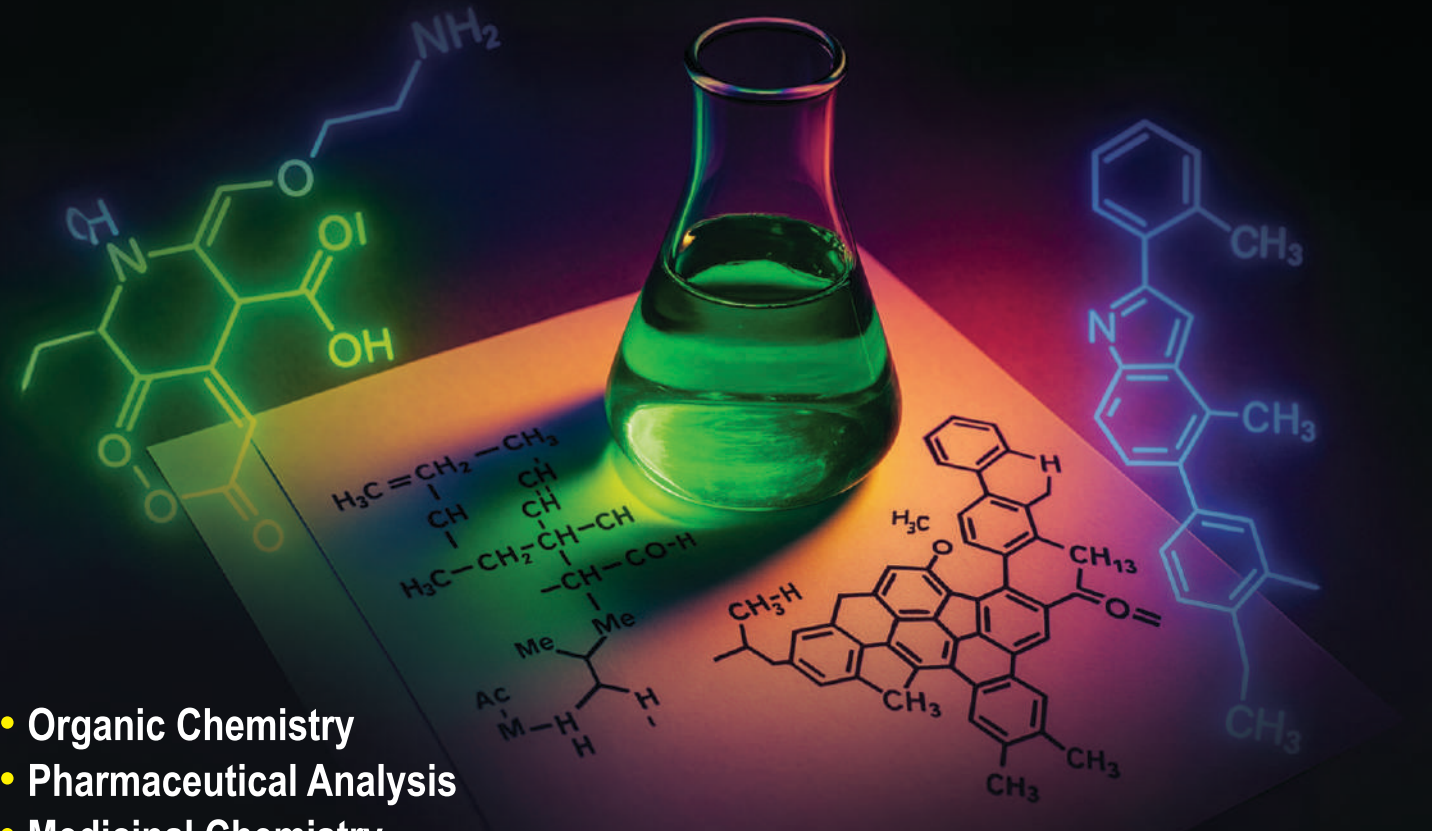
Pharma Pulse - Topper's Tonic

# COMPREHENSIVE PHARMACEUTICAL CHEMISTRY



- Organic Chemistry
- Pharmaceutical Analysis
- Medicinal Chemistry
- Biochemistry
- Physical Chemistry
- Inorganic Chemistry

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A COMPLETE BOOK

Theory and Practice MCQs for GPAT and Other Pharma Competitive Exams

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# IUPAC Nomenclature of Organic Compounds

# 2

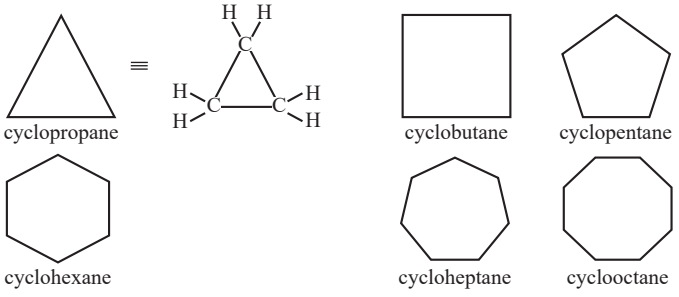
The purpose of the IUPAC system of nomenclature is to establish an international standard of naming compounds to facilitate communication. The goal of the system is to give each structure a unique and unambiguous name, and to correlate each name with a unique and unambiguous structure.

## FUNDAMENTAL PRINCIPLE

IUPAC nomenclature is based on naming a molecule's longest chain of carbons connected by single bonds, whether in a continuous chain or in a ring. All deviations, either multiple bonds or atoms other than carbon and hydrogen, are indicated by prefixes or suffixes according to a specific set of priorities.

**I. Alkanes and Cycloalkanes** Alkanes are the family of saturated hydrocarbons, that is, molecules containing carbon and hydrogen connected by single bonds only. These molecules can be in continuous chains (Called linear or acyclic), or in rings (Called cyclic or alicyclic). The names of alkanes and cycloalkanes are the root names of organic compounds. Beginning with the five-carbon alkane, the number of carbons in the chain is indicated by the Greek or Latin prefix. Rings are designated by the prefix "cyclo". (In the geometrical symbols for rings, each apex represents a carbon with the number of hydrogens required to fill its valence.)

| Molecular Formula | Name |
|---|---|
| $CH_4$ | Methane |
| $CH_3CH_3$ | Ethane |
| $CH_3CH_2CH_3$ | Propane |
| $CH_3[CH_2]_2CH_3$ | Butane |
| $CH_3[CH_2]_3CH_3$ | Pentane |
| $CH_3[CH_2]_4CH_3$ | Hexane |
| $CH_3[CH_2]_5CH_3$ | Heptane |
| $CH_3[CH_2]_6CH_3$ | Octane |
| $CH_3[CH_2]_7CH_3$ | Nonane |
| $CH_3[CH_2]_8CH_3$ | Decane |



## Priorities of Substituents and Functional Groups (Highest to Lowest)

### Group A: Functional Groups (Prefix or Suffix Usage)

| Family of Compound | General Structure | Prefix | Suffix |
|---|---|---|---|
| Carboxylic Acid | R – COOH | carboxy- | -oic acid/-carboxylic acid |
| Aldehyde | R – CHO | oxo-/formyl- | -al/-carbaldehyde |
| Ketone | R– CO – R' | oxo- | -one |
| Alcohol | R – OH | hydroxy- | -ol |
| Amine | $R - NH_2/R - NR_2$ | amino- | -amine |

### Group B: Functional Groups (Suffix Only)

| Family of Compound | General Structure | Prefix | Suffix |
|---|---|---|---|
| Alkene | R – CH = CH – R | — | -ene |
| Alkyne | R – C ≡ C – R | — | -yne |

### Group C: Substituents (Prefix Only, Equal Priority)

| Substituent Type | General Structure | Prefix | Suffix |
|---|---|---|---|
| Alkyl | R– | alkyl- | — |
| Alkoxy | R – O – | alkoxy- | — |
| Halogens | F, Cl, Br, I | fluoro-, chloro-, bromo-, iodo- | — |
| Isobutyl | $–CH_2CH(CH_3)_2$ | isobutyl- | 2-methylpropyl |
| Sec-butyl | $–CH(CH_3)CH_2CH_3$ | sec-butyl- | 1-methylpropyl |
| Tert-butyl | $–C(CH_3)_3$ | tert-butyl- | 1,1-dimethylethyl (t-butyl) |
| Butyl (n-butyl) | $–CH_2CH_2CH_2CH_3$ | butyl- | — |
| Nitro | $–NO_2$ | nitro- | — |
| Vinyl | $–CH = CH_2$ | vinyl- | — |
| Allyl | $–CH_2CH = CH_2$ | allyl- | — |
| Phenyl | $–C_6H_5$ | phenyl- | — |

## Naming Substituted Alkanes and Cycloalkanes (Group C Substituents Only)

When only Group C substituents (Alkyls, halogens, etc.) are present, follow these five steps to construct the IUPAC name:

1. **Identify the Parent Chain:**
   - ❖ Find the longest continuous carbon chain; that is your root.
   - ❖ If a ring is attached to a longer chain, the chain takes priority; otherwise, the ring itself is the parent (Use the prefix "cyclo-").
2. **Number the Parent Chain:**
   - ❖ Assign numbers so that the first substituent encountered (From one end) gets the lowest possible locant.
   - ❖ If there's a tie at the first substituent, compare the second, third, etc., until the tie is broken.

**3. Name and Locate Each Substituent:**

- For each Group C substituent, determine its proper prefix (e.g., methyl-, ethyl-, chloro-).
- Assign the correct position number to each substituent (for N-substituted amines, use "N-" instead of a locant).

**4. Indicate Multiplicity:**

- If the same substituent appears more than once, use di-, tri-, tetra-, etc., to show how many, placing the multiplier directly before the substituent name.

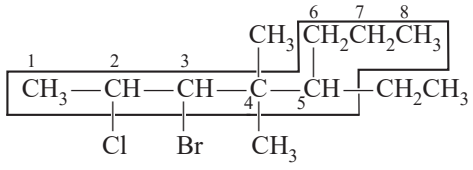
**5. Assemble the Name:**

- List substituent prefixes (With locants and multipliers) in **alphabetical order**, ignoring prefixes di-, tri-, etc., but **including** iso and cyclo.
- Follow this entire sequence by the parent name (Root + "-ane").
- Always include a locant for every substituent, even when redundant.

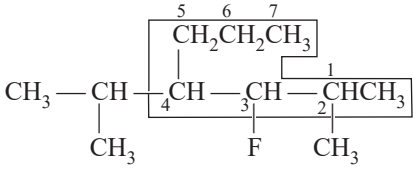
**Example: 3-bromo-2-chloro-5-ethyl-4, 4-dimethyloctane**

1. Octane parent (8-C chain)
2. Numbered from the end giving substituents at C-2, 3, 4, and 5
3. Substituents: bromo (3), chloro (2), ethyl (5), methyl × 2 (4,4)
4. "Di" for two methyl groups → dimethyl
5. Alphabetical order: bromo, chloro, dimethyl, ethyl

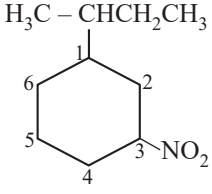
**Examples:**




3-bromo-2-chloro-5-ethyl-4,4-dimethyloctane




3-fluoro-4-isopropyl-2-methylheptane




1-sec-butyl-3-nitrocyclohexane
(Numbering determined by the alphabetical order of substituents)

## Naming Molecules Containing Functional Groups from Group B (Suffix Only)

**1. Alkenes (–C = C–):** Follow the same basic IUPAC steps as alkanes, with the following adjustments:

**Steps for Naming Alkenes:**

**(a) Number the carbon chain** so that the double bond (C = C) gets the **lowest possible position number**, as it has higher priority than any substituents.

**(b) Replace "-ane"** with **"-ene"**.

**(c) Assign the position number** to the first carbon involved in the double bond.

**(d) Indicate stereochemistry** using:

- **cis/trans** for simple systems (Based on symmetry),
- **E/Z** for systems with different groups on double-bonded carbons (Cahn-Ingold-Prelog rules).

**Examples:**

| Compound | IUPAC Name |
|---|---|
| $F_2C = CHCH_3$ (With $CH_3$ at position 3) | 4, 4-difluoro-3-methylbut-1-ene |
| $CH_2 = CH - CH = CH - CF_3$ | 1, 1-difluoro-2-methylbuta-1, 3-diene |
| Cyclopentane ring with $CH_3$ at C – 5 and C = C at 1, 3 | 5-methylcyclopenta-1, 3-diene |

**Special Case:** If the double bond **cannot be part of the main chain**, it is treated as a **substituent**.
**Example:** 3-vinylcyclohex-1-ene

2. **Alkynes (–C ≡ C–):** Similar to alkenes, with naming focused on the triple bond:
**Steps for Naming Alkynes:**
**(a) Number the chain** such that the triple bond (**C ≡ C**) gets the **lowest possible locant**.
**(b) Replace "-ane"** with **"-yne"**.
**(c) Assign the position number** to the **first carbon of the triple bond**.

**Priority Between Alkene and Alkyne: Equal priority**, so:

- Numbering starts from the end **closest to either multiple bond**.
- If a tie occurs, **double bond (Alkene)** takes **precedence in numbering**.
- In the final name, **"ene" comes before "yne"** alphabetically.

**Examples:**

| Compound | IUPAC Name | Notes |
|---|---|---|
| $CH \equiv C - CH_2 - CH = CH_2$ | Pent-1-en-4-yne | "yne" closer to end |
| $CH_2 = CH - C \equiv C - CH_3$ | pent-1-en-3-yne | Double bond gets lower number |
| $CH_3C \equiv CH \equiv C - (CH_3) - CF_2 = CH_2$ | 4, 4-difluoro-3-methylbut-1-yne | Multiple substituents + triple bond |

## ADDITIONAL NOTES

- **Euphony Rule:** Drop the final **"-e"** from "ene" or "yne" if the next part starts with a **vowel** (*e.g., pent-3-en-1-yne, not pent-3-ene-1-yne*).
- **Consonant Rule:** Add **"-a"** between root and "di/triene" etc. (*e.g., buta-1,3-diene, not but-1,3-diene*)

### Examples of Mixed Functional Groups: Group A – Prefix or Suffix

**General Rules for Naming Compounds with Group A, B, and C Functionalities:**

1. **Find the highest priority functional group:**
   - ❖ It will be indicated by **a suffix** in the compound's name.
   - ❖ The **carbon chain** must include this group.
2. **Number the carbon chain:** Start from the end that gives the **highest priority group** the **lowest possible number**.
3. **Incorporate multiple bonds** (from **Group B):**
   - ❖ Use **"-ene"** or **"-yne"** in place of **"-ane"**.
   - ❖ Assign position numbers to double/triple bonds.
4. **Apply the correct suffix:**
   - ❖ Drop the final **"e"** in "ene" or **"yne" if a vowel** follows (e.g., *pent-3-en-1-amine*).
   - ❖ Add an **"a"** between root and suffix when needed for clarity (e.g., *buta-1,3-diene*).
5. **Add other substituents as prefixes:**
   - ❖ Include **Group C** (Alkyl, halogen) and **lower-priority Group A** groups.
   - ❖ List all substituent prefixes in **alphabetical order** with their locants.

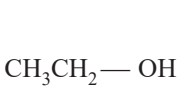
1. **Amines: prefix: amino-; suffix: -amine—substituents on nitrogen denoted by "N"**

| Structure | IUPAC Name | Notes |
|---|---|---|
| $CH_3CH_2CH_2NH_2$ | Propan-1-amine | "1" is optional; amine gets suffix |
| -Cyclohexane-$NH_2$ at position 1 | 3-Methoxycyclohexan-1-amine | Methoxy is a prefix; amine is suffix |
| $CH_2$=CH–CH(N($CH_2CH_3$)$_2$)–$CH_3$ | N, N-Diethylbut-3-en-2-amine | Double bond at C-3; N-substituents use "N" instead of numeric locants |

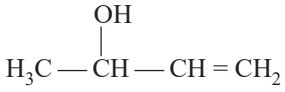
**Quick Notes on Substituent Numbering**

- Always number from the end that gives **the functional group or double/triple bond** the **lowest possible number**.
- When both a double and triple bond are present:
  - Use the group **closer to the chain end**.
  - If equal, **double bond (ene)** gets priority in numbering.
  - In the name: **"ene"** comes before **"yne"** alphabetically.

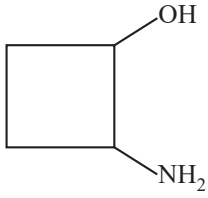
**2. Alcohols:** Prefix: hydroxy-; suffix: -ol



ethanol

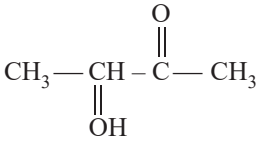


but-3-en-2-ol

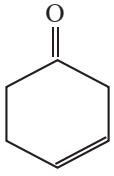


2-aminocyclobutan-1-ol
("1" is optional in this case)

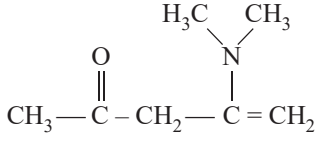
**3. Ketones:** Prefix: oxo-; suffix: -one



3-hydroxybutan-2-one



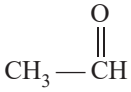
cyclohex-3-en-1-one
("1" is optional in this case)



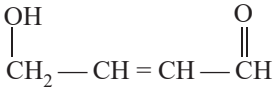
4–(N, N-dimethylamino) pent-4-en-2-one)

**4. Aldehydes:** Prefix: oxo-, or formyl– (O = CH–); suffix: –al (Abbreviation: –CHO).
An aldehyde can only be on carbon 1, so the "1" is generally omitted from the name.

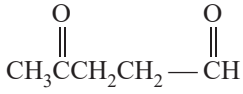
methanal; formaldehyde



ethanal; acetaldehyde

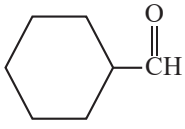


4-hydroxybut-2-enal



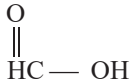
4-oxopentanal

**Specical Case:** When the chain cannot include the carbon of the CHO, the suffix "carbaldehyde" is used:

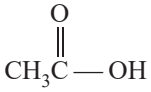


cyclohexanecarbaldehyde

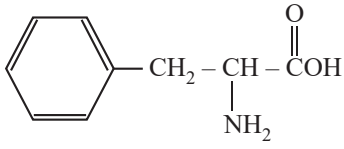
**5. Carboxylic Acids:** Prefix: carboxy–; suffix: –oic acid (Abbreviation: –COOH).
A carboxylic acid can only be on carbon 1, so the "1" is generally omitted from the name.



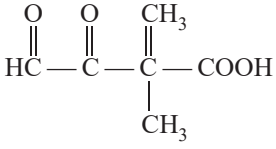
methanoic, acid; formic acid



ethanoic acid; acetic acid



2-amino-3-phenylpropanoic acid

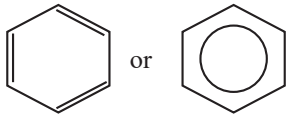


2, 2-dimethyl-3, 4-dioxobutanoic acid

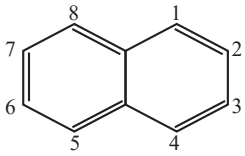
**(Note):** Chemists tradionally use and IUPAC accepts the names "formic acid" and "acetic acid" in place of "methanoic acid" and "ethanoic acid".

**Special Case:** When the chain numbering cannot include the carbon of the COOH, the suffix "carboxylic acid" is used. See example on next page.

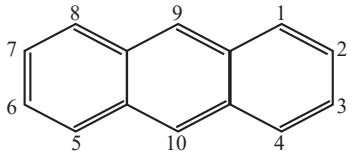
## A. Common Parent Ring Systems:




benzene



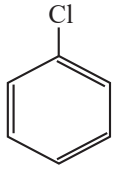

naphthalene



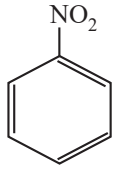

anthracene

## B. Monosubstituted Benzenes:

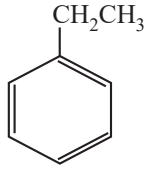
1. Most substituents keep their designation, followed by the word "benzene":




chlorobenzene

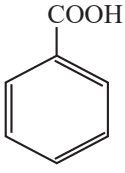



nitrobenzene

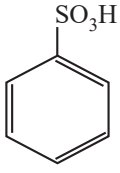



ethylbenzene

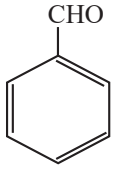
2. Some common substituents change the root name of the ring. IUPAC accepts these as root names, listed here in decreasing priority:



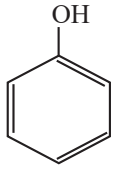

benzoic acid



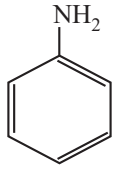

benzene-sulfonic acid



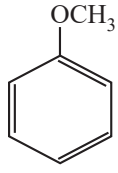

benzaldehyde



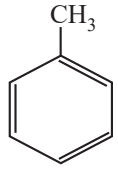

phenol




aniline



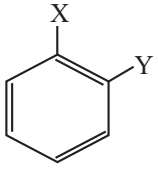

anisole

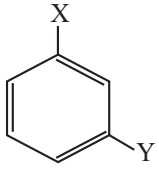


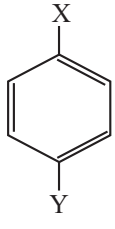

toluene

## C. Disubstituted Benzenes:

1. Designation of substitution–only three possibilities:

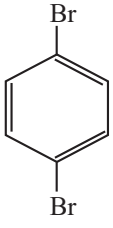


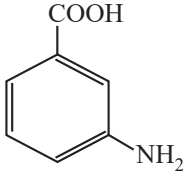




| | | | |
|---|---|---|---|
| common: | *ortho-* | *meta-* | *para-* |
| IUPAC: | 1, 2– | 1, 3– | 1, 4– |

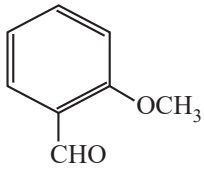
2. Naming disubstituted benzenes–priorities determine root name and substituents:



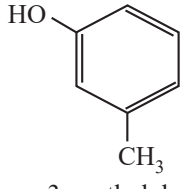

1, 4–dibromobenzene



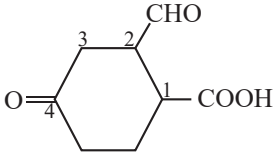

3–aminobenzoic acid




2–methoxybenzaldehyde




3–methylphenol



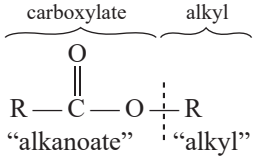

2-formyl-4-oxocyclohexanecarboxylic acid ("Formyl" is used to indicate an aldehyde as a substituent when its carbon cannot be in the chain numbering)

**D. Naming carboxylic acid derivatives:** The six common groups derived from carboxylic acids are salts, anhydrides, esters, acyl halides, amides and nitriles. Salts and esters are most important.

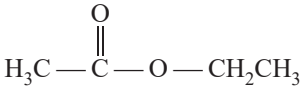
**1. Salts of Carboxylic Acids:** Salts are named with cation first, followed by the anion name of the carboxylic acid, where "ic acid" is replaced by "ate":

| | | |
|---|---|---|
| Acetic acid | Becomes | Acetate |
| butanoic acid | becomes | butanoate |
| cyclohexanecarboxylic acid | becomes | cyclohexanecarboxylate |

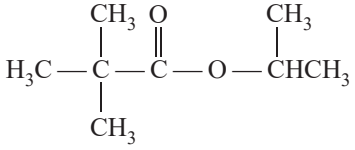
**2. Esters:** Esters are named as "organic salts" that is, the alkyl name comes first, followed by the name of the carboxylate anion. (Common abbreviation: –COOR)



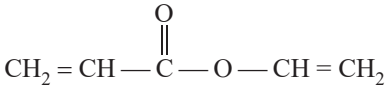

"alkyl alkanoate"



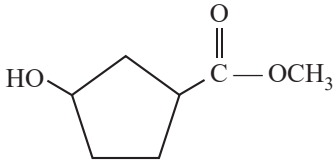

ethyl acetate



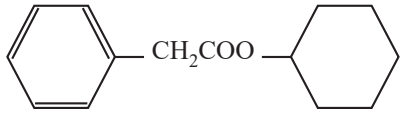

isopropyl 2, 2-dimethylpropanoate




vinyl prop-2-enoate



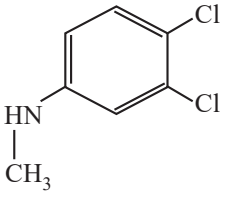

methyl 3-hydroxycyclopentanecarboxylate



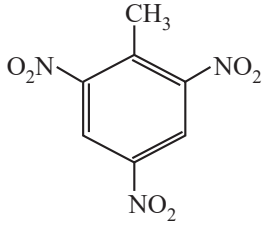

cyclohexyl 2-phenylacetate

**3. Nomenclature of Aromatic Compounds:** "Aromatic" compounds are those derived from benzene and similar ring systems. As with aliphatic nomenclature described above, the process is: determining the root name of the parent ring; determining priority, name and position number of substituents; and assembling the name in alphabetical order. Functional group priorities are the same in aliphatic and aromatic nomenclature.

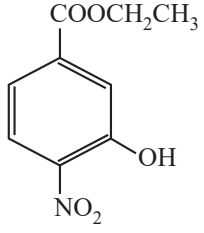
**E. Polysubstituted benzenes:**




3, 4–dichloro-N-methylaniline

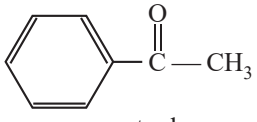



2, 4, 6-trinitrotoluene (TNT)

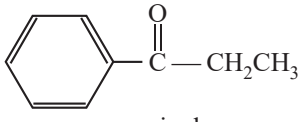



ethyl 4-amino-3-hydroxybenzoate

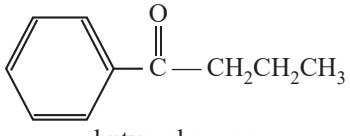
**F. Aromatic ketones:** A special group of aromatic compounds are ketones where the carbonyl is attached to at least one benzene ring. Such compounds are named as "phenones", the prefix depending on the size and nature of the group on the other side of the carbonyl. These are the common examples:



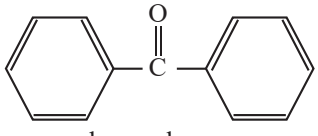

acetophenone




propiophenone




butyrophenone




benzophenone

# IMPORTANT MCQS FOR PRACTICE

**1.** What is the IUPAC name of $CH_3 - CH_2 - CH_3$?
(*a*) Methane (*b*) Propane (*c*) Ethane (*d*) Butane

**2.** What is the correct IUPAC name of $CH_3CH_2CH_2OH$?
(*a*) Propanol (*b*) Propyl alcohol (*c*) Ethanol (*d*) Propan-1-ol

**3.** In the IUPAC system, which has the highest priority when assigning suffixes?
(*a*) Alkene (*b*) Alkyne (*c*) Aldehyde (*d*) Alcohol

**4.** What is the IUPAC name of the compound $CH_3–CH=CH–CH_3$?
(*a*) Butane (*b*) But-1-ene (*c*) But-2-ene (*d*) 2-Butyne

**5.** What is the correct IUPAC name for $(CH_3)_3C–CH_2CH_3$?
(*a*) 2-methylbutane (*b*) 2, 2-dimethylbutane (*c*) 2, 2-dimethylpentane (*d*) 3-methylpentane

**6.** Which of the following is correctly named according to IUPAC rules?
(*a*) 2, 2-dimethylpropane (*b*) 1, 1-dimethylethane (*c*) Isobutane (*d*) Tert-butane

**7.** What is the IUPAC name of $CH_3 - CH = CH - CH_2 - COOH$?
(*a*) Pent-2-enoic acid (*b*) 2-Butenoic acid (*c*) Pent-4-enoic acid (*d*) But-2-enoic acid

**8.** Identify the correct IUPAC name of the compound:
$CH_3 - CH(CH_3) - CH_2 - CH(CH_3) - CH_3$
(*a*) 2, 3-dimethylpentane (*b*) 2, 4-dimethylpentane (*c*) 3, 4-dimethylpentane (*d*) 2, 3-dimethylhexane

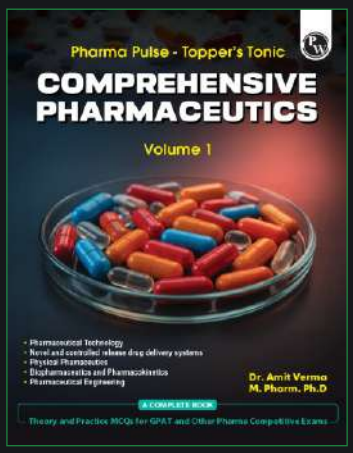
**9.** What is the correct IUPAC name for the compound:
$CH_3 - CH = CH - C(CH_3)_2 - COOH$
(*a*) 2-methyl-3-pentenoic acid (*b*) 3, 3-dimethylpent-2-enoic acid
(*c*) 3, 3-dimethylpent-4-enoic acid (*d*) 3, 3-dimethylpent-2-enoic acid

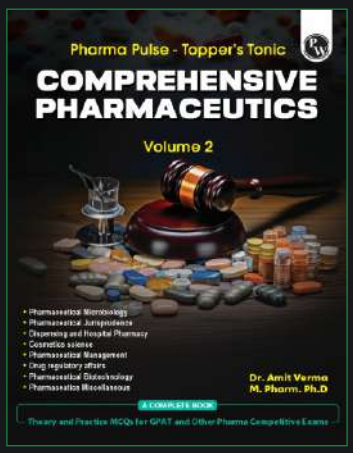
**10.** Which compound has the IUPAC name:
N, N-dimethylpropan-1-amine
(*a*) $CH_3 - CH_2 - CH_2 - NH(CH_3)_2$ (*b*) $CH_3 - NH - CH_2CH_2CH_3$
(*c*) $CH_3 - CH_2 - NH - CH_3$ (*d*) $CH_3 - CH_2 - CH_2 - CH_2 - NH_2$

# ANSWER KEY

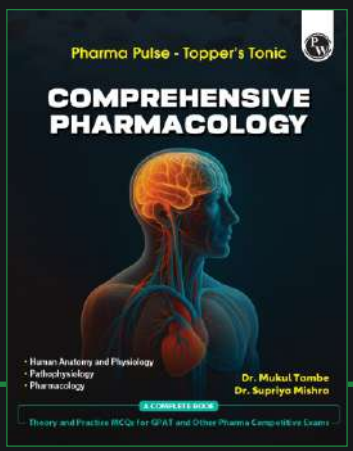
| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **1.** (*b*) | **2.** (*d*) | **3.** (*c*) | **4.** (*c*) | **5.** (*c*) | **6.** (*a*) | **7.** (*a*) | **8.** (*a*) | **9.** (*d*) | **10.** (*a*) |

# Important Books For This Series





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