	***ortho*-xylene**	***meta*-xylene**	***para*-xylene**

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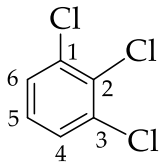
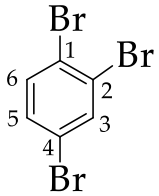
4. Nomenclature of Aromatic Compounds

4.3. How to Name Polysubstituted Benzene

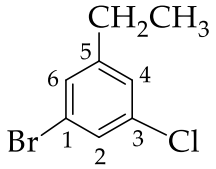
- **If more than two groups are present on the benzene ring, their positions must be indicated using numbers only.**
- **The benzene ring is numbered so as to give the lowest possible numbers to the substituents.**



1,2,3-*Tri*chlorobenzene

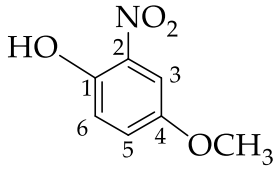


1,2,4-*Tri*bromobenzene

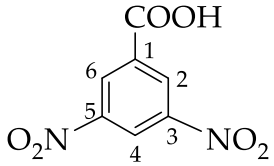


1-Bromo-3-chloro-5 ethylbenzene

- **When a substituent is one that together with the benzene ring gives a new base name, that substituent is assumed to be in position 1 and the new parent's name is used.**



4-Methoxy-2-nitro-phenol



3,5-Dinitrobenzoic acid

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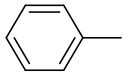
4. Nomenclature of Aromatic Compounds

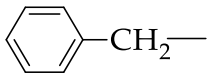
4.4. How to Name Aryl Groups

- When the C_6H_5– group is named as a substituent, it is called a phenyl group (Ph–).
- Benzyl group ($C_6H_5CH_2$-) is an alternative name for the phenylmethyl group.



, C_6H_5- , ph-

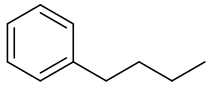
Phenyl group



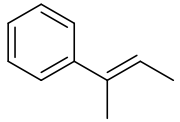
, $C_6H_5CH_2$-

Benzyl group

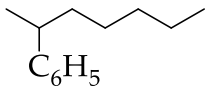
- A hydrocarbon composed of one saturated chain and one benzene ring is usually named as a derivative of the larger structural unit.



Butylbenzene

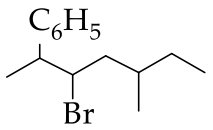


(*E*)-2-Phenyl-2-butene

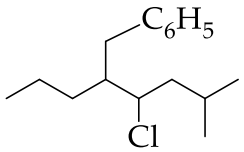


2-Phenylheptane

- If the chain is unsaturated, the compound may be named as a derivative of that chain, regardless of ring size.



3-Bromo-5-methyl-2-phenylheptane



5-Benzyl-4-chloro-2-methyloctane

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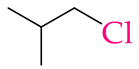
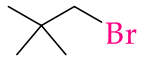
5. Nomenclature of Halogen Compounds

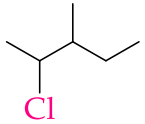
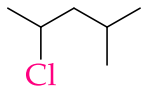
5.1. How to Name Alkyl and Cycloalkyl Halides

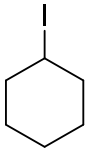
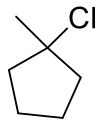
- **Alkanes bearing halogen substituents are named in the IUPAC substitutive system as haloalkanes.**
- **Common nomenclature system, called functional class nomenclature, haloalkanes are named as alkyl halides.**
- **When the parent chain has both a halo and an alkyl substituent attached to it, number the chain from the end nearer the first substituent, regardless of whether it is halo or alkyl.**
- **If two substituents are at equal distance from the end of the chain, then number the chain from the end nearer the substituent that has alphabetical precedence.**
- **Cycloalkyl halides are organic halides in which a halogen atom is attached directly to a carbon atom of a cycloalkane ring.**

	CH_3CH_2Cl	$CH_3CH_2CH_2F$	$CH_3CHBrCH_3$
IUPAC name	Chloroethane	1-Fluoropropane	2-Bromopropane
Common name	Ethyl chloride	Propyl fluoride	Isopropyl bromide

		
IUPAC name	1-Chloro-2-methylpropane	2-Bromo-2-methylpropane
Common name	Isobutyl chloride	*tert*-Butyl bromide

	
IUPAC name	1-Bromo-2,2-dimethyl-propane
Common name	Neopentyl bromide

		
IUPAC name	2-Chloro-3-methylpentane	2-Chloro-4-methylpentane

		
IUPAC name	Iodocyclohexane	1-Chloro-1-methylcyclopentane
Common name	Cyclohexyl iodide	Methylcyclopentyl chloride

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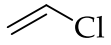
5. Nomenclature of Halogen Compounds

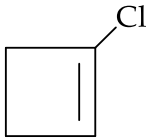
5.2. How to Name Vinylic halides

- **Vinylic halides** are organic halides in which a halogen atom is attached directly to a carbon atom of a C=C double bond.

Common name: Vinyl chloride



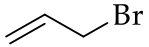
IUPAC name: 1-Chlorocyclobutene



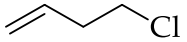
5.3. How to Name Allylic halides

- **Allylic halides** are organic halides in which a halogen atom is attached to a carbon atom adjacent to a C=C double bond.

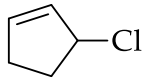
Common name: Allyl bromide



IUPAC name: 3-Bromopropene



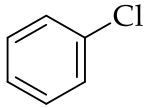
4-Chlorobut-1-ene *or* 4-Chloro-1-butene



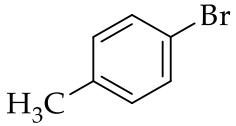
3-Chlorocyclopentene

5.4. How to Name Aryl halides

- **Aryl halides (Ar–X)** are organic halides in which a halogen atom is attached directly to a carbon atom of an aromatic ring.



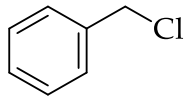
Chlorobenzene



p-Bromotoluene

5.5. How to Name Benzylic halides

- **Benzylic halides (Ar–C–X)** are organic halides in which a halogen atom is attached to a carbon atom adjacent to an aromatic ring.



Benzyl chloride

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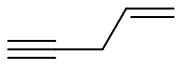
6. Priority of Multiple Bonds in IUPAC Nomenclature

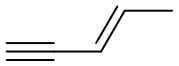
- **When both double and triple bonds are present, number the parent chain to give the multiple bonds the lowest possible set of locants. In case of a tie, the double bond is given the lower locant.**

- **Example 1 – Tie: The double bond is given the lower locant.**



Pent-1-en-4-yne
or **1-Penten-4-yne**

- **Example 2 – No Tie: The lowest set of locants determines the direction of numbering.**



Pent-3-en-1-yne
or **3-Penten-1-yne**

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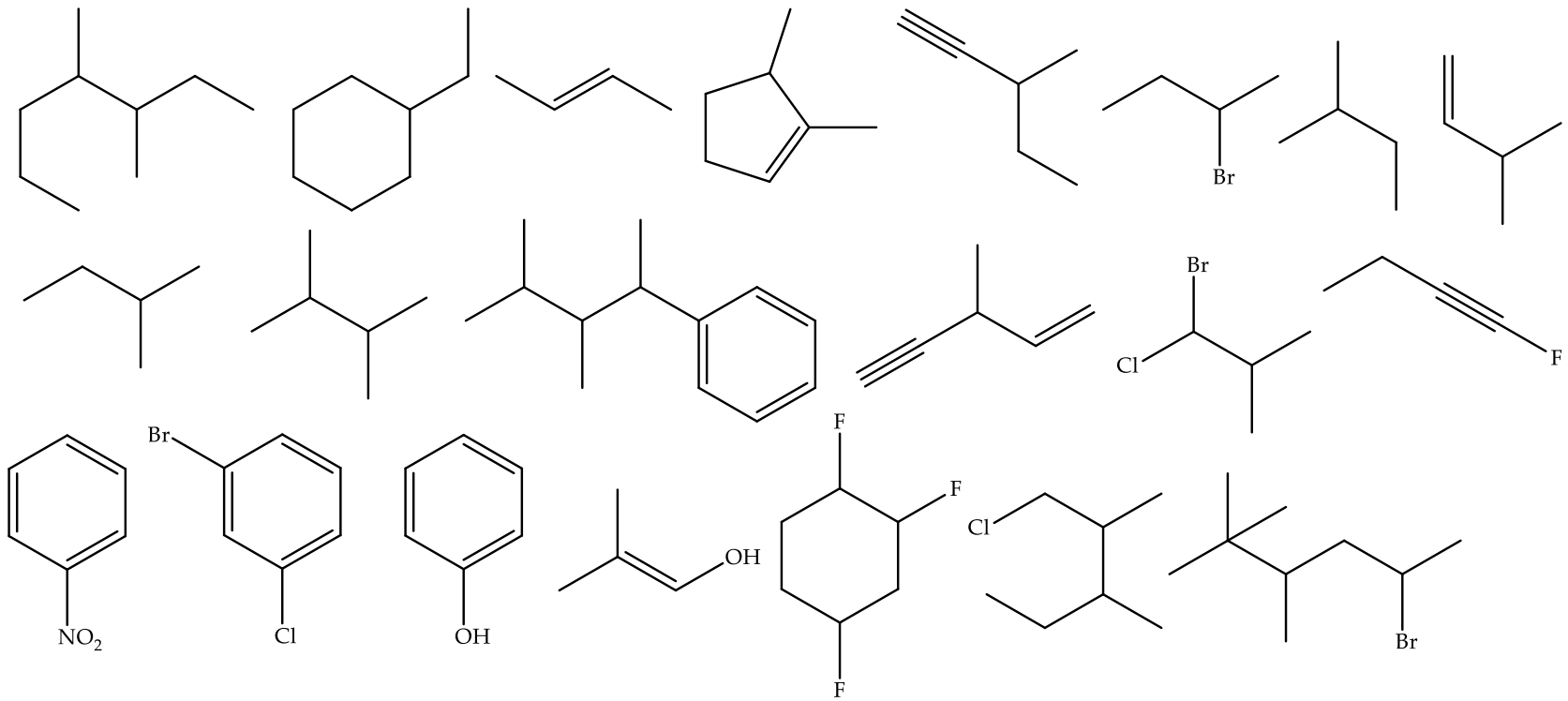
7. Practice Problems

1) Give the IUPAC name of each of the following compounds



2) Write the structural formula for:

a) 2,2,4-trimethylpentane

b) 4-Isopropyl-3,5-dimethyl-2-octene

c) 5-Bromo-4-ethyl-6-methyl-2-nonyne

d) 1,3-Difluoro-4-methylbenzene