JOURNAL OF CHEMICAL EDUCATION

Book and Media Review

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Review of *Spectrometric Identification of Organic Compounds*, 8th Edition

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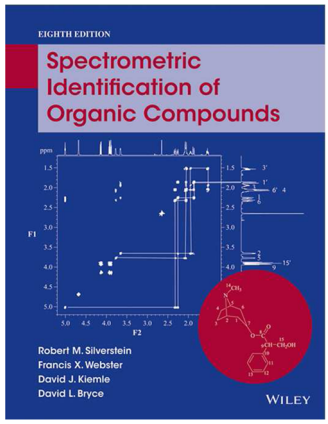
Spectrometric Identification of Organic Compounds, 7th edition by Robert M. Silverstein, Francis X. Webster, David J. Kiemle, and Robert L.Bryce. John Wiley and Sons: Hoboken, NJ, 2015. viii + 455 pp. ISBN 978-0-470-61637-6 (paperback). $190.42

Robert M. Silverstein's *Spectrometric Identification of Organic Compounds* first appeared 50 years ago. Throughout these 50 years, this book has undergone many editions and remained one of the most popular textbooks on organic spectroscopy for chemistry undergraduates. The 8th edition, published in late 2014, is a revised and updated version of the 7th edition[1] that was published 10 years ago.



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The organization of the 8th edition is the same as that of 7th edition, and consists of seven chapters. Chapter 1 presents the technique of mass spectrometry. This chapter is virtually the same as that of the previous edition. The initial portion of the chapter is devoted to instrumental techniques such as ionization methods, mass analyzers, Fourier transform mass spectrometry, and tandem mass spectrometry. The remaining portion of the chapter gives an overview of fragmentation patterns of common organic homologous series. This portion of the chapter gives all the necessary background for understanding organic EI and CI mass spectrometry. For those students who want to go deeper into strategies of data interpretation and fragmentation patterns, J. T. Watson's[2] and F. W. McLafferty's books[3] are two valuable references. Surprisingly, there is hardly any discussion on isotopic patterns of poly-halogenated compounds.

Except for the two additional sections on polymer and phosphorus compounds, Chapter 2 on infrared spectroscopy remains the same as that of the last edition. After initial presentation of the Michelson interferometer, sample handling, and coupled vibrations, the remaining portion of the chapter covers characteristic vibrations of various organic groups. The discussion on characteristic frequencies is extensive and useful in confirming the presence of organic functional groups in a given molecule.

The next four chapters focus on NMR spectroscopy. Naturally, the first of these four chapters covers proton NMR spectroscopy. In this chapter, all the basic theories, concepts and terminologies such as free induction decay, relaxation, chemical shifts, scalar coupling, Pople notation, and chemical and magnetic equivalence are introduced. A few sections have been completely revised. The treatment of chemical equivalence has been shortened and revised. The exposition of this concept is better than that of the 7th edition. The section on the analysis of a complex first-order spectrum, although remaining largely the same as that of the previous edition, is well presented and provides a tool for analyzing this type of spectra methodically. In summary, this chapter covers proton NMR and all the necessary background for the subsequent three chapters.

A few sections in the chapter on carbon-13 NMR have been revised. This chapter mainly covers all the topics such as chemical shifts (various functional groups), T_1 relaxation, phase inversion recovery, broadband decoupling, gated-decoupling technique, nuclear Overhauser effect (NOE) and DEPT. NOE is only introduced in the context of signal enhancement or depletion. No discussion on the physics behind NOE is covered. Conceptually, this is the easiest among the four NMR chapters.

Part of the chapter on two-dimensional NMR has been rewritten to make it much clearer and up-to-date. All current two-dimensional NMR techniques such as DQF-COSY, HETCOR, HMQC, HMBC, INADEQUATE, TOCSY (1-D and 2-D), and ROSEY are presented. HSQC, a variant of HMQC, is not covered. This is not a book for one trying to learn the principles behind pulse sequences. For those who want to have a better understanding of the principles behind pulse sequences, Friebolin's[4] and Claridge's[5] books should be consulted. The original section on pulse field gradient has been revised to include brief discussions on techniques such as ultrafast multidimensional NMR and single-scan NMR. Four compounds, namely, ipsenol, caryophyllene oxide, lactose, and the tetrapeptide VGSE (valine, glycine, serine, and glutamic acid) are used to illustrate the use of 2-D technique for structural elucidation. It starts with the easiest molecule, ipsenol, and ends with a more complicated one, VGSE. Each structure is derived from the given spectra in a systematic way. This part of the chapter remains largely the same as that of 7th edition. To understand how a structure is determined, one has

DOI: 10.1021/acs.jchemed.5b00571
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to go back and forth between various spectra. For VGSE, there are a total of 8 spectra for amino acid identification and sequencing. For those students encountering multidimensional NMR for the first time, this can be confusing on the first read. With patience, one should have no problem understanding the power of multidimensional NMR. If these spectra could be downloaded from the Web and printed out and placed side by side, it would be easier to relate one spectrum to another.

The chapter on multinuclear NMR is devoted to four 1/2-spin nuclei, namely, ^{15}N, ^{29}Si, ^{19}F, and ^{31}P that are commonly found in organic compounds. There are a few revisions. The IUPAC method of referencing chemical shifts for other nuclei is introduced. Simple molecules such as tetramethylsilane and triphenylphosphine are used to illustrate the principles of multinuclear NMR. This chapter provides an introduction to these nuclei. VGSE is used as an example to demonstrate the improved sensitivity of $[(\gamma^1H/\gamma^{15}N)^{3/2}]$ of inverse technique. While the $^1H-^{15}N$ HSQC spectrum shows three types of nitrogen, a 15-hour run of 1-D ^{15}N detects no peaks at all.

The final chapter presents six solved problems using all the common spectroscopic techniques and is virtually the same as that of 7th edition. The introduction gives a recommended set of guidelines on how to tackle a problem. Students are encouraged to explore their own systematic ways. Mass spectra are mainly used to establish molecular weights, and infrared spectra are used for the detection of functional groups such as carbonyl, hydroxyl, and acetylenic methine. NMR is the main workhorse used for structural elucidation. Like the previous chapter, it starts with the easiest molecule and ends with a more complicated one.

As pointed out by the authors in the preface, the goal of *Spectrometric Identification of Organic Compounds* is to teach problem solving. There is hardly any doubt that this book has accomplished this goal. The exposition of the subject matter is clear. It covers all the necessary techniques for spectroscopic identification. The logic used in deducing a given structure from a set of spectra is well presented. Each chapter is packed with problems for students to practice spectrum interpretation. Many useful tables and charts on spectroscopic data are found at the end of each chapter. This book will continue to be a very useful reference for chemists.

As this book is heavily NMR oriented, one should consider other good organic NMR books[6] available in the market before making a purchase of Silverstein's book. This is especially true for those who currently own the 7th edition.

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Notes

The authors declare no competing financial interest.

REFERENCES

(1) Silverstein, R. M.; Webster, F. X.; Kiemle, D. J. *Spectrometric Identification of Organic Compounds*, 7th ed.; John Wiley and Sons: Hoboken, NJ, 2005.

(2) Watson, D. J.; Sparkman, O. D. *Introduction to Mass Spectrometry*, 4th ed.; John Wiley and Sons: West Sussex, England, 2007.

(3) McLafferty, F. W.; Turecek, F. *Interpretation of Mass Spectra*, 4th ed.; University Science Books: Sausalito, CA, 1993.

(4) Friebolin, H. *Basic One- and Two-Dimensional NMR Spectroscopy*, 5th ed.; John Wiley and Sons: Darmstadt, Germany, 2011.

(5) Claridge, T. D. W. *High Resolution NMR Techniques in Organic Chemistry*, 2nd ed.; Elsevier Science: Amsterdam, The Netherlands, 2008.

(6) Simpson, J. T. *Organic Structural Determination Using 2-D NMR Spectroscopy*, 2nd ed.; Academic Press: Waltham, MA, 2012.

DOI: 10.1021/acs.jchemed.5b00571
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