Massachusetts Institute of Technology

Organic Chemistry 5.13

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Assignment and Study Guide for Unit I

Methods for the Elucidation of the Structure of Organic Compounds

> *"…no single tool has had a more dramatic impact upon organic chemistry than infrared measurements. The development, just after the second Great War, of sturdy and simply operated machines for the determination of infrared spectra has permitted a degree of immediate and continuous analytical and structural control in synthetic organic work which was literally unimaginable fifteen years ago… Physical methods, and the principle that they should be used wherever possible, are now part of our armamentarium, and we may expect no surcease of further developments in this direction.*
>
> *"Nuclear magnetic resonance is even now on the horizon, and we shall be surprised if it does not permit another great step forward."*
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> **R. B. Woodward, 1956 (MIT SB '36, PhD '37; Nobel Prize (Chemistry) 1965)**

Reading Assignment   McMurry   Chapter 12   (pp. 393-423)

Chapter 13   (pp. 424-463)

Recommended Problems   McMurry   Chapter 12:   1, 3–4, 8, 10–12, 16, 20, 24, 29, 31, 37, 46, 49, 50.

Chapter 13:   3, 6–9, 14–15, 19–22, 25, 27, 34, 36–38, 43–45, 51, 54.

Methods for the Elucidation of the Structure of Organic Compounds

Study Guide

General Aims of this Unit:

1. We will survey three types of spectroscopy and spectrometry: **Infrared (IR) spectroscopy, mass spectrometry (MS),** and **nuclear magnetic resonance (NMR) spectroscopy (^{1}H and ^{13}C)**. For each method, we will discuss its **physical basis**, how **characteristic data** are affected by molecular structure, and the most useful **applications** of these data in structure elucidation.

2. We will apply the above methods (and others) to the **elucidation of organic molecular structures**, using a **three-stage strategy**: Determination of **molecular formula**, identification of **functional groups**, and elucidation of **connectivity**.

(Nearly) Foolproof Protocol for Organic Structure Determination

A. Molecular Formula
1. Determine molecular formula using **elemental analysis (EA)** and **MS**.
2. Determine **index of hydrogen deficiency (IHD** = # rings + # π-bonds**)** from molecular formula.

B. Functional Groups
1. Identify functional groups using **IR** and **^{13}C NMR** (and ^{1}H NMR occasionally)
2. Determine **symmetry** (a.k.a. degeneracy) by comparing **^{13}C NMR** to molecular formula.

C. Connectivity
1. Identify **molecular fragments** using data from **^{1}H NMR**:
    a. **spin-spin splitting**
    b. **integration**
    c. **chemical shift**
    d. …and **MS fragmentation** (can be done earlier in elucidation)
2. **Assemble** fragments
3. **Confirm** structural assignment – **Must be consistent with ALL data.**