“...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 (MIT SB ’36, PhD ’37; Nobel Prize (Chemistry) 1965)

Reading Assignment
Wade
Chapter 12 (pp. 490-538)
Chapter 13 (pp. 539-599)

Recommended Problems
Text Problems
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 + \# \(\pi\)-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.