

<<有机化学中的光谱方法>>

图书基本信息

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作者：威廉姆斯

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前言

This book is the sixth edition of a well-established introductory guide to the interpretation of the ultraviolet, infrared, nuclear magnetic resonance and mass spectra of organic compounds. It is a textbook suitable for a first course in the application of these techniques to structure determination, and as a handbook for organic chemists to keep on their desks throughout their career. These four spectroscopic methods have been used routinely for several decades to determine the structure of organic compounds, both those made by synthesis and those isolated from natural sources. Every organic chemist needs to be skilled in how to apply them, and to know which method works for which problem. In outline, the ultraviolet spectrum identifies conjugated systems, the infrared spectrum identifies functional groups, the nuclear magnetic resonance spectra identify how the atoms are connected, and the mass spectrum gives the molecular formula. One or more of these techniques nowadays is very frequently enough to identify the complete chemical structure of an unknown compound, or to confirm the structure of a known compound. If they are not enough on their own, there are other methods that the organic chemist can turn to: X-ray diffraction, microwave absorption, the Raman spectrum, electron spin resonance and circular dichroism, among others. Powerful though they are, these techniques are all more specialised, and less part of the everyday practice of most organic chemists. We have kept discussion of the theoretical background to a minimum, since application of the spectroscopic methods is possible without a detailed command of the theory behind them. We have described instead how the techniques work, and how to read each of the four kinds of spectra, including each of the most important 2D N-MR spectra. We have included many tables of data at the ends of Chapters 2, 3 and 4, all of which are needed in the day-to-day interpretation of spectra. Finally in Chapter 5, we work through 11 examples of the way in which the four spectroscopic methods can be brought together to solve fairly simple structural problems, and there are 33 problem sets for you to work through for practice. In preparing a sixth edition, we have almost completely rewritten the book, to reflect our experience teaching the subject, and to respond to changes that have taken place, both of emphasis and of fact, since the fifth edition was published. The chapters on UV and IR spectra are more concise, the chapter on NMR is expanded, and the chapter on MS made more specific to the everyday, rather than to the more specialised, applications of this technique. The appearance of IR absorptions, formerly gathered at the end of the chapter, are now illustrated at the relevant points in the text. Conversely, we have moved the tables of IR data to the end of the chapter, where they are more convenient for reference, and match the arrangement we have always used for the NMR and MS chapters. Most significantly, we have replaced all of the 60 MHz spectra used hitherto to explain the fundamentals of NMR spectroscopy with new and carefully chosen examples at 400 MHz or more. We have also chosen several new compounds with which to illustrate better the common 2D NMR techniques.

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内容概要

本书是一本由英国剑桥大学D. H. Williams和I. Fleming合著的有机化学光谱方法经典教材。

第1版出版于1966年，本书为第6版。

书中讲述了近年来迅猛发展的二维核磁共振（如Tocsy、远¹H-¹³C COSY）、MALDI、FT-ICR、TOF等新技术。

与时俱进，本版较前版在内容上做了较大的改动，有关UV和IR光谱的部分讲述的更加准确；丰富了关于NMR的内容；介绍MS的部分更加讲求结合实际。

全书共分为五章，第1章为紫外和可见光谱，论述了电子吸收光谱在测定有机基团中的应用；第2章红外光谱，阐述了傅里叶红外和喇曼光谱的样品制备、光谱选律以及各官能团的特征吸收频率；第3章核磁共振波谱，主要介绍了¹H和¹³C核磁共振的经验参数、各种二维NMR的具体应用；第4章质谱，介绍了各种粒子谱以及气相和液相色谱与质谱的联用；第5章实例和习题，为读者提供了一些选自研究课题、具有启发性的实例，也为读者巩固所学的知识提供了练习。

本书理论和实践并举，因此也适合有机化学工作者做为手册使用。

读者对象：高校化学系师生、有关研究人员。

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作者简介

作者：(英国) 威廉姆斯 (Williams.D.)

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插图：The energy absorbed by the matrix is transferred indirectly to the sample, which reduces any sample decomposition. The matrix is chosen to have solubility properties similar to those of the sample, in order that the sample molecules are properly dispersed. Higher molecular weight oligomeric 'clumps' are produced as $2M^+$, $3M^+$, and so on, but these are usually minor components of the spectrum if a well-matched matrix is chosen. 4.3.3

Electrospray ionisation (ESI) An 'electrospray' is the term applied to the small flow of liquid (generally 1-10 $\mu\text{l}/\text{min}$) from a capillary needle when a potential difference typically of 3-6 kV is applied between the end of the capillary and a cylindrical electrode located 0.3-2 cm away (Fig. 4.4). The liquid leaves the capillary as a fine mist at or near atmospheric pressure, and consists of highly charged liquid droplets. The charge on these droplets may be selected as positive or negative according to the sign of the voltage applied to the capillary. ESI is especially useful since it can be used to analyse directly the effluent from an HPLC column. The use of a 'sheath' gas or 'nebulising' gas promotes efficient spraying of the solution of the sample from the capillary. Sample molecules dissolved in the spray are released from the droplets by evaporation of the solvent. This evaporation is accomplished by passing a drying gas across the spray before it enters a capillary. As the droplets are multiply charged, and reduced in size by evaporation, the rate of desolvation is increased because of repulsive Coulombic forces. These forces eventually overcome the cohesive forces of the droplet, and an MH^- (or $M - H^+$) molecular ion free of solvent is finally produced. The charged particles are carried, by an appropriate electric field, through a capillary and into an ion analyser.

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