# Chapter 12

# Introduction to Organic Chemistry: Alkanes

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**Chapter 12 suggested problems: 26, 28, 30, 32, 34, 44, 48, 50, 52, 54, 56, 58, 66**

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## Class Notes

I. Organic chemistry - the study of carbon and its compounds

   A. Inorganic chemistry - the study of all other elements and their compounds

   B. Nearly all organic chemicals also contain H; many also contain O, N, S, P, halogens, etc.

   C. Organic chemistry is the basis of biochemistry

II. Families of organic chemicals

   A. The proper (systematic, or IUPAC) name of organic compounds states two pieces of information about the compound: the class of the compound, as determined by its functional group, and the number of carbon atoms in the longest chain containing the most important functional group

   B. Chain length and names (See Table 12.3, p. 338)

| | | |
|---|---|---|
| 1 | $CH_3$- | methyl |
| 2 | $C_2H_5$- | ethyl |
| 3 | $C_3H_7$- | propyl |
| 4 | $C_4H_9$- | butyl |
| 5 | $C_5H_{11}$- | pentyl |
| 6 | $C_6H_{13}$- | hexyl |
| 7 | $C_7H_{15}$- | heptyl |
| 8 | $C_8H_{17}$- | octyl |
| 9 | $C_9H_{19}$- | nonyl |
| 10 | $C_{10}H_{21}$- | decyl |

C. Organic compounds are generally classed by their functional groups, atoms or molecules which determine the general chemistry of the compounds (See Table 12.1, p. 329): note that in most cases naming the compound is based in naming the compound as an alkane and then substituting the appropriate suffix for the class of compounds

| family | family name | functional groups |
|---|---|---|
| alkane | ane | C-C single bonds |
| alkene | ene | C-C double bonds |
| alkyne | yne | C-C triple bonds |
| aromatic | | multiple double bonds, ring compounds |
| alcohol | ol | -OH group |
| ether | ether | C-O-C |
| aldehyde | al | -CHO |
| ketone | one | C-CO-C |
| carboxylic acid | oic acid | -COOH |
| ester | alcohol name + acid name changed to "ate" | COOC |
| amine | amine | organic substituted ammonia |
| amide | amide | CONH |

D. Note that the name of a compound is often based on first naming the compound as an alkane and then modifying the name with the appropriate family suffix

III. Bonding in carbon and other nonmetal atoms

A. Carbon is tetravalent and forms four covalent bonds (nm-nm bonds)

B. Tetrahedral geometry; geometry (shape) is often of paramount importance when studying biological activity of compounds

C. The bonding of other nonmetal atoms (i.e., the number of covalent bonds formed) can easily be determined from the element's position in the periodic table

IV. Hybridization and hybrid orbitals

A. Orbital shapes - s, p, d

B. Orbital overlap is essential for chemical bonding to occur; the greater the overlap the stronger the bond

1. Show overlap between hydrogen and oxygen in water

2. Overlap is an important factor in bond strength but certainly not the only factor

3. If carbon has four valence electrons ($2s^2$ $2p^2$), how can it form four bonds?

a. In the 1930s Linus Pauling suggested that one of the 2s electrons is promoted to the empty 2p orbital, resulting in the formation of four hybrid orbitals that are intermediate in energy and shape

b. Diagram of orbitals vs. energy

c. This hybridization theory can be easily and accurately used to describe bonding in many molecules, and in fact is generally used to describe the covalent bonding of many nonmetallic compounds

| **atom** | **molecule** | **valence configuration** | **hybridization** | **remaining orbitals** |
|---|---|---|---|---|
| Be | $BeH_2$ | $2s^2$ | sp | 2 p orbitals |
| B | $BF_3$ | $2s^2$ $2p^1$ | $sp^2$ | 1 p orbitals |
| C | $CH_4$ | $2s^2$ $2p^2$ | $sp^3$ | none |
| P | $PCl_5$ | $3s^2$ $3p^3$ | $dsp^3$ | 4 d orbitals |
| S | $SF_6$ | $3s^2$ $3p^4$ | $d^2sp^3$ | 3 d orbitals |

C. Hybridization and multiple covalent bonds

1. Double bonds - consist of one sigma bond and one pi bond

a. Sigma bonds

i. Cylindrical probability distribution around the bond axis

ii. Sigma bonds are created by the overlap of hybridized orbitals

b. Pi bonds

i. Probability out of the plane (above and below) the bond axis

ii. Pi bonds are created by the overlap of the unhybridized p orbitals

2. Triple bonds consist of one sigma bond and two pi bonds

3. Summary

| **bond type** | **sigma bonds** | **pi bonds** |
|---|---|---|
| single | 1 | 0 |
| double | 1 | 1 |
| triple | 1 | 2 |

4. The relationship between sigma bonds, hybridization, and molecular geometry

| **bond type** | **hybridization** | **geometry** |
|---|---|---|
| single | $sp^3$ | tetrahedral |
| double | $sp^2$ | tbp |
| triple | sp | linear |

D. An understanding of Lewis structures and hybridization facilitates the prediction of bond strengths, bond lengths, and bond angles, which is important because molecular shape often determines the behavior of the molecule in chemical reactions and in biological systems

V. Molecular and structural formulas: drawing organic structures

A. Molecular formulas indicate the elements and the number of atoms of each element in a substance

B. Structural formulas demonstrate connectivity

C. There are different types of structural formulas: example - pentane

1. Expanded structure: drawn out, all bonds shown

2. Condensed structure: $CH_3CH_2CH_2CH_2CH_3$ - bonds to central carbon backbone are collapsed

3. Skeleton structure: C-C-C-C-C-C - hydrogen is not shown but O, S, etc. are shown

4. Line structure: carbon backbone is represented as a series of zigzags, H is not shown, other atoms are shown

D. "R" groups - used as a general substitution for any organic molecule or fragment of a molecule

VI. Alkanes

A. General information

1. Most commonly obtained from petroleum and natural gas, decomposition of organic material

2. Uses: energy sources, fuels, feed materials for synthetics - most are flammable

3. Low toxicity

4. Odorless or mild odor, colorless, tasteless

5. Generally relatively unreactive except in combustion reactions and with halogens

6. General formula: $C_nH_{2n+2}$

7. Saturated hydrocarbons: each carbon atom is bonded to the maximum number of hydrogen atoms (no C-C double or triple bonds)

B. Naming alkanes

1. Categorization of carbon atoms: primary (1°), secondary (2°), tertiary (3°), quaternary (4°)

2. IUPAC and common names

3. Straight chain alkanes

a. The longest continuous chain forms the base name

b. Functional group contributes name suffix

4. Branched alkanes: indicate side chains by adding them as prefixes to the main compound name

a. Number backbone carbons so numbers are as low as possible

b. Alphabetize names of alkyl groups, ignoring prefixes

c. Use prefixes to indicate numbers of a given alkyl group: di, tri, tetra, penta, hexa, hepta, octa, nona, deca, etc.

d. Use hyphens to separate numbers from words

e. Use commas to separate numbers

5. Common names

a. normal (n) - used for straight chain alkanes

b. n-Propyl and isopropyl

c. n-Butyl, sec-butyl (1-methylpropyl), isobutyl (2-methylpropyl), and tert-butyl (1,1-dimethylethyl)

6. Examples

C. Constitutional isomers of alkanes

1. Isomers: substances with the same molecular formula but that are different compounds

    a. Constitutional isomers (structural isomers): same atoms, different connectivity

        i. Ethanol and dimethyl ether

        ii. 1-pentanol, 2-pentanol, 3-pentanol, and ethyl propyl ether

    b. Geometric isomers: groups on opposite sides of a ring or a double bond

        i. Butane, cis-2-butene, and trans-2-butene

    c. Stereoisomers: same configurations but different spatial arrangements of the atoms; enantiomers and diastereomers; more later in course

2. Constitutional isomers of alkanes

    a. Butane: n-butane, 2-methylpropane

    b. Pentane: n-pentane, 2-methylbutane, 2,2-dimethylpropane

    c. Hexane: n-hexane, 2-methylpentane, 3-methylpentane, 2,2-dimethylbutane, 2,3-dimethylbutane

    d. Heptane: 9 isomers

    e. Octane: 18 isomers

    f. Nonane: 35 isomers

    g. Decane: 75 isomers

    h. $C_{20}H_{42}$: 366,319 isomers

    i. Note: there is no simple way to calculate the number of isomers

D. The shapes of organic molecules: conformations and bond rotation

1. Atoms and molecules are capable of different types of motion: translational, rotational, vibrational, and spin

2. Rotation occur around single bonds

3. Implication: same substance can appear different and yet not be different

E. Cycloalkanes and cis-trans isomerization

1. Cycloalkanes: simple saturated hydrocarbons that exist as closed rings (empirical formula $C_nH_{2n}$)

2. Nomenclature

   a. Count number of carbons in ring

   b. Add "cyclo" prefix without space or hyphen to name that corresponds to the number of ring carbons

   c. Substituents are named before cycloalkane name (do not need to use "1" if only one carbon has substituents)

   d. Other rules as detailed above

   e. Examples

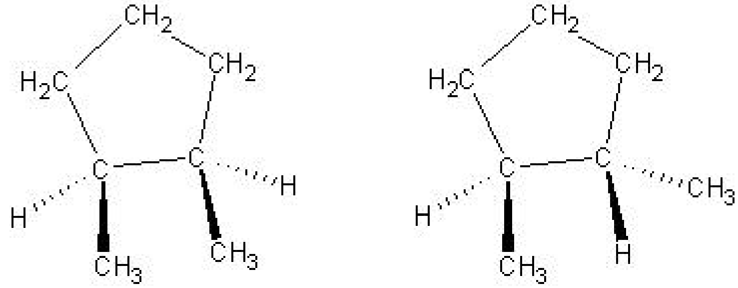
      i. Methylcyclopropane

      ii. 1-butyl-2-propyl-4-ethyl-cyclohexane (alphabetical order takes precedence)

3. Cis-trans (geometric) stereoisomerism: rotation is restricted around rings; compounds can have the same substituents attached to the same carbons but with slightly different spatial orientations

   a. cis and trans isomers have different physical and chemical properties

   b. cis-1,2-dimethylcyclopentane and trans-1,2-dimethylcyclopentane




F. Physical properties of alkanes and cycloalkanes

1. Intermolecular forces: only London forces (induced dipole - induced dipole) interactions in alkanes

2. Strength of bond forces increase with MW and polarizability
3. Shape affects bond strength by increasing the molecular surface area: the greater surface area, the stronger bonds (branched and cycloalkanes)
4. Relatively low BP and MP
5. Poor solubility in polar solvents, good solubility in nonpolar solvents ("like dissolves like")

G. Chemical properties: the reactions of alkanes and cycloalkanes

1. Combustion reactions - reaction with oxygen to liberate energy
    a. Stoichiometry and combustion reactions
2. Halogenation
    a. The halogenation of alkanes is a free-radical reaction, i.e., occurs in a step-wise fashion
        i. $CH_4 + 4\ Cl_2 \rightarrow CCl_4 + 4\ HCl$
    b. Nomenclature: use numbers, prefixes to indicate numbers (di, tri, etc.) and and types of halogens (fluoro, chloro, bromo, or iodo)
    c. As a class of compounds alkyl halides are important as degreasers and cleaning solvents, pesticides, anesthesias, and as intermediates in the synthesis of other organic chemicals

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