Additions and Corrections

Investigation of Cyclopropane Stereomutation by Quasi-classical Trajectories on an Analytical Potential Energy Surface [*J. Am. Chem. Soc.* **1997**, *119*, 5253−5254]. DAVID A. HROVAT, SHU FANG, WESTON THATCHER BORDEN,* AND BARRY K. CARPENTER*

Page 5253: The penultimate sentence of footnote 5 should be replaced by the following: All references to single rotation in this paper imply the second definition of the rate constant for single rotation, and all the ratios of double to single rotations reported refer to the ratio, k_{12}/k_1, of the rate constants for these two processes.

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Book Reviews

Infrared and Raman Spectra of Inorganic and Coordination Compounds, 5th ed., Parts A and B. By Kazuo Nakamoto (Marquette University). Wiley: New York. 1997. Part A: xiii + 387 pp. $64.95. ISBN 0-471-16394-5. Part B: xiii + 384 pp. $69.95. ISBN 0-471-16392-9.

If you want to know something about the vibrational properties (frequencies, normal modes, spectra−structure correlation) of an inorganic or metal-containing molecule, this book is my choice as the first place to look. It has been and will continue to be a classic in this area with this fifth edition. Unlike most entries in the movie industry, this sequel is better than ever. If you liked the fourth edition, you will love the fifth edition. It has its problems because you cannot cover all of vibrational spectroscopy in the 771 pages of these two volumes. Of necessity the material is quite condensed and representative rather than comprehensive. Spectroscopy of purely organic molecules is not treated at all. However, in the general reading list there are references to books on the spectra of organic compounds. Also in the general readings lists, as well as additional books and reviews for subjects covered by Nakamoto, are references for noncovered areas including Fourier transform spectroscopy, adsorbed species, matrix isolation spectroscopy, time-resolved spectroscopy, high-pressure spectroscopy, intensities, advances series, and collections of spectral data. It is these along with the 3541 other references that make Nakamoto's book such a good starting place when a vibrational problem arises.

Infrared and Raman spectroscopy is a mature science so the advances are incremental with few major breakthroughs. This is not a book on what is new, although it does come up to the present, but it rather presents the state of spectral data and its treatment in the whole of inorganic and related fields. The number of pages in the fifth edition is about 50% greater than in the fourth edition, and the number of references is about 40% greater. There are references going into the 1990s for recent work, but most references are not new since basic spectra have not changed. The organization of the material into five sections remains the same as in the previous editions.

Section I, Theory of Normal Vibrations, presents in concise form the theoretical connection of structure to infrared and Raman spectroscopy. This includes most aspects of normal coordinate analysis with the utilization of symmetry properties. For example, the equations are laid out to determine the number of infrared and Raman active normal modes in each symmetry species there are for any structure, and their use is illustrated. Part I is probably too concise to be used as a textbook for a student's first exposure to normal coordinate analysis but is an excellent practical reference. The treatment of the vibrations of crystals has been expanded which is welcome in view of the recent greatly increased interest in solid-state chemistry and materials science. There is a new section on point groups and the symmetry of crystal lattices. The enlarged discussion of spectral analysis of crystals includes correlation methods and a review of vibrations in ceramic superconductors.

Section II deals with inorganic compounds as distinct from coordination and organometallic compounds. This section is divided in several ways. There are divisions based on the number of atoms, e.g., diatomic, triatomic, etc., divisions based on structure, e.g., trigonal bypyramid, octahedral, X_2Y_4, etc., and divisions based on elements, e.g., B, C, Si, etc. Enlargements include whole divisions separately for B, C, Si and Ge, N and P, S and Se, and metal cluster compounds in place of a few paragraphs in earlier editions. In keeping with the expanded coverage of crystals, site symmetry splitting of degenerate Raman bands is illustrated for SnX_3^-.

Section III treating coordination compounds has been expanded in considerable part due to increased interest in biological areas. The old subsection on pyridine, bipyridine, and related molecules has been expanded to two subsections. There is now a subsection for CO and CO_2 complexes to reflect increased interest in their catalytic activation as C_1 compound sources. A new subsection on nitrosyl complexes results from current emphasis on environmental chemistry (NO reduction in auto exhaust) and on NO as a neurotransmitter.

Section IV on organometallic compounds retains the same subsections as previously, but all are expanded. Faster computers which allow detailed normal coordinate analysis of large molecules have allowed this section to now depict all of the normal modes of the cyclopentadienyl group and of benzene.

Section V, Bioinorganic Chemistry, now has a separate subsection for Ligand Binding to Myoglobin and Hemoglobin. Within this is new work on NO adducts of myoglobin and hemoglobin. Another new subsection contains material on the interaction of metal complexes with nucleic acids.

The aim of these books is "to describe fundamental theories of vibrational spectroscopy in a condensed form and to illustrate their application in inorganic" chemistry. In this case "to illustrate" does not mean to just show a few examples but rather to give an introduction to the available data in this area. A nice feature of the presentation is the reproduction in a number of cases of spectral charts which gives a feel for the complexity of real data. It is evident from these that tables of frequencies are an abstraction with much interpretation of complex peaks.

There is no index of compounds so if the spectrum for a particular compound is desired, it must be searched for in the section or subsection for its class of molecule. This is not the most convenient way to find something. Some groups, such as metal clusters, are found in several locations. Some oddities occur such as $LiNaF_2$ (square structures) being included in a section on triatomics where $(MX_2)_2$ types are discussed. Apparently this occurs because of similarities of $(MF_2)_2$ and $LiNaF_2$, but if $LiNaF_2$ was being specifically sought, it would not likely be found. The redeeming feature of Nakamoto's book as a starting place for a search despite the index shortcomings is the well-organized broad coverage and the wealth of general references. The print in my copy of the fifth edition has a more boldface type and the tables are enlarged so it is easier to read than the fourth edition.

In summary this is a book to which anyone doing vibrational infrared or Raman spectroscopy should have access.

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An Introduction to Hydrogen Bonding. By George A. Jeffrey (University of Pittsburgh). Oxford University Press: New York and Oxford. 1997. ix + 303 pp. $60.00. ISBN 0-19-509549-9.

According to the preface, this book is primarily directed toward undergraduates. It contains eleven chapters and four appendices. The first chapter is devoted to a very useful and informative discussion of the history of hydrogen bonds. The second chapter entitled Nature and Properties is devoted to the daunting task of defining exactly what hydrogen bonds are. The next three chapters discuss hydrogen bonds of differing strengths: strong, moderate, and weak. Subsequent chapters deal with various aspects including cooperativity, disorder, proton transfer, water in different states, inclusion compounds, and hydrogen bonding in biological molecules. The final chapter is a review of the various methods generally employed in the study of hydrogen bonding.

The style of the book is similar to that of the author's previous book (with Saenger), *Hydrogen Bonding in Biological Structures*. In fact, several illustrations and tables are common to both. The presentation is episodic, describing particular aspects of hydrogen bonding, usually with reference to specific papers. The author is a crystallographer. Not surprisingly, he refers extensively to the crystallographic literature.

The fact that this book mostly describes work published in specific research papers is both its strongest attribute and its greatest drawback. It is an asset because the published data are presented without smoothing of any kind. However, it is also a drawback because specific interpretations are often presented as if they are generally accepted when there are differing opinions in the literature. For example, it is stated that hydrogen bonds are essentially electrostatic interactions. This analysis is primarily based upon a particular theoretical study of a water dimer. There is no critical discussion of the methodology used to reach this conclusion, nor is there any suggestion that other kinds of hydrogen bonds might have different relative contributions from electrostatic and covalent interactions. While there are many interesting data presented on β-diketoenols, none of the interesting gas-phase studies are discussed.

The chapter on weak hydrogen bonds is particularly useful since many of these interactions have been widely ignored both in chemistry textbooks and by experimental chemists, in general. These H-bonds are most clearly evident from crystallographic studies. The greater appreciation of these interactions by experimental and biochemical chemists (other than crystallographers) is certainly desirable. In this context, this book does a very valuable service. The chapter on cooperativity, etc., presents this phenomenon mostly from the crystallographic point of view, once again. That is, cooperativity is discussed in terms of hydrogen bonding distances. The question of nonadditive cooperativity (in energetic terms) is not addressed at all.

The chapter on water includes an interesting discussion of the various ice polymorphs. That on hydrogen bonding in biological molecules presents interesting examples from nucleic acid, peptide, and polysaccharide chemistry. A recent controversial topic, low barrier hydrogen bonds and enzyme catalysis, is mentioned but not discussed at any length.

The final chapter deals with various methods (infrared, Raman, gas-phase microwave, and NMR spectroscopy, neutron scattering, deuterium nuclear quadrapole coupling, neutron and X-ray diffraction, computational chemistry, and thermochemical measurements) that are used in the study of hydrogen bonding. Much of this chapter is quite informative and extremely useful to undergraduate students. However, one important method, electron diffraction, is curiously omitted. Also, the description of theoretical methods is surprisingly superficial compared with the rest of the chapter.

As a whole, this book is a very useful addition to the chemical literature. Its greatest benefit is the presentation of real experimental data which often provide examples that are different from what undergraduates might expect from the rather rudimentary (and often inaccurate) treatment hydrogen bonding generally receives in textbooks. On the other hand, one could wish for more critical analysis of the experimental data that are presented.

All things considered, this is probably the best place for any undergraduate interested in hydrogen bonding to begin reading. It will, also, be extremely useful to researchers who would like to learn about hydrogen bonds.

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Carbohydrates in Drug Design. Edited by Zbigniew J. Witczak and Karl A. Nieforth (University of Connecticut). Marcel Dekker: New York. 1997. ix + 703 pp. $175.00. ISBN 0-8247-9982-8.

This book offers a timely account of various applications of carbohydrates in drug design. Approximately five areas of carbohydrate research are covered with scholarly reviews from leading researchers in the field. The discussion of future prospects, in each of the areas covered, is a particularly appealing aspect of the book.

Chapter one briefly presents the carbohydrate-based drugs currently in use and those that hold the greatest hope for future application; it is somewhat of an outline of the chapters that are to follow. Sialoglycoconjugates is the topic of the next three chapters. Their potential application as antimicrobial agents is presented by Mark von Itzstein and Milton Kiefel. Rene Roy has contributed an informative chapter on sialoside mimetics as antiinflammatory and antiviral agents, while Akira Hasagawa and Makato Kiso report on the synthesis of various analogues that probe selectin binding. Each of these chapters presents a unique perspective on the chemistry and potential of sialic acid-based drugs. Polysulfated drugs are covered in chapters five, six, and seven. Eric De Clerq, Miriam Witvrouw, and Chrisophe Pannecouque describe their work on the development of antiviral drugs. They also include significant experimental details, making their contribution especially valuable. Susanne Alban examines the anticoagulant and antithrombic properties of sulfated carbohydrates whereas Robert Linhardt and Toshihiko Toida discuss analogue development of heparin oligosaccharides. Here again the individual perspective of each chapter is a strength of the book; however, there is quite a bit of overlap in the introductions. For example, the several different types of sulfated sugars and their sources are presented in all three chapters. The chemoenzymatic synthesis of *myo*-inositol analogues is presented in chapter eight by Shoichiro Ozaki and Ling Lei. Targeting phosphatidylinositol-specific phospholipase C is discussed by Karol Bruzik, and aminocyclitol antibiotics are presented by Seichiro Ogawa. A chapter on azasugars and their potential as anti-HIV drugs is written by Leon van den Broek. The antiviral potential of nucleosides is also represented in the work of Stanislas Czernecki and Jean Valery. Chapter thirteen, which is written by Warren Beach, discusses interesting synthetic work directed toward the preparation of 3′-heteronucleosides. Unfortunately the editing of this chapter is substandard with poorly rendered structures and reaction schemes. In Chapter fourteen, Waldemar Priebe and Roman Perez-Soler present the chemistry of sugar-modified anthracyclines as potential targets against multidrug resistance. The final two chapters of the book include an in-depth perspective of lincomycin chemistry by Osman Achmatowicz and Barbara Szechner and a discussion of the antitumor activity of fungal (1−3)-β-D-glucans written by Akira Misaki and Mariko Kakuta.

It should be pointed out that this book is not an exhaustive account of the use of carbohydrates in drug design. Instead, the intent was to provide the reader with developments that have major clinical implications. To that extent the editors were successful. However, the price of the book is difficult to justify. There are no aspects of its production that appear to be particularly costly.

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