

---

---

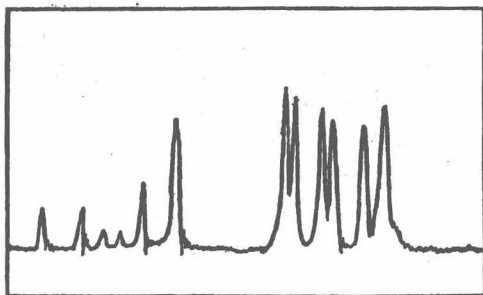
# Physical Methods in ORGANIC CHEMISTRY

edited by

J. C. P. SCHWARZ

M.A., B.SC., PH.D.,

Lecturer in Chemistry  
University of Edinburgh



OLIVER & BOYD  
EDINBURGH & LONDON

1964

---

---

---

## EDITOR'S PREFACE

Physical methods for the determination of structure now play a vital part in the daily work of the organic chemist. This book is intended to provide an introduction to these methods, primarily for undergraduate and post-graduate students, but also for more senior chemists who wish to assess the relevance of these modern techniques to their own work.

The basic principles are presented in simple terms and the scope of each method is illustrated by examples of structural problems to which it can be applied. Important analytical applications are also mentioned. The aim has been to provide a readable introduction to the various techniques rather than an exhaustive survey of data and applications; references are given to monographs and reviews which provide more detailed information. Methods which are of outstanding importance (particularly infrared spectroscopy) are discussed in greater detail than the others. In the opening chapter the methods are assessed as a whole.

The Oxford University Press and Pergamon Press Ltd. are thanked for providing the line blocks for the Figures on p. 298 and p. 309. Permission to copy diagrams from other sources mentioned in the text is also gratefully acknowledged. Finally the authors and the editor wish to express their special thanks to the many colleagues and students who have stimulated the writing of this book and who have read part or all of the manuscript.

PETER SCHWARZ

*Edinburgh*

**OLIVER AND BOYD LTD**

**Tweeddale Court  
Edinburgh 1**

**39A Welbeck Street  
London W.1**

**First published . . . . . 1964**

**© 1964, The Authors**

**Printed in Great Britain by  
Robert Cunningham & Sons, Ltd., Alva**

# CONTENTS

	<i>Page</i>
EDITOR'S PREFACE	v
 <i>Chapter</i>	
1. INTRODUCTION .. .. . <i>J. C. P. Schwarz</i>	1
Historical	2
The 'theoretical' and 'empirical' approaches	3
The electromagnetic spectrum	4
A survey of the methods	7
Reference works	19
 2. ULTRAVIOLET, VISIBLE AND INFRARED	
SPECTROSCOPY .. .. . <i>P. Bladon and G. Eglinton</i>	22
General introduction	22
The origin of light absorption	23
The measurement of light absorption	24
Applications of ultraviolet, visible and infrared spectroscopy	31
 3. INFRARED AND RAMAN SPECTROSCOPY .. <i>G. Eglinton</i>	35
Introduction	35
 PART I. INFRARED SPECTROSCOPY—THEORY AND PRACTICE	36
Molecular vibrations and their interaction with infrared radiation	36
Instruments and sampling methods	42
The applications of infrared spectroscopy	44
The correlation and interpretation of infrared spectra	48
Factors affecting group frequencies	55
Physical state and group frequencies	57
Intramolecular factors and group frequencies	62
Prediction of approximate values for group frequencies	73

PART II. INFRARED SPECTROSCOPY—EXAMPLES OF APPLICATIONS	78
1. Solvents	80
2. Functional group absorptions (i) In simple alicyclic systems	80
3. Functional group absorptions (ii) In the 5 $\alpha$ -cholestane skeleton	84
4. Straight- and branched-chain hydrocarbons	89
5. The gem-dimethyl group and double bond absorptions	90
6. Polynuclear aromatic hydrocarbons	93
7. A reaction study. The photochemistry of verbenone	95
8. Long-chain acids and esters	98
9. Synthetical confirmation of a natural product structure	101
10. Chelate systems	104
11. Ethers, ketals and carbohydrates	106
12. Amines, amine salts and alkaloids	108
13. Carboxylic acid salts and amino-acids	110
14. The total synthesis of griseofulvin	113
PART III. RAMAN SPECTROSCOPY	116
Origin of Raman spectra	116
Apparatus and sampling	120
Applications	121
4. ULTRAVIOLET AND VISIBLE SPECTROSCOPY .. <i>P. Bladon</i>	126
Theoretical aspects	126
Experimental technique	129
The absorptions of some common structural types	132
Absorption due to carbon-carbon multiple bonds	133
Absorption due to carbonyl groups	138
Absorption of compounds containing nitrogen or sulphur	144
Light absorption of saturated compounds containing heteroatoms	145
Absorption due to aromatic chromophores	146
Applications of ultraviolet and visible spectra	155
The literature of electronic spectra	164
5. MAGNETIC RESONANCE SPECTROSCOPY .. <i>L. M. Jackman</i>	168
Introduction	168
The spectroscopic method (N.M.R.)	170
Proton nuclear magnetic resonance	173
The chemical shift	173
Time-dependent effects	178
Types of shielding	179
Spin-spin coupling	183
Examples of applications	193
Electron spin resonance	203

# CONTENTS

xi

6. OPTICAL ROTATION .. .. .	<i>J. C. P. Schwarz</i>	210
Introduction		210
The measurement of optical rotations		212
The theory of optical rotation		217
The correlation of structure and optical rotation		220
The presence or absence of optical activity		222
Cotton effect curves		223
Circular dichroism		232
Plain curves		234
Rotations at a single wavelength		235
Summary		242
7. THE DETERMINATION OF MOLECULAR WEIGHT .. .. .	<i>C. T. Greenwood</i>	244
Introduction		244
Molecular weights of up to 2,000		248
Molecular weights in the range 2,000–20,000		259
Molecular weights above 20,000		262
8. DIFFRACTION METHODS .. .. .	<i>G. A. Sim</i>	276
Introduction		276
The crystalline state		278
X-Ray diffraction: experimental procedure		285
X-Ray diffraction: structure analysis		292
X-Ray diffraction: applications		300
9. MASS SPECTROMETRY .. .. .	<i>R. I. Reed</i>	306
Theory and operation		306
Applications of isotopic abundance measurements		310
Thermochemistry and cracking patterns		312
Structural applications of mass spectrometry		313
10. DIPOLE MOMENTS .. .. .	<i>B. L. Shaw</i>	323
Introduction		323
General results		326
Contributions to the electronic theory of organic chemistry		327
Problems in stereochemistry		331
Organometallics		334
INDEX OF COMMON GREEK SYMBOLS		338
INDEX		339

## Chapter 1

J. C. P. Schwarz

---

### INTRODUCTION

Methods based on relationships between structural features and physical properties are now making an ever-increasing contribution to organic chemistry, not only in the elucidation of structure, but also in analytical and preparative work. The advantages of these methods are numerous: (i) they can give much more precise information about molecular structure than a classical chemical approach, (ii) the amount of sample required is small and it can generally be recovered, (iii) the information is usually obtained rapidly, often in the form of a permanent record on a chart, (iv) many of the methods provide analytical techniques of high selectivity and sensitivity, invaluable in the analysis of complex mixtures and in the detection of impurities, (v) continuous analysis is often possible, facilitating kinetic work and the automatic control of process variables in industry, (vi) systems can be examined without disturbing their composition, an obvious advantage over chemical analysis in the study of tautomeric, conformational and other equilibria. It is therefore not surprising that the growing availability of physical methods has altered both the scope and pace of organic chemistry. Many recent successes in the determination of the structures of complex natural products would have remained out of reach without them, and their contribution in widening our understanding of the reactivity of organic compounds can hardly be overestimated.

The various physical techniques of greatest interest to the organic chemist are discussed individually in the following chapters. The aim of this introduction is to provide a broad survey of the methods and of their applications, particularly in the determination of the structures of complex molecules, e.g. natural products. The first few pages are devoted to general considerations, and then the salient features of the various methods will be presented, largely in tabular form. Details of the principles and applications of the methods must be sought in the

individual chapters, and cross-references for this purpose are provided.

**Historical.** Physical properties have always played an important part in the practice of organic chemistry. They form the basis of separation techniques, both classical and modern, and also provide criteria of purity and identity which are indispensable in laboratory work. Furthermore, two physical methods—molecular weight determination and the detection of molecular asymmetry by optical rotation—were of great importance in the early growth of structural theory. Otherwise the classical approach to the elucidation of structure depended almost entirely on the systematic investigation of chemical reactions. Although there were many attempts, even in the nineteenth century, to relate physical properties and structure, these yielded little of interest to the organic chemist; in fact, readily determined properties such as melting point, boiling point, density and refractive index give little direct information about structural features.

During the first three decades of the present century, advances in physics began to make major contributions to the concept of molecular structure. It became apparent that certain physical properties (e.g. spectra, X-ray diffraction, dielectric behaviour, etc.) could provide numerical data about the relative positions of the atoms in a molecule and the nature of the bonds between them. This led to a much more precise picture of molecular structure than could be obtained by purely chemical means and laid the basis of modern theories of reaction mechanisms.

At the same time it was found that some physical properties, particularly absorption spectra, could be related empirically to the presence of certain functional groups, even though the rigorous theoretical basis of the relations was not fully understood. Methods based on these properties began to be used in both structural and analytical work, and by 1930 the fundamentals of most of the techniques discussed in this book were well established. Nevertheless, the impact of these methods on the laboratory practice of organic chemistry was still comparatively small. With the apparatus available at the time, the measurement of physical properties such as absorption spectra was tedious and required considerable skill. For this reason, most of the methods remained in the hands of specialists, who were usually more interested in the fundamental basis of the effects and in the fine structure of simple molecules than in the investigation of the more complex molecules with which the average organic chemist has to deal.

The fact that physical methods now play such an important part in the work of the organic chemist is due only in a minor degree to further



knowledge of their fundamental theory. Advances in instrumentation, many of which were stimulated by military needs during the second world war, were probably the most important factor in establishing physical methods as routine tools. These advances came at a time when the need for new methods of approach was widely felt. Complex natural products (e.g. steroid hormones), often available only in very small quantities, were providing structural problems of a new order of complexity. Developments in the chemical industry underlined the need for rapid and powerful analytical methods. Moreover, an increasing interest in reaction mechanisms and in the interpretation of relative reactivities inevitably drew attention to physical methods of investigation. Organic chemists were therefore quick to take advantage of the new methods which had come within their reach. Economic factors also played a part in these developments; the increasing financial support for scientific research, both academic and industrial, stimulated the instrument manufacturer—a vital link between the physicist and the organic chemist—to undertake the development and production of the costly equipment required for the routine exploitation of many of the physical techniques.

**The 'theoretical' and 'empirical' approaches.** Many of the physical methods discussed in this book can be considered from two different, though not unrelated, points of view. In the first approach, structural information is obtained by interpreting the experimental data in terms of fundamental physical theories. This 'theoretical approach' can provide detailed information, not only about molecular geometry, but also about electron distributions, polarisabilities, molecular energetics and other aspects of fine structure.<sup>1-3</sup> In general this approach is limited to fairly simple molecules (e.g. ethane, benzene, etc.) and its exploitation belongs to the realms of physical chemistry and physics, although the organic chemist may often profit by the results.

The second approach may be called the 'empirical approach', as it depends on the empirical correlation of certain physical properties with structural features. It is particularly successful with spectroscopic methods, and its general principles are explained and illustrated in Chapter 3 (pp. 48 and 80). It depends on two related assumptions: (i) that the physical characteristic in question can be associated with a particular portion of the molecule, and (ii) that it is more or less unaffected by changes in other parts of the molecule. The utility of a particular physical property thus depends greatly on the extent to which it can be regarded as 'localised'. Highly localised physical properties (e.g. characteristic infrared absorption peaks) can be used to detect the

presence of functional groups even in molecules of completely unknown structure. By contrast, methods depending on less localised physical properties (e.g. optical rotation) can seldom be used profitably unless a considerable amount of structural information is already available. (Often they are restricted to the problem of deciding between two or three alternative structures, the physical behaviour of which can be predicted from that of closely analogous compounds; cf. p. 220.)

The application of physical methods to organic chemistry is largely based on the empirical approach because, even for molecules of only moderate complexity, a more fundamental approach is usually impossible. Moreover, the arguments used in the empirical approach are congenial to the organic chemist since they are rather similar to those employed in deducing structure from chemical evidence. The theoretical approach is usually more demanding and specialised; it is therefore unprofitable to adopt it unless otherwise inaccessible information about fine structure is sought. However, even when a largely empirical approach is used, considerations based on fundamental theory often play an important part; they provide a rational background for the collection and qualitative interpretation of empirical data, and frequently lead to useful predictions about the physical behaviour of compounds for which direct analogies are not available. For example, the effect of structural environment on the light absorption characteristics of a group can often be predicted on theoretical grounds (cf. p. 62).

In the diffraction methods (Chapter 8) a simple empirical approach is not possible, and the theoretical evaluation of the results is rather complex and time-consuming. The diffraction methods have therefore remained in the hands of specialists. However, since the structural information given by these methods (particularly by X-ray diffraction) is of great importance to organic chemistry, they have nevertheless been included in this book. Thanks to the development of electronic computers, X-ray diffraction may now provide a quicker route to the structure of a complex organic compound than a chemical approach, especially if the chemistry is complicated by rearrangements or if the material is difficult to obtain in quantity.

**The electromagnetic spectrum.**<sup>†</sup> Many of the physical methods which are of greatest value to the organic chemist depend on the interaction of matter with electromagnetic radiation of various wavelengths. The most familiar type of electromagnetic radiation is visible light. Early

<sup>†</sup> Readers who are familiar with the fundamentals of the absorption and diffraction processes characteristic of the various regions of the electromagnetic spectrum (Fig. 1) can omit this section and proceed to the section beginning on p. 7.

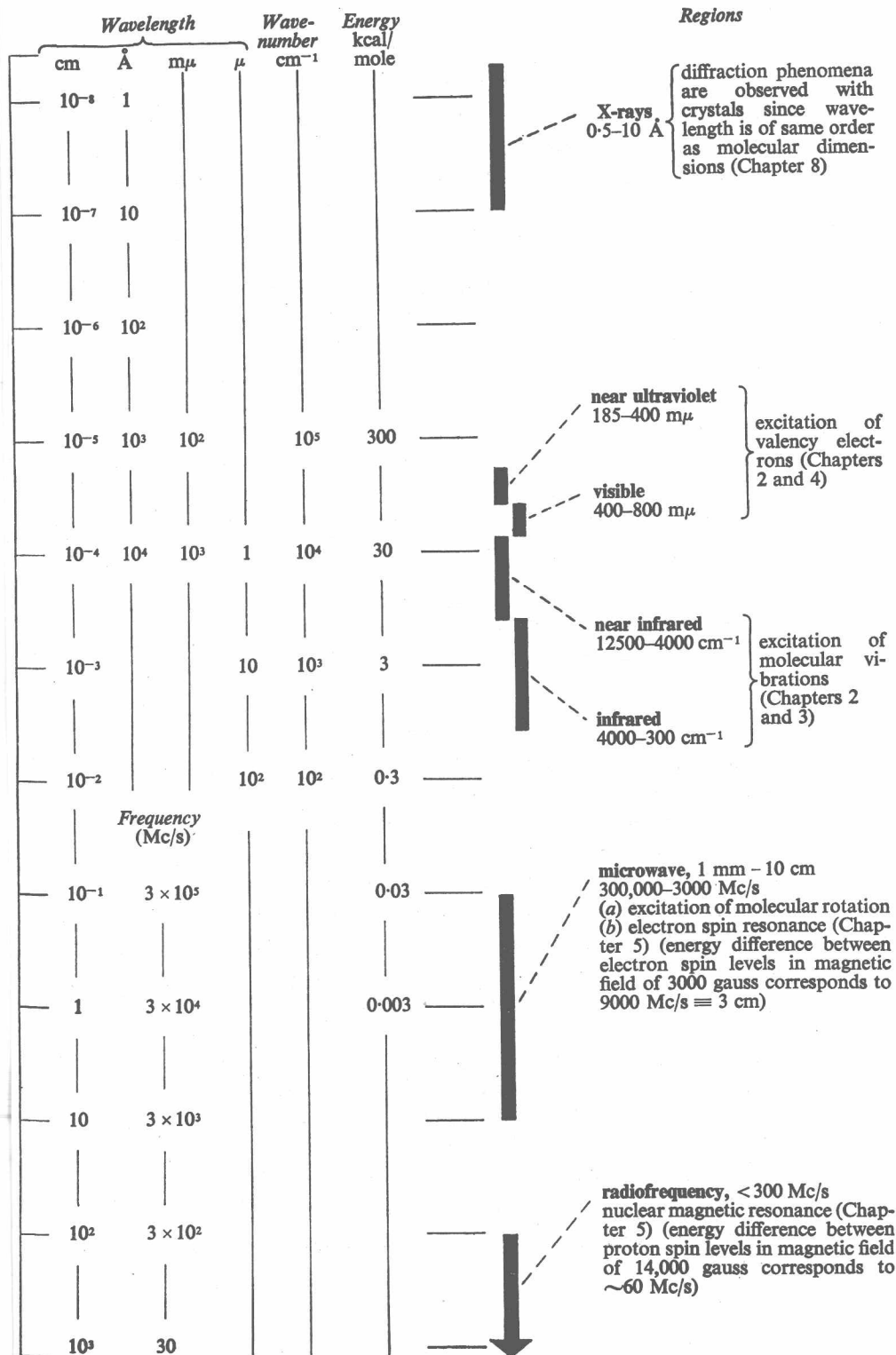


Fig. 1. The electromagnetic spectrum

in the nineteenth century it was found that the spectrum extends outside the visible region, and the adjacent parts of it were named the ultra-violet and infrared. It is now known that these regions form part of a continuous spectrum embracing microwaves and radiowaves at one end, and X-rays and  $\gamma$ -rays at the other. The boundaries of most of the regions are not rigidly defined; those of greatest interest to the organic chemist are indicated approximately in Fig. 1.

*Units.* The electromagnetic spectrum covers a very wide range of wavelengths, and different units are therefore used in the different regions. For convenience, the units used in the later chapters are briefly summarised here (see also Fig. 1).

X-rays have wavelengths of the order of  $10^{-8}$  cm and in this region the Ångström ( $1 \text{ Å} = 10^{-8}$  cm) is the preferred unit of wavelength. In the visible and ultraviolet regions, wavelengths are usually expressed either in Ångströms or in millimicrons† ( $1 \text{ m}\mu = 10^{-7}$  cm =  $10 \text{ Å}$ ). In the infrared region, wavelengths are expressed in microns ( $1 \mu = 10^{-4}$  cm). An alternative convention, commonly used in the infrared region and less frequently in the ultraviolet and visible, is to give the number of waves per cm. This is known as the *wavenumber* and is expressed in  $\text{cm}^{-1}$ . It is clear that

$$\text{wavenumber (cm}^{-1}\text{)} = \frac{1}{\text{wavelength in cm}} = \frac{10^4}{\text{wavelength in } \mu}$$

A wavelength of  $4 \mu$  ( $= 4 \times 10^{-4}$  cm) therefore corresponds to a wavenumber of  $2500 \text{ cm}^{-1}$ .

Many infrared spectroscopists loosely refer to the wavenumber as 'frequency' and represent it by the symbol  $\nu$  (the symbols  $\tilde{\nu}$  or  $\sigma$  are preferable, but less common among organic chemists). The term 'frequency' and the symbol  $\nu$  are therefore used in this sense in Chapters 2 and 3. The true frequency, also represented by  $\nu$ , is given by

$$\text{frequency} = \frac{\text{velocity of light}}{\text{wavelength}}$$

and is preferred in microwave and radiofrequency spectroscopy (see Chapter 5), the usual unit being megacycles per second ( $1 \text{ Mc/s} = 10^6$  cycles per second). A wavelength of 1 cm (in vacuo) corresponds to a frequency of *ca.* 30,000 Mc/s.

*Types of interaction.* Interaction of radiation with matter may occur in a number of ways. X-ray diffraction (see Chapter 8) depends on

† The term 'nanometer' ( $1 \text{ nm} = 1 \text{ m}\mu$ ) is also used, particularly in the German literature.

elastic scattering of the radiation—there is usually no permanent transfer of energy between the radiation and the molecules. Many of the other methods are based on interactions which involve an exchange of energy. The molecule may either emit radiant energy at the expense of its internal energy, or it may absorb radiant energy, being promoted to an excited state. The spectroscopic methods of greatest interest to the organic chemist all depend on the latter process.

According to the quantum theory, the energy content of a molecule cannot change continuously, but is confined to certain discrete values (*energy levels*). Furthermore, a molecule will absorb radiation only when the (true) frequency ( $\nu$ ) of the radiation is related to the energy difference ( $\Delta E$ ) between two energy levels by the equation  $\Delta E = h\nu$ , where  $h$  is Planck's constant. Since the relative positions of the energy levels depend characteristically on the molecular structure, absorption spectra (i.e. observations on the intensity with which a compound absorbs at various frequencies) provide subtle tools for structural investigation.

A molecule can become excited in a variety of ways, corresponding to absorption in different regions of the spectrum. The various processes and the approximate energy differences involved are summarised in Fig. 1; details may be found in the individual chapters. The practical applications of the various absorption methods and of the other physical techniques are compared and contrasted below. Rotational spectra (see Fig. 1) are not considered further; although they provide an accurate method for the determination of the geometry of simple molecules, they are of little direct interest to organic chemists. Quantised absorption of X-rays can occur and involves the excitation of electrons in the inner shells of atoms, but this process is also of little significance in the determination of organic structures (see however p. 304).

**A survey of the methods.** The effective and economic use of physical tools in organic chemistry clearly depends on an appreciation of the theoretical and practical capabilities and limitations of the various methods. The following chapters are intended to provide a basis on which such an appreciation can be built. Unfortunately, since the methods differ widely both in principle and practice, it is difficult to discuss them as a whole in a systematic way; indeed even the sequence in which the various methods are presented in this book is determined more by their relative importance than by any more logical physical or chemical criteria. Nevertheless, an attempt to survey some outstanding features will now be made.

Factors which determine the choice of the methods to be used in any particular problem are (i) the information required and the type and complexity of the compound under investigation, (ii) the amount of relevant empirical data already in the literature and/or the availability of relevant reference compounds, (iii) the quantity of sample available, (iv) certain physical characteristics of the sample, e.g. its solubility in the permissible solvents, (v) the importance of the problem, i.e. the amount of time and effort which it justifies and (vi) the accessibility and cost of the apparatus required. A full appreciation of these factors

TABLE 1. A survey of

1. <i>Method</i>	2. <i>Principle</i>	3. <i>Time required†‡</i>	4. <i>Approximate amount of sample</i>	5. <i>State of sample‡</i>
INFRARED SPECTROSCOPY (Chapters 2 and 3; see Tables 1, 2 and 3, Chapter 2 for comparison with ultraviolet spectroscopy)	quantised absorption of infrared radiation leading to vibrational excitation of molecules (pp. 23 and 36)	mins, hrs	1–10 mg	solid (usually mull), liquid film, dilute solution in suitable solvent (not, in general, water), alkali halide disc or vapour (see p. 42)
RAMAN SPECTROSCOPY (Chapter 3, p. 116)	scattering of visible or ultraviolet light with quantised absorption of <i>some</i> of the energy, leading to vibrational excitation of molecules (p. 116)	mins, hrs	50 mg–10 g	fairly concentrated solution, clear and colourless (p. 120)

† Time required for experimental observations (including preparation of solutions, etc.) on one compound and for their immediate interpretation (see p. 16); mins = 5 minutes to 1 hour, hrs = 1 hour to 1 day, days = 1 day to 1 month, months = 1 month to 1 year, years = more than one year.

‡ Bold type signifies 'much more common', italic type means 'relatively rare'.

necessitates a basic knowledge of the individual methods (see the following chapters) and some practical experience in their use. However, it is hoped that Table 1, which summarises the salient features of the methods, will prove useful as a preliminary guide. Cross-references to the following chapters are provided for many of the entries and the Table can be used later for revision purposes and to gain perspective. It must be emphasised that the Table does not cover every circumstance and should be regarded only as a general guide; many of the statements are not without exceptions.

[discussion of Table 1 continued on p. 16]

the physical methods

6. <i>Approximate cost of apparatus</i>	7. <i>Availability</i> §	8. <i>Information obtained and applications</i>
£1,500–5,000	bench, service	<p>Presence and environment of functional groups, esp. those containing X – H bonds (e.g. O – H) or multiple bonds (e.g. C = O) (see p. 38 <i>et seq.</i> and p. 48 <i>et seq.</i>). Diagnosis of finer structural detail, e.g. conformation (p. 70), intramolecular hydrogen bonding (pp. 66, 76 and 105), <i>cis-trans</i> isomerism (pp. 72 and 101), etc.</p> <p>Analytical applications include qualitative and quantitative analysis (e.g. pp. 32, 45 and 46), investigation of reaction rates and equilibria (including intermolecular hydrogen bonding, p. 61), examination of crude reaction products (p. 95), detection of impurities (p. 45), industrial production control (p. 46), etc.</p>
£2,500 (photographic)– 6,000 (photoelectric) –18,000	specialist, service	<p>As for infrared but less widely applicable, mainly because of sampling restrictions. However, aqueous solutions can be used (not easy in infrared). Functional groups which have weak infrared absorption often give strong Raman spectra and vice versa (p. 119)</p>

§ Bench = apparatus suitable for operation after only brief instruction is widely available, service = available as a service in most laboratories, service = available as a service in many laboratories, service = available as a service in relatively few laboratories, specialist = to a large extent in the hands of specialists.

TABLE 1. A survey of

1. <i>Method</i>	2. <i>Principle</i>	3. <i>Time required†‡</i>	4. <i>Approximate amount of sample</i>	5. <i>State of sample‡</i>
ULTRAVIOLET AND VISIBLE SPECTROSCOPY (Chapters 2 and 4; see Tables 1, 2 and 3, Chapter 2 for comparison with infrared spectroscopy)	quantised absorption of ultraviolet or visible radiation leading to electronic excitation (pp. 23 and 126)	mins, hrs	0.1–10 mg	dilute solution in transparent solvent (p. 130)
NUCLEAR MAGNETIC RESONANCE (Chapter 5)	quantised absorption of radiation giving rise to transitions between different spin orientations of nuclei (commonly protons) in a magnetic field (p. 168)	mins, hrs, days (for analysis of complex spin-spin coupling)	ca. 0.5 ml of 0.1–1M soln., i.e. ca. 5–100 mg	fairly concentrated solution, commonly in CCl <sub>4</sub> , CDCl <sub>3</sub> or D <sub>2</sub> O
ELECTRON SPIN RESONANCE (electron paramagnetic resonance) (Chapter 5, pp. 168 and 203)	quantised absorption of radiation giving rise to transitions between opposite spin orientations of unpaired electrons in a magnetic field (pp. 168 and 203)	mins, hrs, days (for analysis of complex spectra)	10 <sup>-11</sup> mole of radicals detectable, but larger quantity required for structural studies	solution or solid
OPTICAL ROTATION (Chapter 6) (a) at a single wavelength, e.g. sodium D line	rotation of the plane of plane polarised light by asymmetric molecules in solution (theory is complex, p. 217)	mins	1–200 mg (depending on apparatus and specific rotation)	solution



the physical methods—cont.

6. Approximate cost of apparatus	7. Availability§	8. <i>Information obtained and applications</i>
£700 (non-recording)– 1,500 (recording)– 5,000	bench, service	<p>Presence and nature of unsaturation, particularly conjugated double bonds (p. 133 <i>et seq.</i>) and aromatic rings (p. 146 <i>et seq.</i>). Stereochemistry of conjugated systems (pp. 135 and 159). Detection of certain (relatively few) functional groups, e.g. ketonic or aldehydic C=O (pp. 138 and 155).</p> <p>Analytical applications: similar to infrared, except that</p> <ul style="list-style-type: none"> <li>(a) restricted mainly to conjugated and aromatic compounds</li> <li>(b) aqueous solutions can be used</li> <li>(c) often more sensitive, i.e. very dilute solutions can be examined. (pp. 32, 152 and 160)</li> </ul>
£10,000–20,000	service, specialist	<p>Environment of nuclei (esp. protons), hence unambiguous detection of certain functional groups (p. 193) and information about the environment of many others (p. 174 <i>et seq.</i>). Counting of protons of various types in a molecule (p. 173). Determination of proton sequences (e.g. p. 195) and hence of relative points of attachment of functional groups. Assignment of configuration and conformation (p. 191). Can be used for quantitative analysis including study of reaction rates and equilibria, but requires more material than u.v. or i.r. spectroscopy—however sometimes applicable when these fail (an advantage is that the intensity of the signal from a nucleus is independent of its molecular environment). Study of fast reactions (pp. 178 and 191) and of hydrogen bonding (pp. 178 and 196).</p>
£5,000–10,000 (depends on resolution)	specialist	<p>Detection and estimation of free radicals and diagnosis of their structure and electron distribution (p. 205). Applications include study of free radicals in irradiation products and in complex biological material. Organometallic compounds with unpaired electrons can also be studied.</p>
£150 (visual)– 500 (photoelectric)– 1,500	bench, service	<p>Determination of relative and absolute configurations of asymmetric centres (p. 236). Location of functional groups in certain types of compound (e.g. steroids, p. 240). Information about conformation. Criterion of purity and identity esp. valuable when m.p. and spectra are indefinite (e.g. carbohydrates).</p>