

Spectroscopic and Structure Determination Methods Texts and References

Dr. Allen D. Hunter, Department of Chemistry

March 31st, 1997

I. General References on NMR Spectroscopy, Books

1. J. K. M. Sanders and B. K. Hunter, "Modern NMR Spectroscopy: A Guide for Chemists", Second Edition, 1993, Oxford University Press, New York. QD 96.N8 s24 1993
2. **J. K. M. Sanders, E. C. Constable, B. K. Hunter, & C. M. Pearce "Modern NMR Spectroscopy: A Workbook of Problems", Second Edition, 1993, Oxford University Press, New York. (Requested, December 1996)**
3. J. K. Akitt, "NMR and Chemistry: An Introduction to Modern NMR Spectroscopy", Third Edition, 1992, Chapman & Hall, New York. **(Being Processed in Maag Library, March 17th 1997)**
4. K. Nakanishi, "One-Dimensional and Two-Dimensional NMR Spectra by Modern Pulse Techniques", 1990, University Science Books, Mill Valley, CA. **(Being Processed in Maag Library, March 17th 1997)**
5. S. W. Homans, "A Dictionary of Concepts in NMR", Revised Edition, 1992, Clarendon Press, Oxford. QD 96.N8 H65 1992
6. H. Duddleck and W. Dietrich, "Structure Elucidation by Modern NMR: A Workbook", Second Edition, 1992, Springer-Verlag, New York. QD 96.N8 D83 1989
- *7. E. Breitmaier, "Structure Elucidation by NMR in Organic Chemistry: A Practical Guide", 1993, John Wiley & Sons, New York. QD 476.B6713 1993
8. A. E. Derome, "Modern NMR Techniques for Chemistry Research", 1987, Pergamon Press, New York. QD 96.N8 D47 1987 (Oversize)
9. **R. K. Harris and B. E. Mann, "NMR and the Periodic Table", 1978, Academic Press, New York.**
10. C. H. Dungan & I. R. Van Wazer, "Compilation of Reported ¹⁹F Chemical Shifts", 1970, Wiley Interscience, New York. QD 462.F8 D8
11. **R. K. Harris, "Nuclear Magnetic Resonance Spectroscopy", 1986, Longman, London.**
12. **J. W. Emsley and J. C. Lindon, "NMR Spectroscopy Using Liquid Crystal Solvents", 1975, Pergamon Press, New York.**
13. D. Shaw, "Fourier Transform NMR Spectroscopy", Second Edition, 1984, Elsevier, New York. QC 762.S45 1984
14. J. D. Memory and N. K. Wilson, "NMR of Aromatic Compounds", John Wiley & Sons, 1982, New York. QD 331.M45 1982
15. G. C. Levy, R. L. Lichter & G. L. Nelson, "Carbon-13 Nuclear Magnetic Resonance Spectroscopy", Second Edition, John Wiley & Sons, 1980, New York. QD 272.S6 L474 1980

16. Nuclear Magnetic Resonance Spectroscopy, Chapter 2 in E. A. V. Ebsworth, D. W. H. Rankin, & S. Craddock, "Structural Methods in Inorganic Chemistry", Second Edition, CRC Press, 1991, Boca Raton. [1st edition, 1987, QD 95.E29 1987]
17. C. Brevard and P. Granger, "Handbook of High Resolution Multinuclear NMR", 1981, Wiley, New York. QD 96.N8 B75
18. **J. Mason, "Multinuclear NMR", 1987, Plenum, New York (Requested, February 24th, 1997).**
19. J. B. Roberts, Editor, "NMR at Very High Fields", Volume 25 of NMR (Series), 1991, Springer-Verlag, NY. QC 490.N2 vol. 25
20. J. H. Noggle and R. E. Schirmer, "The Nuclear Overhauser Effect: Chemical Applications", 1971, Academic Press, NY. QC 490.N58
21. A. Ha-ur-Raman, "Nuclear Magnetic Resonance Basic Principles", 1986, Springer-Verlag, New York. QD 96.N8 R34 1986
22. R. J. Abraham, J. Fisher and P. Loftus, "Introduction to NMR Spectroscopy", 1988, John Wiley & Sons, New York. QD 96.N8 A27 1988
23. **D. G. Gorenstein, "Non-Biological Aspects of Phosphorus-31 NMR Spectroscopy", in Progress in NMR spectroscopy, vol. 16, pp. 1-98, 1983.**
24. H. Friebolin, "Basic One- and Two-Dimensional NMR Spectroscopy", 1991, VCH, NY. **(on order, 01-21-97)**
25. **E. D. Becker, "High Resolution NMR: Theory and Chemical Application's, 2nd edition, 1980, Academic Press, NY. [1st edition, 1969. QD 476.B358]**
26. **D. Neuhaus and M. P. Williamson, "The Nuclear Overhauser Effect in Structural and Conformational Analysis", 1989, VCH, NY.**
27. **L. D. Quin and J. G. Verkade, "Phosphorus-31 NMR Spectral Properties in Compound Characterization and Structural Analysis", 1994, VCH, NY. (Requested, December 1996)**
28. **G. E. Martin and A. S. Zektzer, "Two-Dimensional NMR Methods for Establishing Molecular Connectivity", 1988, VCH, NY. (out of print)**
29. **J. G. Verkade and L. D. Quin, "Phosphorus-31 NMR Spectroscopy in Stereochemical Analysis", 1987, VCH, NY.**
30. **K. Pihlaja and E. Kleinpeter, "Carbon-13 NMR Chemical Shifts in Structural and Stereochemical Analysis", 1994, VCH, NY. (Requested, December 1996)**
31. **W. R. Croasmun and R. M. K. Carlson, "Two-Dimensional NMR Spectroscopy: Applications for Chemists and Biochemists", 1994, VCH, NY. (Exceptional Book, Rinaldi Article) (Order Canceled because publisher didn't respond, resubmit in 1997/98)**
32. **G. C. Levy and R. L. Lichter, "Nitrogen-15 Nuclear Magnetic Resonance Spectroscopy", 1979, John Wiley & Sons, NY.**
33. **J. L. Marshall, "Carbon-Carbon and Carbon-Proton NMR Couplings: Applications to Organic Stereochemistry and Conformational Analysis", 1983, VCH, Deerfield Beach, Florida.**
34. **W. Bremser, B. Franke, and H. Wagner, "Chemical Shift Ranges in Carbon-13 NMR Spectroscopy", 1982, VCH, Deerfield Beach, Florida.**

35. E. O. Stegskal and J. D. Memory, "High resolution NMR in the Solid State: Fundamentals of CP/MAS", 1994, Oxford University Press, NY. QC 176.8.06 S74 1994

II Organic Spectroscopy/Structural Methods Texts

1. **R. M. Silverstein, G. C. Bassler, T. C. Morrill, "Spectroscopic Identification of Organic Compounds", now in its 5th edition, 1991, John Wiley & Sons, NY. (\$67.50 from Bookstore)**

2. **J. B. Lambert, H. F. Shurvell, D. A. Lightner, R. G. Cooks, "Introduction to Organic Spectroscopy", 1987, Macmillan, NY.**

3. K. Feinstein, "Guide to Spectroscopic Identification of Organic Compounds", 1995, CRC Press, Boca Raton, Florida. (would be \$34.95 if sold by Bookstore) **(Being Processed in Maag Library, March 17th 1997)**

4. V. M. Parikh, "Absorption Spectroscopy of Organic Molecules", 1974, Addison-Wesley Publishing, Menlo Park, CA.

5. **R. H. Shapiro, C. H. DePuy, "Exercises in Organic Spectroscopy", 2nd edition, 1977, Saunders College, Philadelphia.**

6. **W. Kemp, "Organic Spectroscopy", 3rd edition, 1991, W. H. Freeman, NY (Requested, February 24th, 1997).** [1st edition, 1975. QD 272.S6 S74 1986]

7. A. J. Baker, G. Eglinton, F. J. Preston, and T. Cairns, "More Spectroscopic Problems in Organic Chemistry", 2nd edition, 1975, Heyden & Son Ltd., London. QD 95.M6 1975

8. S. Sternhell and J. R. Kalman, "Organic Structures from Spectra", 1986, John Wiley & Sons, NY. QD 272.S6 S74 1986

9. **D. H. Williams and I. Fleming, "Spectroscopic Methods in Organic Chemistry", 5th Edition, 1995, McGraw-Hill, NY. (\$66.60 from Bookstore)** [2nd edition, 1973. QD 272.S6 W54 1973 ; 4th edition, 1987. QD272.S6 W54 1987]

10. L. D. Field, S. Sternhell, and J. R. Kalman, "Organic Structures from Spectra", 2nd edition, 1995, John Wiley & Sons, NY. (\$34.95 from Bookstore) **(on order 01-22-97)**

11. D. W. Brown, A. J. Floyd, and M. Sainsbury, "Organic Spectroscopy", 1988, John Wiley, NY. QD 272.S6 B76 1988

12. S. F. Dyke, "Organic Spectroscopy: An Introduction", 1978, Longman, NY. QD 272.S6 O72 1978

III Inorganic Spectroscopy/Structural Methods Texts

1. E. A. V. Ebsworth, D. W. H. Rankin, & S. Cradock, "Structural Methods in Inorganic Chemistry", Second Edition, 1991, CRC Press, Boca Raton, Florida, QD 95.E29.1991b [1st edition, 1987, QD 95.E29 1987] (\$69.95 from Bookstore)

IV Polymer Spectroscopy/Structural Methods Texts

1. **D. Campbell and J. R. White, "Polymer Characterization: Physical Techniques", 1989, Chapman and Hall, NY. (\$41.95 from Bookstore)**

2. **T. R. Crompton, "Analysis of Polymers: An Introduction", 1989, Pergamon Press, NY (Requested, February 24th, 1997).**
3. A. R. Cooper, Editor, "Determination of Molecular Weight", 1989, John Wiley & Sons, NY. **(on order 01-21-97)**
4. J. L. Koenig, "Spectroscopy of Polymers", 1992, American Chemical Society, Washington, DC. **(Being Processed in Maag Library, March 17th 1997)**
5. E. Schroder, G. Muller, and K.-F. Arndt, "Polymer Characterization", 1989, Hanser Publishers, NY. **(on order, 10-31-96)**
6. H. G. Barth and J. W. Mays, "Modern Methods of Polymer Characterization", 1991, John Wiley & Sons, NY. **(on order 01-21-097)**
7. **K. S. Schmitz, "An Introduction to Dynamic Light Scattering by Macromolecules", 1990, Academic Press, NY.**
8. **B. Chu, "Laser Light Scattering: Basic Principles and Practice", Second Edition, 1991, Academic Press, NY. [1st edition, 1974. QC 446.2.C48]**
9. **M. E. Brown, "Introduction to Thermal Analysis: Techniques and Applications", 1988, Chapman and Hall, NY (Requested, February 24th, 1997).**
10. **B. Wunderlich, "Thermal Analysis", 1990, Academic Press, NY (Requested, February 24th, 1997).**
11. J. D. Randall, Editor, "NMR and Macromolecules: Sequence, Dynamics, and Domain Structure", ACS Symposium Series #247, 1984, American Chemical Society, Washington, D. C. QD 380.N57 1984
12. F. A. Bovey, "High Resolution NMR of Macromolecules", 1972, Academic Press, NY. QD 381.B66 1972.
13. A. C. Woodward and F. A. Bovey, Editors, "Polymer Characterization by ESR and NMR", ACS Symposium Series #142, 1980, American Chemical Society, Washington, D. C. QD 471.P68
14. E. D. Craver and T. Provder, Editors, "Polymer Characterization: Physical Property, Spectroscopic, and Chromatographic Methods", Advances in Chemistry Series, 1990, American Chemical Society, Washington, D. C. QD 1.A355 no. 227
15. W. W. Wendlant, "Thermal Analysis", 1986, Wiley, NY. QD 79.T38 W45 1986
16. **K. Schmidt-Rohr and H. W. Spiess, "Multidimensional Solid-State NMR and Polymers", 1994, Academic Press, NY.**
17. H. Saechtling, "International Plastics Handbook: for the Technologist", 1995, Hanser, NY. **(on order 01-22-97)**
18. **D. Braun, "Simple Methods for Identification of Plastics", 1995, Hanser, NY. (Requested, December 1996) [old edition TP 1140.B7213 1982]**
19. E. Schroder, G. Muller, and K. F. Arndt, "Polymer Characterization", 1989, Hanser, NY. QD 134.P6 S3713 1989.
20. **H. Ulrich, "Introduction to Industrial Polymers", 1993, Hanser, NY. (on order 01-21-97)**
21. **H. Ulrich, "Raw Materials for Industrial Polymers", 1988, Hanser, NY. (on order 01-22-97)**
22. W. W. Wendlandt, "Thermal Analysis", 1986, Wiley, NY. QD 79.T38 W45 1986

V. Tabulations of Spectroscopic Data

1. **Pretsch, Clerc, Seibl, & Simon "Tables of Spectral Data for Structure Determination of Organic Compounds", Second Edition, 1989, Springer-Verlag, New York.**
2. C. J. Pouchert, "Aldrich Library of NMR Spectra", 1974, Aldrich Chemical Company, Milwaukee, W. I. QD 96.N8 P68
3. Aldrich Library of ¹H and ¹³C FT-NMR Spectra, Aldrich Chemical Company. QD 462.85.A44 1996 (reserve)

VI. Useful Review Articles and Papers on Aspects of NMR Spectroscopy

1. R. K. Harris, *Can. J. Chem.*, 1964, *47*, 2275. (Virtual coupling, AA'XnXn')
 2. T. R. Hoye, P. R. Hanson and J. R. Vyvyan, *J. Org. Chem.*, 1994, *59*, 4096-4103.
 3. **E. A. Williams, "NMR Spectroscopy of Organosilicon Compounds", Chapter 8 in "The Chemistry of Organic Silicon Compounds", S. Patai and Z. Rappoport eds., 1989, John Wiley and Sons, NY. (reorder, previous order canceled for some reason)**
- R. S. Drago, "Organometallics", 1995, *14*, 327-331, (¹⁹F NMR as a probe of bonding, e.g., FC₆H₄ Pt(PEt₃)₂X).

VII. General Organic Lab Manuals that have Useful Spectroscopy Sections

1. D. Pasto, C. Johnson, and M. Miller, "Experiments and Techniques in Organic Chemistry", 1992, Prentice Hall, Englewood Cliffs, New Jersey.
2. L. M. Harwood and C. J. Moody, "Experimental Organic Chemistry: Principles and Practice", 1989, Blackwell Scientific Publications, Boston.

VIII. X-Ray Crystallography References

- A. Acta Crystallographica. Section A. Foundation of Crystallography. QD 901.A25
 - B. Acta Crystallographica. Section B. Structural Science. QD 901.A26
 - C. Acta Crystallographica. Section C. Crystal Structure Communications. QD 901.A27
 - D. Acta Crystallographica. Section D. Biological Crystallography. QD 901.A28
 - E. International Tables of X-Ray Crystallography. Current Volumes in X-Ray Lab. Old Edition: QD 945.I55 1965 V.1 V.2 V.3
1. J. P. Glusker, M Lewis, and M. Rossi, "Crystal Structure Analysis for Chemists and Biologists", 1994, VCH, NY. QD 945.G583 1994
 2. J. P. Glusker, "Crystal Structure Analysis: A Primer", 2nd Edition, 1985, Oxford University Press, NY. QD 945.G58 1985. [1st edition with J. P. Glusker and K. N. Trueblood as authors, 1972. QD 945.G58]

3. M. C. F. Ladd and R. A. Palmer, "Structure Determination by X-Ray Diffraction", 3rd Edition, 1993, Plenum, NY. [1st edition: QD 945.L32 (1977). 2nd edition: QD 945.L32 1985.] **(Being Processed in Maag Library, March 17th 1997)**
4. I. Hargittai and M. Hargittai, "Symmetry Through the Eyes of a Chemist", 1995, Plenum, NY. QD 461.H268 1995
5. R. Jenkins and R. Snyder, "Introduction to X-Ray Powder Diffractometry", 1993, Wiley, NY. QD 482.D5 J46 1996
6. G. Rhodes, "Crystallography Made Crystal Clear: A Guide for Users of Macromolecular Models", 1993, Academic Press, San Diego. QP 551.R48 1993
7. L. E. Alexander, "Diffraction Methods in Polymer Science", 1969, Wiley-Interscience, NY. QD 945.A365
8. J. L. Amoros, "The Laue Method
9. L. V. Azaroff, "Elements of X-ray Crystallography", 1968, McGraw-Hill, NY. QD 945.A85
10. L. V. Azaroff et al, "X-ray Diffraction", 1974, McGraw-Hill, NY. QC 482.D5 X7 1974
11. H. Brumberger, "Small-Angle X-ray Scattering; Proceedings of the Conference held at Syracuse University, June 1965", 1967, Gordon and Breach, NY. QC 482.S52
12. M. J. Buerger, "The Precession Method in X-ray Crystallography", 1964, Wiley, NY. QD 945.B79
13. G. B. Carpenter, "Principles of Crystal Structure Determination", 1969, W. A. Benjamin, NY. QD 945.C35
14. J. P. Glusker, Editor, "Structural Crystallography in Chemistry and Biology", 1981, Hutchinson Ross Pub. Co., Stroudsburg, PA. QD 945.S87
15. J. W. Jeffery, "Methods in X-ray Crystallography", 1971, Academic Press, NY. QD 945.J36 1971
16. A. Guinier, "X-ray Diffraction in Crystals, Imperfect Crystals, and Amorphous Bodies", 1963, W. H. Freeman, San Francisco. QD 945.G943
17. H. Lipson, "Interpretation of X-ray Powder Diffraction Patterns", 1970, St. Martin's Press, NY. QD 945.L52
18. H. Lipson, "Crystals and X-rays", 1970, Wykeham, London. QD 945.L522
19. A. McPherson, "Preparation and Analysis of Protein Crystals", 1982, Wiley, NY. QP 551.M364 1982
20. G. H. W. Milburn, "X-ray Crystallography; An Introduction to the Theory and Practice of Single Crystal Structure Analysis", 1973, CRC Press, Cleveland, OH. QD 945.M5 1973.
21. E. W. Nuffield, "X-ray Diffraction Methods", 1966, Wiley, NY. QD 945.N83
22. H. W. Wyckoff, C. H. W. Hirs, and Serge N. Timasheff, "Diffraction Methods for Biological Macromolecules/Part A", 1985, Academic Press, Orlando, FL. QP 601.M49 vol. 114
23. H. W. Wyckoff, C. H. W. Hirs, and Serge N. Timasheff, "Diffraction Methods for Biological Macromolecules/Part B" 1985, Academic Press, Orlando, FL. QP 601.M49 vol. 115
24. R. Rudman, "Low-temperature X-ray Diffraction: Apparatus and Techniques", 1976, Plenum Press, NY. QD 945.R77

25. D. Sherwood, "Crystals, X-rays, and Proteins", 1976, Wiley, NY. QD 945.S46 1976
26. G. H. Stout, "X-ray Structure Determination; A Practical Guide", 1968, Macmillan, NY. QD 945.S8
27. B. K. Tanner, "X-ray Diffraction Topography", 1976, Pergamon Press, NY. QD 945.T36 1976
28. B. E. Warren, "X-ray Diffraction", 1969, Addison-Wesley, Reading, MA. QD 945.W33
29. A. J. Cochran Wilson, "Elements of X-ray Crystallography", 1970, Addison-Wesley, Reading, MA. QD 945.W49
30. M. M. Woolfson, "An Introduction to X-ray Crystallography", 1970, Cambridge University Press, Cambridge. QD 945.W58
31. J. R. Wormald, "Diffraction Methods", 1973, Clarendon Press, Oxford. QD 945.W63