
Contents

Preface ix
Note to the Instructor xii

Chapter **1** STRATEGIES FOR INTERPRETING SPECTRA OF ORGANIC MOLECULES 1

- I. Organic Molecules 2
- II. Types of Spectroscopy 3
- III. General Strategies for Interpretation of Spectra 5
 - A. Identification of a Predicted Reaction Product 5
 - B. Identification of Reaction By-products 6
 - C. Identification of an Unknown Compound 7

Chapter **2** INFRARED SPECTROSCOPY 11

- I. Theory 12
- II. Experimental Considerations 14
- III. Interpretation of the Infrared Spectrum 18
 - A. The Frequency Assignment Approach 18
 - B. The Heteroatom Approach 47
- References 51

Chapter **3** NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY 53

- Theory 53
 - A. The Absorption Process 53
 - B. Relaxation 56
 - C. Chemical Shifts 56
 - D. Chemical Equivalence 63
 - E. Spin-spin Splitting 64

- F. First-order Spectra 71
- G. Complex Spectra 71
- II. Experimental Considerations 71
- III. Interpretation of the NMR Spectrum 75
 - A. Integrated Intensity 75
 - B. Chemical Shift 76
 - C. Spin-spin Splitting 80
- IV. Examples 84
- References 95

Chapter 4 ^{13}C NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY 97

- I. Theory 97
 - A. The Proton-coupled ^{13}C NMR Spectrum 100
 - B. The Broad-band Decoupled Spectrum 101
 - C. The Off-resonance Decoupled Spectrum 102
- II. Experimental Considerations 105
- III. Interpretation of the ^{13}C NMR Spectrum 106
 - A. Identification of Functional Groups 106
 - B. Confirmation of Previous Assignments 113
- References 115

Chapter 5 MASS SPECTROSCOPY 117

- I. Theory 118
- II. Experimental Considerations 121
- III. Interpretation of the Mass Spectrum 123
 - A. Initial Examination 123
 - B. Confirmation of Structures 128
- References 151

Appendix A Masses and Isotopic Abundance Ratios for Various Combinations of Carbon, Hydrogen, Nitrogen, and Oxygen 153

Appendix B Expected Fragmentation Patterns According to Compound Type 166

Index 169