

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."

R. B. Woodward, 1956

Reading Assignment	Wade	Chapter 12 (pp. 500-543) Chapter 13 (pp. 544-609)
Recommended Problems	Text Problems	Chapter 12: 3-7, 10, 14-16, 20, 23 - 25. Chapter 13: 2, 3, 5-10, 13-18, 21, 24, 26, 30-36, 38, 40, 43-45, 47-48.

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Study Guide

General Aims of this Unit:

1. We will develop a qualitative understanding of how molecular structure affects the position of absorption bands in **infrared (IR) spectra**.
2. We will learn how to use IR reference tables to interpret **infrared (IR) spectra**, identifying what functional groups are present in a molecule of unknown structure.
3. We will use **mass spectrometry (MS)** to determine chemical formulas and structure.
4. We will develop a qualitative understanding of the physical basis of **nuclear magnetic resonance (NMR)**, including the factors that determine **chemical shift** and **spin-spin splitting**.
5. We will learn how to interpret **proton (^1H) and carbon (^{13}C) NMR spectra** with the aid of reference tables, and we will learn how to employ NMR spectroscopy in conjunction with IR spectroscopy, elemental analysis, and mass spectrometry to elucidate the structure of organic molecules.