

Contents

Preface — VII

Foreword — 1

1 Introduction — 2

2 Simple First-Order ^1H NMR Multiplets: Pascal's Triangle — 4

3 Complex First-Order ^1H NMR Multiplets: Infographic Walk-Through — 8

3.1 Doublet of Doublet of Triplets [ddt] — 8

3.1.1 Step 1: Integration — 8

3.1.2 Step 2: Symmetry and 2^n Rule — 10

3.1.3 Step 3: Coupling Constants — 12

3.1.4 Step 4: J -Tree Diagram — 16

3.1.5 Step 5: The Completed "Puzzle" — 18

3.1.6 The Infographic [ddt] — 20

3.2 Triplet of Triplets [tt] — 24

3.2.1 Step 1: Integration — 24

3.2.2 Step 2: Symmetry and 2^n Rule — 26

3.2.3 Step 3: Coupling Constants — 28

3.2.4 Step 4: J -Tree Diagram — 30

3.2.5 Step 5: The Completed "Puzzle" — 32

3.2.6 The Infographic [tt] — 34

3.3 Doublet of Doublet of Doublet of Doublets [dddd] — 38

3.3.1 Step 1: Integration — 38

3.3.2 Step 2: Symmetry and 2^n Rule — 40

3.3.3 Step 3: Coupling Constants — 42

3.3.4 Step 4: J -Tree Diagram — 44

3.3.5 Step 5: The Completed "Puzzle" — 46

3.3.6 The Infographic [dddd] — 48

4 Mnemonic rules — 52

5 Exercises — 58

5.1 Introductory Level: Doublet of Doublets [dd] — 58

5.1.1 Introductory Exercises — 59

5.1.2 Introductory Answers — 63

5.2 Intermediate Level: Doublet of Doublet of Doublets [ddd] — 68

5.2.1 Intermediate Exercises — 69

5.2.2 Intermediate Answers — 80

- 5.3 Advanced Level: Doublet of Doublet of Doublet of Doublets [dddd] — **92**
 - 5.3.1 Advanced Exercises — **93**
 - 5.3.2 Advanced Answers — **118**
- 5.4 Expert Level: Doublet of Doublet of Doublet of Doublet of Doublets [ddddd] — **144**
 - 5.4.1 Expert Exercises — **145**
 - 5.4.2 Expert Answers — **152**
- 6 Classification of Protons in ^1H NMR Spectra — 158**
 - 6.1 Diastereotopic Protons: Questions — **162**
 - 6.2 Diastereotopic Protons: Answers — **170**
- 7 ^1H NMR Multiplet Prediction: ^1H , ^1H Coupling — 178**
 - 7.1 Introductory Level: Doublet of Doublets [1–12] — **180**
 - 7.1.1 Introductory ^1H NMR Questions — **180**
 - 7.1.2 Introductory ^1H NMR Answers — **183**
 - 7.2 Intermediate Level: Doublet of Doublet of Doublets [13–20] — **186**
 - 7.2.1 Intermediate ^1H NMR Questions — **186**
 - 7.2.2 Intermediate ^1H NMR Answers — **188**
 - 7.3 Advanced Level: Doublet of Doublet of Doublet of Doublets [21–36] — **190**
 - 7.3.1 Advanced ^1H NMR Questions — **190**
 - 7.3.2 Advanced ^1H NMR Answers — **194**
 - 7.4 Expert Level: Doublet of Doublet of Doublet of Doublet of Doublets [37–60] — **198**
 - 7.4.1 Expert ^1H NMR Questions — **198**
 - 7.4.2 Expert ^1H NMR Answers — **204**
- 8 ^{19}F NMR Multiplet Prediction: ^{19}F , ^{19}F and ^{19}F , ^1H Coupling — 210**
 - 8.1 ^{19}F NMR Questions — **212**
 - 8.2 ^{19}F NMR Answers — **218**
- 9 ^1H NMR Multiplet Prediction: ^1H , ^1H and ^1H , ^{19}F Coupling — 224**
 - 9.1 Intermediate Level: Doublet of Doublet of Doublets [81–84] — **225**
 - 9.1.1 Intermediate ^1H NMR Questions (Mixed Coupling) — **225**
 - 9.1.1 Intermediate ^1H NMR Answers (Mixed Coupling) — **226**
 - 9.2 Advanced Level: Doublet of Doublet of Doublet of Doublets [85–92] — **228**
 - 9.2.1 Advanced ^1H NMR Questions (Mixed Coupling) — **228**
 - 9.2.2 Advanced ^1H NMR Answers (Mixed Coupling) — **230**

- 9.3 Expert Level: Doublet of Doublet of Doublet of Doublet of Doublets [93–100] — 232
 - 9.3.1 Expert ^1H NMR Questions (Mixed Coupling) — 232
 - 9.3.2 Expert ^1H NMR Answers (Mixed Coupling) — 234

Appendix — 237

Acknowledgments — 245

References — 247