

# Analysis of Simple Organic Compounds

## Introduction

The analysis of organic compounds is the process of determining the identity, structure, and purity of a substance. In the laboratory, this transition from an "unknown" to a known structure involves a combination of classical chemical methods (wet chemistry) and modern spectroscopic techniques. While chemical tests identify specific functional groups, spectroscopy provides a "fingerprint" or a detailed map of the molecular framework.

## Learning Objectives

By the end of this module, you will be able to:

- Apply chemical methods to identify functional groups in simple organic compounds.
- Interpret spectroscopic data (IR, NMR, and Mass Spec) to elucidate molecular structures.
- Integrate analytical data to transition from a molecular formula to a complete structural representation.

## Key Concepts and Definitions

Term	Definition
<b>Spectroscopy</b>	The study of the interaction between matter and electromagnetic radiation to determine structure.
<b>Infrared (IR) Spectroscopy</b>	A technique used to identify functional groups by measuring the vibrations of chemical bonds.
<b>Nuclear Magnetic Resonance (NMR)</b>	A technique used to map the carbon-hydrogen framework by

	measuring the magnetic properties of atomic nuclei.
<b>Mass Spectrometry (MS)</b>	A technique that measures the mass-to-charge ratio of ions to determine molecular weight and formula.
<b>Chemical Shift (<math>\delta</math>)</b>	The position on an NMR spectrum that indicates the electronic environment of a nucleus.
<b>Wavenumber (<math>\text{cm}^{-1}</math>)</b>	The unit of frequency used in IR spectroscopy; proportional to the energy of vibration.

## Detailed Discussion

### Why Multiple Analytical Techniques Are Required

No single analytical method can fully determine the structure of an organic compound. Each technique provides different but complementary information:

- **Chemical tests** quickly indicate the presence of specific functional groups.
- **IR spectroscopy** confirms functional groups through characteristic bond vibrations.
- **NMR spectroscopy** reveals the hydrogen and carbon framework of the molecule.
- **Mass spectrometry** determines molecular weight and fragmentation patterns.

Accurate structural identification requires **correlating results from all methods**, not relying on a single test.

### Chemical Methods for Functional Group Identification

Before expensive instrumentation, chemists used "wet" chemical tests to narrow down functional groups. These are still used for rapid qualitative analysis:

- **Unsaturation (Alkenes/Alkynes):** Bromine Test ( $\text{Br}_2$  in  $\text{CCl}_4$ ); disappearance of reddish-brown color indicates a double or triple bond.
- **Alcohols:** Lucas Test (using  $\text{ZnCl}_2$  in  $\text{HCl}$ ); identifies primary, secondary, or tertiary alcohols based on the speed of cloudiness (formation of alkyl halide).
- **Aldehydes/Ketones:** 2,4-Dinitrophenylhydrazine (2,4-DNP); formation of yellow/orange precipitate indicates a carbonyl group ( $\text{C=O}$ ).

- **Carboxylic Acids:** Sodium Bicarbonate Test ( $\text{NaHCO}_3$ ); evolution of  $\text{CO}_2$  gas (effervescence) indicates acidity.

## Spectroscopic Techniques (The Modern Approach)

Modern structural elucidation relies on the synergy of three main spectroscopic methods.

### 1. Infrared (IR) Spectroscopy: Functional Group "Fingerprinting"

IR measures bond stretching and bending. Different bonds absorb specific frequencies of light.

- **O-H (Alcohol):** Broad, strong peak around  $3200\text{--}3600\text{ cm}^{-1}$ .
- **C=O (Carbonyl):** Sharp, strong peak around  $1700\text{ cm}^{-1}$ .
- **C-H (Alkanes):** Just below  $3000\text{ cm}^{-1}$ .

### 2. Nuclear Magnetic Resonance (NMR): The Structural Map

NMR (especially  $^1\text{H}$  and  $^{13}\text{C}$ ) provides info on the connectivity of the molecule.

- **Chemical Shift ( $\delta$ ):** Indicates the type of proton/carbon (e.g., aromatics appear at  $6.5\text{--}8.5\text{ ppm}$ ).
- **Integration:** Shows the number of protons in that environment.
- **Splitting (n+1 rule):** Reveals the number of neighboring protons (e.g., a triplet means there are 2 neighboring protons).

### 3. Mass Spectrometry (MS): Weight and Formula

MS knocks an electron off a molecule to create a “molecular ion” ( $\text{M}^+$ ).

- The highest mass peak (base peak or molecular ion) gives the **molar mass**.
- Fragmentation patterns act as unique pieces of a puzzle.

### 4. Limitations of Common Spectroscopic Techniques

Correct structure determination relies on integrating all data sources, not interpreting spectra in isolation.

- **IR spectroscopy** cannot determine the exact carbon skeleton.
- **NMR spectra** may overlap in complex molecules.
- **Mass spectrometry** does not directly show functional group positions.

## Strategy for Structure Elucidation

Analyzing an unknown follows a logical sequence:

1. **Molecular Weight (MS):** Determine the size of the molecule.

$$\text{Degree of Unsaturation} = \frac{2C + 2 - H - N - X}{2}$$

Where:

- C = number of carbons
- H = number of hydrogens
- N = number of nitrogens
- X = number of halogens

Each degree represents either:

- One double bond
- One Ring

2. **Degrees of Unsaturation:** Calculate from the molecular formula to see how many rings or double bonds exist.
3. **Functional Groups (IR):** Identify groups like -OH or C=O.
4. **Hydrogen/Carbon Framework (NMR):** Use the shifts and splitting to assemble the pieces found in IR and MS.

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