Lecture 4

Trivial, rational and IUPAC nomenclatures of organic compounds

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Aim and Objectives

Aim: to study the trivial, rational and IUPAC nomenclature systems, and understand their principles, differences and applications.

1. Define organic nomenclature and its importance
2. Explain the principles of trivial nomenclature
3. Describe rational nomenclature and its structural basis
4. Study the systematic naming rules of IUPAC
5. Identify functional groups, parent chains and substituents
6. Compare the three systems using examples
7. Develop practical skills in naming organic compounds

Introduction to Organic Nomenclature

Rules for assigning names to organic compounds by composition, structure and functional groups. With millions of compounds, standard naming is essential.

- Identifies chemical substances clearly
- Distinguishes compounds with different structures
- Indicates functional groups
- Supports research, pharmaceuticals and industry

Trivial

Common or historical names

Rational

Derivatives of simpler parents

IUPAC

International systematic rules

Trivial Nomenclature

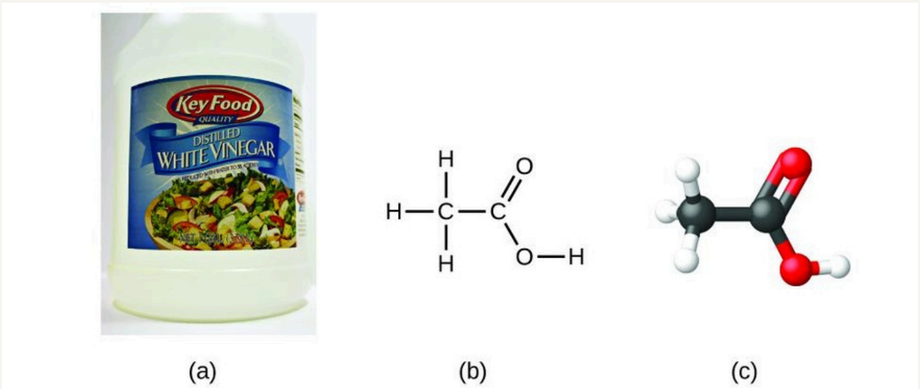
Common or historical names taken from natural sources, properties, discoveries or practical uses.

Characteristics

- Names are not always related to molecular structure
- Common in everyday life and industry
- Often based on the original source of a compound
- Simple, familiar names are often retained

Examples

- Acetic acid, CH_3COOH → ethanoic acid
- Formic acid, $HCOOH$ → methanoic acid
- Acetone, CH_3COCH_3 → propan-2-one
- Ethylene, C_2H_4 → ethene
- Glycerol, $C_3H_8O_3$ → propane-1,2,3-triol



Acetic Acid
Derived from the Latin word acetum, meaning vinegar.
Formula: CH_3COOH

Formic Acid
Derived from the Latin word formica, meaning ant**.**

Citric Acid
Named after citrus fruits, in which it naturally occurs.
Formula: $C_6H_8O_7$

Origin of Trivial Names

Many names come from natural materials or historical preparation methods.

Acetic acid

CH_3COOH

From Latin *acetum*, vinegar

Formic acid

$HCOOH$

From Latin *formica*, ant

Citric acid

$C_6H_8O_7$

Named after citrus fruits, where it occurs

Trivial names preserve historical and practical origins, though they do not always describe structure.

Rational Nomenclature

Compounds are treated as derivatives of simpler parent substances. The name identifies the alkyl or aryl groups attached to a reference compound or functional class.

Main principles

- The compound is related to a basic structural unit
- Attached alkyl or aryl groups are named
- Names show relationships between fragments
- Mostly met in older terminology

Examples

- CH_3CH_2OH: ethyl alcohol (ethanol)
- CH_3OCH_3: dimethyl ether (methoxymethane)
- CH_3COCH_3: dimethyl ketone (propan-2-one)
- $CH_3CH_2NH_2$: ethylamine (ethanamine)

Principles of Rational Nomenclature

Alcohol

CH_3CH_2OH

Ethyl alcohol

Ethyl group + alcohol

Ether

$CH_3–O–CH_2CH_3$

Ethyl methyl ether

Methyl + ethyl + ether

Ketone

$CH_3–CO–CH_2CH_3$

Ethyl methyl ketone

Methyl + ethyl + ketone

Alkyl / aryl groups + functional class → rational name

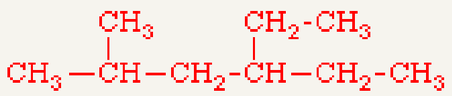
IUPAC Nomenclature

The internationally standardized system of the International Union of Pure and Applied Chemistry.

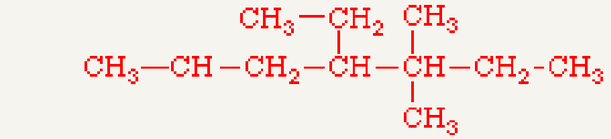
1. Select the parent structure
2. Identify the principal functional group
3. Number the parent structure by the rules
4. Identify and name substituents
5. Indicate positions with locants
6. Combine prefixes, parent name and suffixes

$CH_3–CH(CH_3)–CH_2–CH_3$ = 2-methylbutane

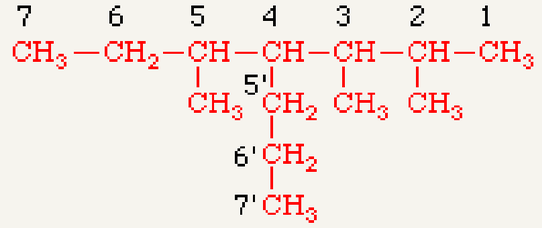
Parent: butane · substituent: methyl · position: carbon 2



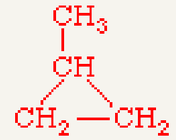
4-ethyl-2-methylhexane



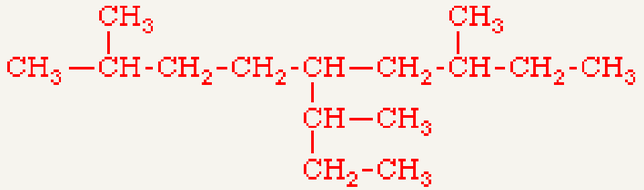
4-ethyl-3,3-dimethylheptane



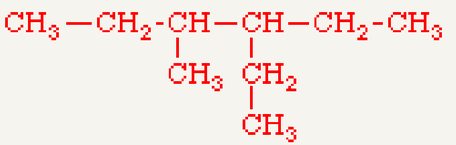
2,3,5-trimethyl-4-propylheptane
(NOT: 2,3-dimethyl-4-sec-butylheptane)



methylcyclopropane



5-sec-butyl-2,7-dimethylnonane



3-ethyl-4-methylhexane

Parent Chains and Root Names

For saturated hydrocarbons, the number of carbon atoms sets the root name.

CH_4 → methane · $CH_3–CH_2–CH_3$ → propane · $CH_3–(CH_2)_3–CH_3$ → pentane

C atoms	Root	Alkane
1	Meth-	Methane
2	Eth-	Ethane
3	Prop-	Propane
4	But-	Butane
5	Pent-	Pentane

C atoms	Root	Alkane
6	Hex-	Hexane
7	Hept-	Heptane
8	Oct-	Octane
9	Non-	Nonane
10	Dec-	Decane

Functional Groups in IUPAC Names

Functional groups set chemical properties and usually the suffix of the systematic name.

Alcohol

–OH

suffix -ol · ethanol

Aldehyde

–CHO

suffix -al · ethanal

Carboxylic acid

–COOH

suffix -oic acid · ethanoic acid

Alkyne

C≡C

suffix -yne · ethyne

Amine

–NH_2

suffix -amine · ethanamine

Ester

–COOR

suffix -oate · methyl ethanoate

Ketone

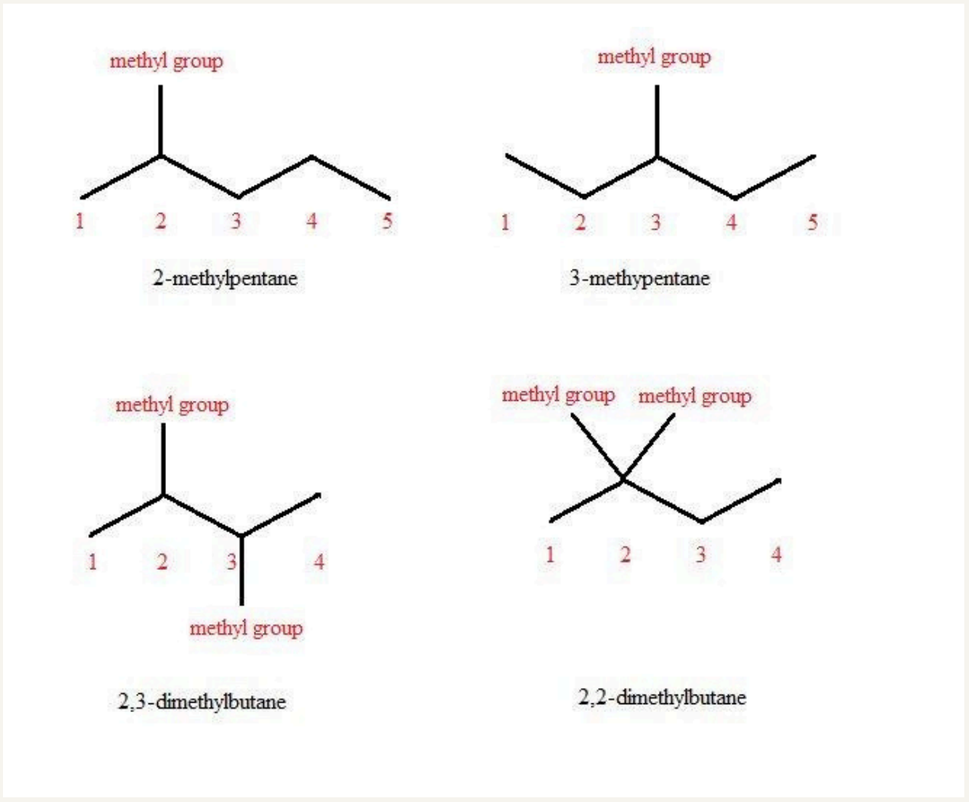
–CO–

suffix -one · propanone

Alkene

C=C

suffix -ene · ethene



Naming Branched Compounds

1. Select the parent chain
2. Number it for the lowest locants
3. Identify the substituents
4. Give the position of each
5. List prefixes alphabetically

2-methylpropane

$CH_3–CH(CH_3)–CH_3$

2,3-dimethylbutane

$CH_3–CH(CH_3)–CH(CH_3)–CH_3$

3-methylpentane

$CH_3–CH_2–CH(CH_3)–CH_2–CH_3$

Unsaturated Compounds

Compounds with carbon–carbon double or triple bonds. A locant gives the position when needed.

Alkenes (C=C)

$CH_2{=}CH{-}CH_3$

Propene

Suffix -ene

Alkynes (C≡C)

$CH_3{-}C{\equiv}C{-}CH_3$

But-2-yne

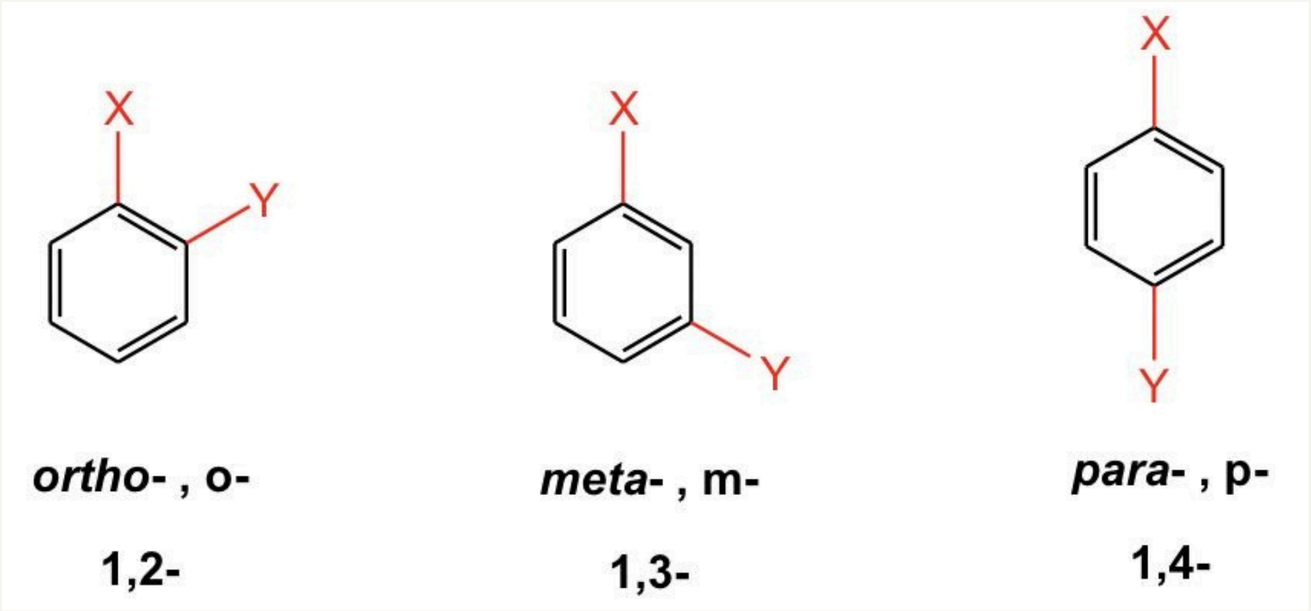
Suffix -yne

Position

$CH_2{=}CH{-}CH_2{-}CH_3$

But-1-ene

Numbered locant



Aromatic Compounds

Benzene (C_6H_6) is the most common aromatic ring. Substituted benzenes are named by their groups and positions.

- Toluene, $C_6H_5–CH_3$ → methylbenzene
- Phenol, $C_6H_5–OH$ → phenol (retained IUPAC name)
- Aniline, $C_6H_5–NH_2$ → benzenamine (aniline is retained)
- Nitrobenzene, $C_6H_5–NO_2$ → nitrobenzene

ortho (o-)
1,2-position

meta (m-)
1,3-position

para (p-)
1,4-position

These descriptors are widely used; systematic names use numerical locants.

Comparison of the Three Systems

Feature	Trivial	Rational	IUPAC
Basis	History, common usage	Structural relationships	Standardized rules
Structural information	Often limited	Partial	Usually detailed
Standardization	Limited	Varies	International
Main use	Everyday, traditional	Functional-class naming	Scientific communication
Example	Acetone	Dimethyl ketone	Propan-2-one

The systems are not strictly separate: some traditional or functional-class names are also accepted by IUPAC.

More Examples Across Systems

Each line reads: trivial name → rational name → IUPAC name.

- Wood alcohol → methyl alcohol → methanol
- Grain alcohol → ethyl alcohol → ethanol
- Acetone → dimethyl ketone → propan-2-one
- Diethyl ether → diethyl ether → ethoxyethane
- Methyl ethyl ketone → ethyl methyl ketone → butan-2-one

Some names are the same in two systems, which shows the systems overlap.

Practice and Exercises

Example 1

$CH_3–CH_2–OH$

Rational: ethyl alcohol
IUPAC: ethanol

Example 2

$CH_3–CO–CH_3$

Trivial: acetone
Rational: dimethyl ketone
IUPAC: propan-2-one

Example 3

$CH_3–CH(CH_3)–CH_2–CH_3$

Butane parent, methyl at C2
IUPAC: 2-methylbutane

Questions

1. IUPAC name of CH_3COOH?
2. Rational name of CH_3OCH_3?
3. How many carbon atoms in hexane?
4. Which group is –CHO?

Conclusion

1. Trivial: historical names and traditional usage
2. Rational: structural fragments and functional classes
3. IUPAC: internationally standardized systematic rules
4. Correct naming needs parent structure, functional groups, substituents and positions

IUPAC is the principal international standard, while trivial and rational names remain important in chemistry, medicine and industry.

References: IUPAC Blue Book (2013); Clayden, Greeves & Warren; McMurry; Smith (March’s)