

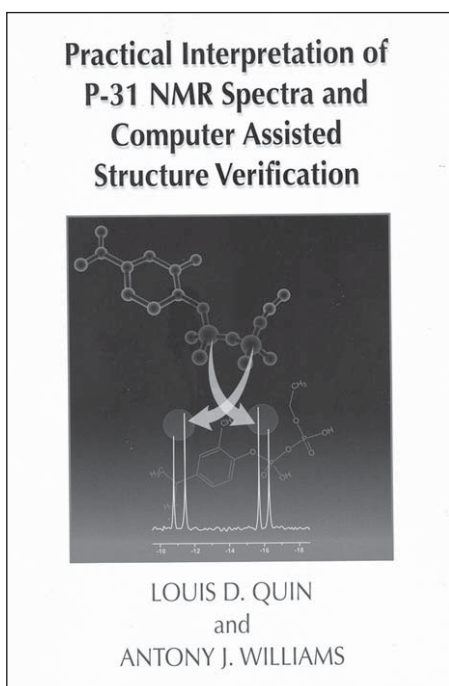
Книжнина • Reviews

ПОЛЕЗНО РЪКОВОДСТВО ЗА ХИМИЦИ-ОРГАНИЦИ

Louis D. Quin, Antony J. Williams. *Practical Interpretation of P-31 NMR Spectra and Computer-Assisted Structure Verification*. Advanced Chemistry Development, 90 Adelaide Street West, Suite 600, Toronto, M5H 3V9, 416-368-5596, info@acdlabs.com, ISBN 0-9735913-0-7

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Резюме. Направено е кратко представяне на книгата на проф. Луис Д. Куин и Антони Уилямс “Практическа интерпретация на ^{31}P ЯМР спектри и проверка на структурата с помощта на компютри”. Подчертано е, че въпреки наличието на много добри обзори по ^{31}P ЯМР, тази книга попълва празнината от подробен наръчник по факторите, влияещи върху химичното отместване на най-важните фосфорсъдържащи функционални групи. Тези фактори са илюстрирани на повече от 400 фосфор съдържащи съединения. Представено е накратко съдържанието на книгата, като е изтъкнато, че изследовател, търсещ ^{31}P ЯМР сравнение, може да отиде до съответната глава и бързо да намери необходимата информация само като знае типа на съединението, с което работи. В книгата са представени и съвременните компютърни методи за предсказване на ^{31}P ЯМР спектри, като са изследвани различните съвременни софтуерни инструменти, които са в помощ на химика за проверка и изясняване на структурата на фосфор съдържащи химични съединения. Тази книга би била необходима за всеки студент или новодошъл в областта на ^{31}P ЯМР. Добавянето на повече дискусия по константите на спин-спиново взаимодействие между ^{31}P и ^1H или ^{13}C би могло да се желае в следващо издание на книгата.



The phosphorus nucleus ^{31}P has a spin quantum number of $\frac{1}{2}$ and is the only natural isotope of this element. Therefore ^{31}P NMR has been widely used from very beginning of NMR spectroscopy era. The chemical shift of ^{31}P is highly indicative of the particular phosphorus functional group, and is generally predictable from studying the effects of structural change. Said that, it is well recognized that ^{31}P NMR shifts can be influenced by structural changes, and anyone reporting ^{31}P chemical shifts should rationalize the data with the structure at phosphorus to avoid assignment errors. Chemists and Analysts should be observant about any unusual effects that might be operating on the shielding phenomenon. This book is designed to aid the researcher, especially students or newcomers to the field, in these tasks, and to help in developing an un-

derstanding of the factors that lead to a certain shift.

The existing literature contains many fine reviews on ^{31}P NMR published in the last decades. However a book, focused on the chemical shift effect for various functional groups presenting them in an instructional and comprehensive mode, is not available. This book fulfills that need.

In this text, Dr. Louis D. Quin (Adjunct Professor, University of North Carolina-Wilmington; James B. Duke Professor Emeritus, Duke University; and Professor Emeritus, University of Massachusetts-Amherst) summarizes his comprehensive knowledge of phosphorus chemistry to provide a through grounding for the chemist in the NMR properties of the nucleus. By coupling this capability, in a single book, with a review and validation of the software tools to aid in the interpretation of ^{31}P NMR, the authors have provided a first-class handbook on phosphorus NMR.

Book Description

This is a book oriented to functional groups and contains information about ^{31}P chemical shifts in a concise and well-edited format. The book consists of 16 chapters. They include not only the introduction to ^{31}P NMR Spectroscopy (Chapter 1) and computer assisted structure verification (Chapter 16), but survey the chemical shift effects of most important phosphorus-containing functional groups. These effects were illustrated on more than 400 compounds.

Chapter 1 is an introduction to ^{31}P NMR Spectroscopy and focuses on factors influencing ^{31}P chemical shifts. The reader will find an array of 9 such factors, which control the ^{31}P chemical shifts. Knowledge of these factors is fundamental in developing interpretive skills in this field. The main sources of ^{31}P NMR spectral data are reviewed. The reader should remember that the purpose of quoting spectral data in the text is not to supply a source of preferred shifts, but to use data to illustrate structural effects on chemical shifts.

Chapters 2-15 discuss the chemical shifts of important phosphorus derivatives including natural phosphorus compounds, which are well recognized to play vital roles in living systems. The compounds are divided into specific categories and ^{31}P NMR chemical shifts expected for different substitutions are discussed. Any researcher looking for phosphorus NMR comparison can go to the specific chapter and easily find the information just by knowing the type of compound one is working with.

The discussion of ^{31}P NMR chemical shifts of phosphorus containing compounds and the 9 factors influencing these shifts continue during the entire book and cover phosphoric acid derivatives (Chapter 2), phosphonic and phosphinic acids and derivatives (Chapter 3), thio and selenoderivatives of phosphates, phosphonates and phosphinates (Chapter 4), phosphonous and phosphinous acid esters and amides (Chapter 5), halophosphines (Chapter 6), 3-coordinated phosphorous acid derivatives (Chapter 7), phosphines (Chapter 8), phosphine oxides, sulfides and selenides (Chapter 9), phosphonium salts and ylides (Chapter 10), heterophosphonium salts (Chapter 11), compounds with 5- and 6-coordinated phosphorus (Chapter 12), compounds with P-P bonds (Chapter 13), phosphorus compounds with true multiple bonds to P (Chapter 14), special families of heterocyclic phosphines (Chapter 15).

Chapter 16 not only presents how the NMR prediction technology works, but also examines a number of software tools that are available today in order to assist a chemist in structure verification and elucidation of phosphorus containing chemical entities. The ^{31}P NMR prediction using ACDLABS suite of programs is illustrated using suitable structures, figures and program windows.

The list of reference consists of 79 sources, which includes not only the well known by NMR spectroscopists books and reviews, but also recent reports on specific problems.

Any student or newcomer to the field of ^{31}P NMR should find this handbook indispensable. The experienced NMR spectroscopists should find it a helpful addition to their libraries. Possible new edition of the book would benefit from the supplement of more discussion on ^{31}P - ^1H and ^{31}P - ^{13}C coupling constants.

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