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Organische Peroxo-Verbindungen

Methoden der Organischen Chemie (Houben-Weyl), Band E13 (I/II)

Georg Thieme Verlag, Stuttgart, 1988, XLIV + 1768 pp. (in German).

This book is a comprehensive survey of the synthesis and chemistry of organic peroxo compounds and mirrors the present and applications in this field. Both organic chemists and specialists working in the field of organic peroxo compounds will discover this book an indispensable desk reference for new insights into their research objectives. Most contributors are directly involved in research and development in the fields they are reviewing; even though there are many contributors, the chapters are all consistently well-written. The organization is well balanced and the presentation is uniformly succinct. After a brief introductory chapter on nomenclature, we come upon shorter treatises on the structure and properties, thermochemical data, and naturally occurring hydroperoxides and peroxides (a possible source of criticism is the omission of peroxide intermediates in enzymic transformations, e.g., pterin- and flavin-dependent oxydases and oxygenases). A short section dealing with handling precautions is also included. Written from an organic chemical perspective, the book is divided into four main sections dealing with syntheses, reactions, applications, and analyses of organic peroxo compounds. A solid two-thirds of the book is devoted to preparative methods. Many chapter sections are large and contain scores of diverse reaction examples. In selecting detailed synthetic procedures, the authors have adhered to general reaction patterns and utility in synthetic applications as their major criteria. While the methods discussed are generalized for applicability to many situations, there are extensive references to the literature for those who wish to find more details. A large section of the book deals with the reactions of organic peroxo compounds. The reactions are grouped by type; one of the most useful features of the treatment is the authors' attempt to provide enough mechanistic information to enable the reader to evaluate the applicability of the model reaction to other systems. One goal of this section is to demonstrate how syntheses involving organic peroxides may be dissected into a number of simple, fundamental chemical transformations. The section dealing with the applications of peroxo compounds in organic synthesis covers general reactions of carbon and heteroatoms. The latter are grouped by type within the framework described above, and numerous examples are provided, primarily from the synthetic organic literature. A great many useful reactions are covered in this section and it provides an excellent overview of synthetic applications of organic peroxo compounds. A short, but highly representative section on the analysis of organic peroxo compounds, including a survey of chemical, spectroscopic and chromatographic techniques augments the value of the book. The book also contains the bibliography as well as the author and subject index. The organic chemist who takes the time to familiarize himself with the layout and contents of this book will find it a comprehensive and valuable guide to a rapidly growing area of organic chemistry. All in all, this is a very good book with an urging appeal to all organic chemists. However, due to the general importance of some of the topics covered, the book should also be of interest to a wide audience.

M. POJE

L. Sommer

Analytical Absorption Spectrophotometry in the Visible and Ultraviolet

Studies in Analytical Chemistry #8, Akadémia Kiadó, Budapest 1989, 311 pp.

One might wonder if UV/VIS spectrophotometry, being one of the commonest analytical methods used for more than a century, deserves a whole book. However, the method is still

widely used in many modern analytical instruments (e.g. HPLC) and, besides, recently there have been significant technical advances in the field (e.g. diode-array spectrophotometry).

Therefore, the book written by L. Sommer (Professor of Analytical Chemistry, Purkine University at Brno, Czechoslovakia) will undoubtedly find a large audience.

The book comprises eight chapters: Basics of UV/VIS spectrophotometry, Principles of measurement, Errors in spectrophotometry, Evaluation of analyte concentration, Optimization of spectrophotometric procedures, Special approaches, Complexation and spectrophotometry, Some Applications of UV/VIS spectrophotometry, accompanied by a list of comprehensive books on spectrophotometry and a Subject Index.

On the whole, the book is very informative and some chapters (e.g. 3, 4, 5) were written with outstanding competence. An additional merit of the book can be found in the author's extensive use of Eastern European and Soviet papers which, for linguistic and other reasons, frequently escape the attention of Westerners.

Several, though minor, objections can be raised: modern chemometric methods of spectral information processing (principal components factor analysis) are not covered, dimensional inconsistency of some equations, inadequate description of the physical background of UV/VIS spectra,... and, last but not least, the book's English is far from perfect, even hardly understandable in places.

However, the general impression is still favourable: the book is written competently, all important topics are covered, the literature references are up to date and, indeed, very copious.

VL. SIMEON

A. E. Martell and R. J. Motekaitis

The determination and Use of Stability Constants

VCH Publishers, New York 1988, 215 pp. + floppy disk, price USD 34.50

Although the determination of the stability constants of coordination compounds is not nowadays as fashionable as it was in the fifties and sixties, this activity still remains important not only in (bio)inorganic chemistry but also in a number of diverse scientific and technical fields (analytical chemistry, agriculture, corrosion, ecology, oceanography, tensides, galvanic plating, etc.). Therefore, the need for an authoritative book on the stability constants determination is and will be welcomed by many chemists, specialists in the field and those who use this kind of data. Even more so, since the senior author of the book is one of the world's most distinguished inorganic chemists.

The contents of the book is the following: Introduction/Equilibrium Constants, Protonation Constants, Formation Constants/Experimental Methods for Measuring Equilibrium Constants/Experimental Procedure for Potentiometric p[H] Measurement of Metal Complex Equilibria/Common Errors and Their Elimination or Minimization/Examples of Stability Constant Determination/Macroscopic and Microscopic Constants/Determination of Stability Constants and Species Concentrations of Complex/Critical Stability Constants and Their Selection/Development of a Complete Critical Metal Complex Data Base/Appendix I: Program PKAS/Appendix II: Program BEST/Appendix III: Program SPE/Appendix IV: Scientific and Technical Fields Requiring Stability Data..

The above table of contents shows that all essential topics are mentioned, with the emphasis on glass-electrode potentiometry. Especially valuable are numerous examples of computational treatment of (potentiometric) data, using Martell's and Motekaitis' program BEST. Another useful part are the chapters on the experimental methods and the sources of errors. Finally, the book contains the listing of three of the authors' programs (PKAS, BEST, SPE), as well as a floppy disk containing not only the symbolic (Fortran 77) text of these programs but also several sample data files and the executable program (running admirably on several PC compatibles, as checked by the reviewer).

VL. SIMEON

Theoretical Models of Chemical Bonding, (Zvonimir B. Maksić, Ed.)

Springer Verlag Berlin-Heidelberg, 1990).

Part 1: XXVIII + 324 pp., DM 350,—; Part 2: X + 642 pp., DM 450,—.

This is an attractively composed collection of essays written by well selected, leading experts in the field of theoretical chemistry. Part 1 contains 9 chapters in addition to the Prologue (Modelling — Search for Simplicity) written by the Editor (Z.B.M.). The chapters are: The Concept of Molecular Structure (B. T. Sutcliffe), Topology and Properties of Molecules (O. E. Polansky), Symmetry in Molecules (J. P. Dahl), Chirality of Molecular Structures — Basic Principles and Their Consequences (L. D. Barron), Interplay of Experiments and Theory in Determining Molecular Geometries. A. Experiments, B. Theoretical methods (J. E. Boggs), Molecular Mechanics alias Mass Points and Elastic Springs Model of Molecules (A. Y. Meyer), Atoms in Molecular Environments (K. B. Wiberg) and The Modelling of Molecules as Collections of Modified Atoms (Z.B.M.).

Part 2 contains 14 chapters: The Physical Origin of the Chemical Bond (W. Kutzelnigg), Absolute Electronegativity and Absolute Hardness (R. G. Pearson), Valence in Molecular Orbital Theory (K. Jug and M. S. Gopinathan), The Magnetic Description of Conjugated Hydrocarbons (J.-P. Malrieu), Directional Properties of Covalent Bonding in Molecules (Z.B.M.), The Two-Electron Bond as a Molecular Building Block (P. R. Surjan), Interpretation of Molecular Behaviour by Localized Molecular Orbitals (LMOs) (C. Edminton), Properties of the Fermi Hole and Electronic Localization (W. L. Luken), The Diatomics-in-Molecules Method and the Chemical Bond (P. J. Kuntz), Calculation of Electron Correlations by Using Local Operators (P. Fulde), The Concept of the Chemical Bond in Solids (M. Grodzicki), Chemical Implication of Local Features of the Electron Density Distribution (E. Kraka and D. Cremer), Electron Deformation Densities and Chemical Bonding in Transition Metal Complexes (A. A. Low and M. B. Hall), Fundamentals of Relativistic Effects in Chemistry (W. H. E. Schwarz).

Each chapter is self-contained and, therefore, some overlapping is unavoidable. However, it is very modest and in fact useful in that each chapter can be read without looking into others. The tactical approach to the treated topics (and to the reader) varies considerably between the chapters; in some of them the essayistic (or even philosophical) note is dominant whereas others are closer to the textbook or review type of writing, but each chapter is well balanced in its scope and makes enjoyable reading. For whom? Certainly not for the novice. Some knowledge not only of quantum mechanical concepts and formalism is a prerequisite for understanding, but to get the best of the chapters some experience and previous pondering on the questions treated are necessary. The Editor should be congratulated for having assembled so many excellent authors and produced such a useful book. The only regrettable aspect is the price. Individuals will hardly be able to afford purchasing the whole series (two more parts are forthcoming) and, very likely, only department libraries will do it.

DUŠAN HADŽI

Brian Webster

Chemical Bonding Theory

Blackwell Scientific publications, Oxford 1990

ISBN 0-632-01619-1

276 pages

This book stems from the experience of the author, who has taught bonding theory to beginners and advanced students for over 20 years, testing much of the material in lectures, workshop sessions and tutorials. The principal objective of the book is to instruct beginners in the modern views on the chemical bond, adhering to an elementary level. The author has endeavoured to keep the tradition of a sound chemical approach to chemical bonding, mostly derived from Gilbert Lewis and Linus Pauling, but he also incorporates the results of *ab initio* molecular orbital calculations to illustrate a modern description of chemical bonding.

The book incorporates 10 Chapters which are divided into four parts: 1. Electron Pairs and the Shape of Molecules, 2. The Orbital Model of Atomic Structure, 3. Diatomic Molecules, and 4. Polyatomic Molecules, which also treats orbital symmetry, complex ions, and molecular attractions. The book ends with a data section that provides values for fundamental constants and other physical data required in the problems.

Some instructors may appreciate the author's suggestion to use the book by taking only Chapters 1, 2, 3, 5, and 7 for classes of moderate ability and if time is restricted. In fact, this selection provides a short elementary course in bonding theory, having no spectroscopic component and requiring little mathematical skill.

Some other features of the book that should be pointed out are: (i) The SI system of units is used throughout the text; (ii) Learning outcomes are given at the beginning of each part so that students know exactly what skills they should have acquired on completion of that part; (iii) Examples with solutions are given at appropriate points to illustrate the use of an equation or chemical idea; (iv) All mathematical illustrations are derived from solutions of the wave equation by an ab initio molecular orbital method or are based on the relevant equation; (v) Each chapter ends with a selection of problems.

In conclusion, the book can be recommended, as one of the best in this teaching field, both to students and to instructors.

MARIJAN PRIBANIĆ

*Nomenclature of Inorganic Chemistry
Recommendations 1990*

G. J. Leigh (Editor)

Blackwell Scientific Publications, Oxford 1990

(Issued by the Commission on the Nomenclature of Inorganic Chemistry, International Union of Pure and Applied Chemistry)

ISBN 0-632-02319-8

Ta knjiga predstavlja dopunjavanje pravila za nazivlje, koje se dopunjavanje obično javlja kao posljedica razvitka kemije kao i novih tumačenja kemijske veze te otkrića novih struktura kemijskih spojeva. IUPAC-ova Komisija za nazivlje anorganske kemije sastavila je 1938. i objavila 1940. godine prva pravila koja su se poslije mijenjala, dopunjavala i objavljivala 1957, 1960, 1971, 1978. i sada 1990.

Iako nije istaknuto u naslovu, ta je knjiga prvi dio (Part I), od budućih nekoliko dijelova u kojima će biti opisana pravila za nazivlje specijalnih područja anorganske kemije. Komisija je nastojala uvrstiti u taj prvi dio temeljna pravila za osnovne spojeve kao što su jednostavne molekule, oksokiseline i njihovi derivati, koordinacijski spojevi i jednostavni borovi spojevi. Komisija izražava nadu da taj prvi dio neće pretrpjeti velike promjene zbog budućeg razvitka kemije, što se ne može očekivati za druge dijelove koji će se kasnije pojaviti, a u kojima će se obraditi posebna područja poput anorganskih polimera, polioksoaniona, organometalnih spojeva itd.

Knjiga predstavlja desetogodišnji rad članova Komisije kao i brojnih drugih pojedinaca uz sudjelovanje nekoliko ostalih srodnih IUPAC-ovih komisija. Od 1981. do 1987. bio je član Komisije prof. dr. Vladimir Simeon kao predstavnik Jugoslavije.

Knjigu preporučujem svakom istraživaču iz područja anorganske kemije, a poglavito nastavnicima anorganske kemije.

MARIJAN PRIBANIĆ

Nenad Raos

Konformacijska analiza

Školska knjiga, Zagreb, 1988

164 str.

Ovo je djelo Dr. Nenada Raosa (s Instituta za medicinska istraživanja u Zagrebu) izdano u seriji *Suvremena kemija* koju izdaje izdavačko poduzeće »Školska knjiga« iz Zagreba. Započela je izlaziti pred 18 godina i do sada je objavljeno svega 6 djela. Izgleda da se domaći autori vrlo teško odlučuju na pisanje knjiga u području kemije. U svjetlu te činjenice valja pozdraviti stvaralački napor Dr. Raosa koji je našoj kemijskoj javnosti ponudio vrelu informacija o konformacijskoj analizi na hrvatskom jeziku.

Konformacijska je analiza zaista dio suvremene kemije. Iako su njeni korijeni u prošlom stoljeću, ona je kao samostalna disciplina stara svega dvadesetak godina. IUPAC tek 1976. prihvaća naziv »konformacija«. Razvoj je konformacijske analize u našem vremenu uvjetovan upravo nevjerovatnim razvojem eksperimentalnih metoda, kao i teorijskih metoda, čija je pak primjena omogućena pojavom brzih elektroničkih računala.

Djelo *Konformacijska analiza* sastoji se od Predgovora, 8 poglavlja, 5 priloga i literaturnih referencija, a tematski je podijeljeno u tri cjeline. U prvom dijelu (koji se sastoji od prva tri poglavlja) pristupa se konformacijskoj analizi sa stajališta organskog kemičara, u drugom dijelu (koji se sastoji od druga tri poglavlja) sa stajališta fizikalnog i teorijskog kemičara), a treći tematski dio (koji se sastoji od posljednja dva poglavlja) od interesa je prije svega biokemičarima, biofizičarima i teorijskim biologima. Prva tri poglavlja govore o izomeriji i konfomeriji (prvo poglavlje, 17 str.), o prikazivanju molekula u prostoru (drugo poglavlje, 6 str.) i o konformaciji jednostavnih molekula (treće poglavlje, 15 str.). Druga tri poglavlja govore o silama u molekuli (četvrto poglavlje, 15 str.), o eksperimentalnim metodama kojima se istražuje struktura i ravnoteža konformera (peto poglavlje, 27 str.) i o teorijskim metodama koje služe kao osnovica za proračunavanje geometrije, energije i drugih relevantnih parametara konformera (šesto poglavlje, 27 str.). Posljednja dva poglavlja govore o konformaciji prirodnih spojeva (sedmo poglavlje, 33 str.) i o interakciji između biomolekula (osmo poglavlje, 11 str.). U dodacima se redom govori o simetrijskim svojstvima molekula ili konformera (Prilog A, 2 str.), o transformaciji koordinata (Prilog B, 3 str.), o Diracovoj bra-ket notaciji (Prilog C, 1 str.), o gradijentnim metodama za minimalizaciju konformacijske energije (Prilog D, 3 str.) i o parametrima uzvojnice (Prilog E, 3 str.).

Već smo naglasili da ova monografija Dr. Raosa obiluje mnoštvom podataka o konformacijskoj analizi, a osobito o teorijskoj konformacijskoj analizi. Međutim u nekim dijelovima nije potpuna (npr. Tablica 1.2 ili prikaz Karplusove jednadžbe na str. 69), a i neke definicije nisu sasvim uspjele (npr. definicija kiralnog kromofora). Autor također upotrebljava nazivlje koje je manje primjereno hrvatskom jeziku (kao npr. hiralan umjesto kiralan, hirooptički umjesto kiroptički, dihiroizam umjesto dikroizam). No, bez obzira na sve manjkavosti, djelo Dr. Raosa vrijedan je prilog stručnoj literaturi iz kemije na hrvatskom jeziku, pa ga stoga preporučamo svakom domaćem kemičaru bez obzira na uži interes.

NENAD TRINAJSTIĆ