Summary and Notes for Exam Preparation: Introduction to Organic Compounds

Introduction to Organic Chemistry

Organic chemistry is the branch of chemistry that focuses on the study of carbon-based compounds. Carbon's unique ability to form four covalent bonds allows it to create a vast variety of molecules, ranging from simple ones like methane (CH_4) to complex polymers and biomolecules.

Key Concepts in Organic Chemistry

1. **Organic Molecules:** Organic molecules are primarily composed of carbon atoms, often in combination with hydrogen, oxygen, nitrogen, sulfur, and halogens (such as chlorine and bromine). These molecules can form long chains, branched structures, rings, and complex three-dimensional shapes.
2. **Functional Groups:** Functional groups are specific groups of atoms within molecules that determine the characteristics and chemical reactivity of those molecules. Common functional groups include hydroxyl (-OH), carbonyl (C=O), carboxyl (-COOH), amino ($-NH_2$), and halogens (e.g., -Cl, -Br).
3. **Hydrocarbons:** Hydrocarbons are the simplest organic molecules and consist entirely of carbon and hydrogen atoms. They are categorized into alkanes, alkenes, alkynes, and aromatic hydrocarbons based on the types of bonds between carbon atoms.
    - **Alkanes:** Saturated hydrocarbons with single C-C bonds (general formula: C_nH_{2n+2}).
    - **Alkenes:** Unsaturated hydrocarbons with one or more C=C double bonds (general formula: C_nH_{2n}).
    - **Alkynes:** Unsaturated hydrocarbons with one or more C≡C triple bonds (general formula: C_nH_{2n-2}).
    - **Aromatic Hydrocarbons:** Hydrocarbons containing benzene rings (C_6H_6) or similar ring structures.
4. **Representation of Organic Molecules:** Organic chemists use various notations to represent organic molecules, including empirical, molecular, structural, displayed, and general formulas.

Representation of Organic Molecules

1. **Empirical Formula:** The empirical formula represents the simplest whole-number ratio of atoms of each element in a compound. It does not provide information about the actual number of atoms, just their ratio.
   Example:

- For glucose ($C_6H_{12}O_6$), the empirical formula is CH_2O, as the ratio of carbon to hydrogen to oxygen is 1:2:1.

2. **Molecular Formula:** The molecular formula gives the exact number of atoms of each element in one molecule of the compound. It is a multiple of the empirical formula.
   Example:
   - For glucose, the molecular formula is $C_6H_{12}O_6$.
3. **Structural Formula:** The structural formula shows the arrangement of atoms within the molecule, indicating how the atoms are bonded to each other.
   Example:
   - The structural formula of ethanol (C_2H_5OH) is: H3C−CH2−OH
4. **Displayed Formula:** The displayed formula (or fully displayed formula) shows all the atoms and all the bonds between them. It provides a clear picture of the molecule's structure.

5. **General Formula of Hydrocarbons:** The general formula of a class of hydrocarbons provides a way to represent any member of that class using a single formula.
   Examples:
   - **Alkanes:** The general formula is C_nH_{2n+2}, where n is the number of carbon atoms.
     - For example, for n = 3 (propane), the formula is C_3H_8.
   - **Alkenes:** The general formula is C_nH_{2n}, where n is the number of carbon atoms.
     - For example, for n = 3 (propene), the formula is C_3H_6.
   - **Alkynes:** The general formula is C_nH_{2n-2}, where n is the number of carbon atoms.
     - For example, for n = 3 (propyne), the formula is C_3H_4.

Detailed Examples with Explanations

Example 1: Ethane (C_2H_6)

- **Empirical Formula:** The empirical formula of ethane is CH_3 because the ratio of carbon to hydrogen atoms is 2:6, which simplifies to 1:3.
- **Molecular Formula:** The molecular formula is C_2H_6.
- **Structural Formula:** H3C−CH3\text{H}_3\text{C} - \text{CH}_3H3C−CH3
- **General Formula (Alkane):** C_nH_{2n+2} (for n = 2, it becomes C_2H_6).

Example 2: Propene (C_3H_6)

- **Empirical Formula:** The empirical formula of propene is CH_2 because the ratio of carbon to hydrogen atoms is 3:6, which simplifies to 1:2.
- **Molecular Formula:** The molecular formula is C_3H_6.
- **Structural Formula:** H2C=CH−CH3
- **General Formula (Alkene):** C_nH_{2n} (for n = 3, it becomes C_3H_6).

Example 3: Butyne (C_4H_6)

- **Empirical Formula:** The empirical formula of butyne is C_2H_3 because the ratio of carbon to hydrogen atoms is 4:6, which simplifies to 2:3.
- **Molecular Formula:** The molecular formula is C_4H_6.
- **Structural Formula:** H3C−C≡C−CH3
- **General Formula (Alkyne):** C_nH_{2n-2} (for n = 4, it becomes C_4H_6).

Practice Questions and Answers

1. **Question:** What is the empirical formula of butane (C_4H_{10})?
    - **Answer:** The empirical formula of butane is C_2H_5 because the ratio of carbon to hydrogen atoms is 4:10, which simplifies to 2:5.
2. **Question:** Determine the molecular formula of a compound with an empirical formula of CH_2O and a molar mass of 180 g/mol.
    - **Answer:** The molar mass of the empirical formula CH_2O is 30 g/mol (C: 12, H: 2, O: 16).
    - The molecular formula is found by dividing the molar mass of the compound by the molar mass of the empirical formula:
    - 180 g/mol/ 30 g/mol=6
    - Therefore, the molecular formula is $C_6H_{12}O_6$.
3. **Question:** Write the displayed formula for ethene (C_2H_4).
    - **Answer:** The displayed formula for ethene is:

      H2C=CH2
4. **Question:** Explain the difference between the structural formula and the displayed formula of propane (C_3H_8).
    - **Answer:** The structural formula of propane shows the arrangement of atoms and the connections between them without showing all bonds: H3C−CH2−CH3 The displayed formula of propane shows all atoms and all bonds

Functional Groups

Functional groups are specific groups of atoms within molecules that have characteristic properties and reactivities. Understanding functional groups is crucial for naming organic compounds, predicting their reactivities, and understanding their properties.

1. **Hydroxyl Group (-OH):**
    - Found in alcohols.
    - Example: Ethanol (CH_3CH_2OH).
2. **Carbonyl Group (C=O):**
    - Found in aldehydes and ketones.
    - Example of aldehyde: Ethanal (CH_3CHO).
    - Example of ketone: Propanone (CH_3COCH_3).
3. **Carboxyl Group (-COOH):**
    - Found in carboxylic acids.
    - Example: Ethanoic acid (CH_3COOH).
4. **Amino Group (-NH_2):**
    - Found in amines.

- Example: Ethylamine ($CH_3CH_2NH_2$).

5. **Halides (R-X):**
   - Found in alkyl halides.
   - Example: Chloromethane (CH_3Cl).
6. **Nitrile Group (-CN):**
   - Found in nitriles.
   - Example: Ethanenitrile (CH_3CN).
7. **Nitro Group (-NO_2):**
   - Found in nitro compounds.
   - Example: Nitrobenzene ($C_6H_5NO_2$).

Naming Organic Compounds

The IUPAC system provides a systematic method for naming organic compounds. The name of an organic compound consists of three parts: the prefix, the root, and the suffix.

1. **Prefix:**
   - Indicates the substituents attached to the main carbon chain.
   - Example: Methyl, ethyl, chloro, bromo.
2. **Root:**
   - Indicates the number of carbon atoms in the longest continuous chain.
   - Example: Meth- (1 carbon), eth- (2 carbons), prop- (3 carbons).
3. **Suffix:**
   - Indicates the functional group present in the molecule.
   - Example: -ane (alkane), -ene (alkene), -yne (alkyne), -ol (alcohol), -al (aldehyde), -one (ketone), -oic acid (carboxylic acid).

Steps to Naming Organic Compounds:

1. Identify the longest continuous carbon chain.
2. Number the carbon atoms in the chain starting from the end nearest to a substituent or functional group.
3. Identify and name the substituents.
4. Combine the names of the substituents with the root and suffix, using appropriate locants (numbers) to indicate the positions of the substituents.

Examples:

1. **2-Chloropropane:**
   - Longest chain: 3 carbons (propane).
   - Substituent: Chlorine on the second carbon.
   - Name: 2-Chloropropane.
2. **3-Methylpent-2-ene:**
   - Longest chain: 5 carbons (pent-).
   - Double bond starting at the second carbon (pent-2-ene).
   - Substituent: Methyl group on the third carbon.
   - Name: 3-Methylpent-2-ene.

Bonding in Organic Molecules: Sigma (σ) and Pi (π) Bonds

In organic molecules, covalent bonds can be classified as sigma (σ) and pi (π) bonds.

1. **Sigma (σ) Bonds:**
    - Formed by the head-on overlap of atomic orbitals.
    - Every single bond consists of one σ bond.
    - Example: The C-H bonds in methane (CH_4) are all σ bonds.
2. **Pi (π) Bonds:**
    - Formed by the side-on overlap of p orbitals.
    - Found in double and triple bonds.
    - A double bond consists of one σ bond and one π bond.
    - A triple bond consists of one σ bond and two π bonds.
    - Example: The C=C double bond in ethene (C_2H_4) consists of one σ bond and one π bond.

Examples and Practice Problems

Example 1: Ethene (C_2H_4)

- Contains a C=C double bond.
- One σ bond and one π bond between the two carbon atoms.

Example 2: Ethyne (C_2H_2)

- Contains a C≡C triple bond.
- One σ bond and two π bonds between the two carbon atoms.

Practice Problems:

1. **Draw and identify the types of bonds in propene (C_3H_6).**
    - Solution:
      mathematica
      Copy code
        H2C=CH-CH3
        1. There is one double bond (one σ bond and one π bond) between the first and second carbon atoms, and single bonds (σ bonds) between the second and third carbon atoms and between each carbon and hydrogen.
2. **Name the following compound: $CH_3CH_2CH_2OH$.**
    - Solution:
        1. Longest chain: 3 carbons (propane).
        2. Functional group: Hydroxyl (-OH) on the first carbon.
        3. Name: Propan-1-ol.
3. **Determine the empirical and molecular formulas of a compound with 40% carbon, 6.7% hydrogen, and 53.3% oxygen by mass, with a molar mass of 180 g/mol.**
    - Solution:
        1. Assume 100 g of the compound:

        - 40 g C, 6.7 g H, 53.3 g O.
2. Convert to moles:
        - Moles of C = 40 g / 12 g/mol = 3.33 mol.
        - Moles of H = 6.7 g / 1 g/mol = 6.7 mol.
        - Moles of O = 53.3 g / 16 g/mol = 3.33 mol.
3. Simplify ratio:
        - C:H
          = 3.33:6.7:3.33 = 1:2:1.
4. Empirical formula: CH_2O.
5. Molecular formula:
        - Molar mass of CH_2O = 30 g/mol.
        - Molecular formula = (180 g/mol) / (30 g/mol) = 6.
        - Therefore, molecular formula = $C_6H_{12}O_6$.

Structural Isomerism

Structural isomers are compounds with the same molecular formula but different structural formulas. This means the atoms are connected in different ways, leading to different compounds with unique properties.

Types of Structural Isomerism:

1. **Chain Isomerism:**
    - Occurs when carbon chains are arranged differently.
    - Example: Butane (C_4H_{10}) can be n-butane (straight chain) or isobutane (branched chain).

2. **Position Isomerism:**
    - Occurs when functional groups are attached at different positions on the same carbon chain.
    - Example: Butan-1-ol ($CH_3CH_2CH_2CH_2OH$) vs. Butan-2-ol ($CH_3CH_2CHOHCH_3$).
3. **Functional Group Isomerism:**
    - Occurs when compounds have the same molecular formula but different functional groups.
    - Example: Propanal (CH_3CH_2CHO, an aldehyde) vs. Propanone (CH_3COCH_3, a ketone).

Stereoisomerism

Stereoisomers have the same molecular and structural formulas but differ in the spatial arrangement of atoms. The two main types of stereoisomerism are cis-trans isomerism and optical isomerism.

1. **Cis-Trans Isomerism (Geometric Isomerism):**
    - Occurs in alkenes and cyclic compounds where restricted rotation around a bond results in different spatial arrangements.
    - Example: 2-butene can exist as cis-2-butene (CH_3 groups on the same side) and trans-2-butene (CH_3 groups on opposite sides).

2. **Optical Isomerism:**
    - Occurs in molecules with a chiral center (a carbon atom bonded to four different groups).
    - These molecules exist as non-superimposable mirror images called enantiomers.
    - Example: 2-hydroxypropanoic acid (lactic acid) exists as two enantiomers.

Practice Problems and Examples

Structural Isomerism:

1. **Draw and name all the structural isomers of C_5H_{12} (pentane).**
    - n-Pentane: $CH_3CH_2CH_2CH_2CH_3$
    - Isopentane (2-methylbutane): $(CH_3)_2CHCH_2CH_3$
    - Neopentane (2,2-dimethylpropane): $(CH_3)_4C$
2. **Identify the type of isomerism between the following pairs:**
    - CH_3CH_2OH and CH_3OCH_3: Functional group isomerism.
    - $CH_3CH_2CH_2CH_2OH$ and $CH_3CH_2CHOHCH_3$: Position isomerism.

Cis-Trans Isomerism:

1. **Draw the cis and trans isomers of 1,2-dichloroethene ($C_2H_2Cl_2$).**
    - Cis-1,2-dichloroethene: ClHC=CHCl (Cl atoms on the same side).
    - Trans-1,2-dichloroethene: ClHC=CHCl (Cl atoms on opposite sides).
2. **Explain why cis-2-butene and trans-2-butene have different boiling points.**
    - Cis-2-butene has a higher boiling point than trans-2-butene because the polar C-H bonds on the same side cause a dipole-dipole interaction, whereas trans-2-butene has a more symmetrical structure, resulting in a lower boiling point.

Optical Isomerism:

1. **Identify the chiral centers in the following molecule: $CH_3CH(OH)CH_2CH_3$.**
    - The carbon atom bonded to OH, H, CH_3, and CH_2CH_3 is a chiral center.
2. **Draw the enantiomers of 2-butanol ($CH_3CH(OH)CH_2CH_3$).**
    - Enantiomer 1: $CH_3CH(OH)CH_2CH_3$ with OH on the right.
    - Enantiomer 2: $CH_3CH(OH)CH_2CH_3$ with OH on the left

Mechanisms of Organic Reactions

Organic reactions occur through various mechanisms that describe the step-by-step process of bond breaking and forming.

1. **Homolytic Fission:**
    - **Definition:** Homolytic fission involves the equal splitting of a covalent bond, with each atom taking one electron from the bond, resulting in the formation of free radicals.
    - **Example:** The homolytic fission of a chlorine molecule under UV light produces two chlorine radicals. Cl2→2Cl.

2. **Heterolytic Fission:**
    - **Definition:** Heterolytic fission involves the unequal splitting of a covalent bond, where one atom takes both bonding electrons, leading to the formation of ions.
    - **Types of Ions Formed:**
        - **Carbocation:** Positively charged carbon ion (e.g.CH_3^+).
        - **Carbanion:** Negatively charged carbon ion (e.g., CH_3^-).
    - **Example:** The heterolytic fission of a hydrogen chloride molecule. $HCl \rightarrow H^+ + Cl^-$

Free Radical Mechanism

Free radicals are highly reactive species with an unpaired electron. Free radical reactions typically involve three stages:

1. **Initiation:** Formation of radicals.
    - Example: Chlorine radicals are formed by homolytic fission. $Cl_2 \rightarrow 2Cl$.
2. **Propagation:** Radicals react with stable molecules to form new radicals.
    - Example: Chlorine radical reacts with methane to form methyl radical and HCl. $Cl\cdot + CH_4 \rightarrow CH_3\cdot + HCl$
3. **Termination:** Radicals combine to form stable molecules.
    - Example: Two methyl radicals combine to form ethane. $2CH_3\cdot \rightarrow C_2H_62$

Electronic Effects in Organic Chemistry

1. **Inductive Effect:**
    - **Definition:** The shifting of electrons in a sigma bond in response to the electronegativity of nearby atoms.
    - **Example:** In chloromethane (CH_3Cl), the electron density is pulled towards the chlorine atom, creating a partial negative charge on chlorine and a partial positive charge on carbon.
2. **Electromeric Effect:**
    - **Definition:** The temporary shifting of electrons in a double bond or a conjugated system in response to the presence of a reagent.
    - **Example:** When a proton attacks ethene, the pi electrons shift towards one carbon, creating a carbocation intermediate.
3. **Mesomeric Effect (Resonance Effect):**
    - **Definition:** The delocalization of electrons in molecules with conjugated systems, resulting in resonance structures.
    - **Example:** The delocalization of electrons in benzene leads to resonance structures that stabilize the molecule.

Reaction Intermediates

1. **Carbocations:** Positively charged carbon species with three bonds and an empty p-orbital.
2. **Carbanions:** Negatively charged carbon species with three bonds and a lone pair of electrons.

3. **Free Radicals:** Neutral species with an unpaired electron.

Types of Organic Reactions

1. **Addition Reactions:**
    - **Definition:** Two molecules combine to form a single product.
    - **Example:** Hydrogenation of ethene to form ethane. $C2H4+H2\rightarrow C2H6$
2. **Elimination Reactions:**
    - **Definition:** A single molecule splits into two products, usually involving the removal of a small molecule.
    - **Example:** Dehydration of ethanol to form ethene. $C2H5OH\rightarrow C2H4+H2O$
3. **Substitution Reactions:**
    - **Definition:** An atom or group of atoms in a molecule is replaced by another atom or group of atoms.
    - **Example:** Halogenation of methane. $CH4+Cl2\rightarrow CH3Cl+HCl$
4. **Reduction Reactions:**
    - **Definition:** Gain of electrons or hydrogen atoms, or loss of oxygen atoms.
    - **Example:** Reduction of a ketone to a secondary alcohol. $R2C=O+H2\rightarrow R2CHOH$
5. **Oxidation Reactions:**
    - **Definition:** Loss of electrons or hydrogen atoms, or gain of oxygen atoms.
    - **Example:** Oxidation of a primary alcohol to an aldehyde. $RCH2OH+[O]\rightarrow RCHO+H2O$
6. **Hydrolysis Reactions:**
    - **Definition:** Breaking of a bond in a molecule using water.
    - **Example:** Hydrolysis of an ester to form an alcohol and a carboxylic acid. RCOOR'+H2O→RCOOH+R'OH

Electrophiles and Nucleophiles

1. **Electrophiles:**
    - **Definition:** Electron-deficient species that seek electrons.
    - **Examples:** H+\text{H}^+H+, NO2+\text{NO}_2^+NO2+, Br2\text{Br}_2Br2.
2. **Nucleophiles:**
    - **Definition:** Electron-rich species that donate electrons.
    - **Examples:** OH−\text{OH}^-OH−, CN−\text{CN}^-CN−, NH3\text{NH}_3NH3.

Practice Problems

1. **Draw the mechanism for the chlorination of methane.**
    - Include initiation, propagation, and termination steps.
    - Show formation of methyl chloride and hydrogen chloride.
2. **Explain the inductive effect in the following molecules:**
    - CH_3CH_2Cl vs. CH_3CH_2OH
    - Which is more electron-withdrawing and why?
3. **Draw all possible resonance structures for the nitrate ion (NO_3^-).**
    - Explain how these structures contribute to the stability of the ion.
4. **Identify the type of isomerism in the following pairs:**

  - CH_3CH_2OH vs. CH_3OCH_3
  - Cis-2-butene vs. trans-2-butene
5. **Predict the products of the following reactions and classify the reaction type:**
  - Ethene + Br_2
  - 2-bromopropane + KOH (ethanol)
  - Benzene + HNO_3 (with H_2SO_4 as catalyst)