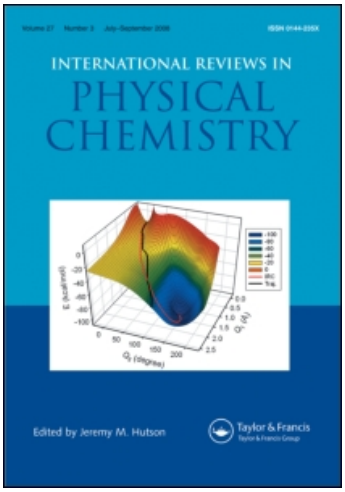

International Reviews in Physical Chemistry
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713724383

Book Reviews

To cite this Article (1987) 'Book Reviews', International Reviews in Physical Chemistry, 6: 1, 91 — 92
To link to this Article: DOI: 10.1080/01442358709353402
URL: http://dx.doi.org/10.1080/01442358709353402

INTERNATIONAL REVIEWS IN PHYSICAL CHEMISTRY, 1987, VOL. 6, NO. 1, 91–92

Book reviews

Orbitals, Terms and States. By M. GERLOCH (John Wiley & Sons, 1986.) [Pp. 176.] £7·95. ISBN 0 471 90936 X.

This useful little book applies itself to a number of the tricky prolems that abound in the application of quantum mechanics to chemical problems. As those involved in the teaching of quantum chemistry to chemistry undergraduates are aware, compromises invariably are needed since there is rarely the space for the full rigour of quantum mechanics to be taught. For this reason, much must be taken on trust or justification sought through the use of physical models. As a result, in each area of quantum chemistry there are points and concepts of some substance that can profitably stand amplification and illustration, particularly if this can be done in an interesting and readable fashion.

In *Orbitals, Terms and States,* Gerloch illuminates a number of dark corners of quantum chemistry that are known to cause students conceptual problems and he achieves this in a text that is both lively and instructive. The subjects tackled are mainly those concerned with the electronic structure of atoms. There is a preamble on angular momentum and its central role in atomic theory, including an extended discussion on the spherical harmonic functions. Many-electron atoms are then described in some detail with a full chapter on spin–orbit coupling; thus, the vexing question of what constitutes an orbital, an atomic term, and a state, can be carefully defined. Stark and Zeeman effects are also treated.

Following this quite coherent treatise on atomic theory, the selection of topics chosen in the remainder of the book strikes the reviewer as less clearly defined and related. Perhaps the most useful section is that on electronic states of diatomic molecules, although the omission of rotational angular momentum means that the section is reduced in value as a teaching aid in spectroscopy. The non-crossing rule, Hilbert space, diagonalization and a number of other topics are discussed and undoubtedly the student will be further enlightened by the discussion, but the thread linking these disparate areas is not clearly apparent.

After reading this book, elegantly written and lively as it is, it is difficult not to see the need that this text fills as a symptom of a deeper malaise in our teaching of quantum mechanics. In truth it represents a patching up operation that is necessary because, apart from some specialized courses in theoretical chemistry or chemical physics, a complete and detailed description of the quantum theory is not normally contained in the chemistry curriculum. An alternative strategy to revealing layer after layer of understanding onion skin-like would be to recognize that quantum mechanics is a proper subject as a foundation in modern chemistry. In this spirit, then, the reviewer would recommend Atkins's *Molecular Quantum Mechanics* at *c.* £16 as a source of deeper and longer lasting enlightenment than Gerloch at £7·95. Our curricula being what they are, however, Gerloch's book performs a useful function at a modest price.

A. J. MCCAFFERY
University of Sussex

Fourier Transform Infrared Spectrometry. By PETER A. GRIFFITHS and JAMES A. DE HASETH. (Wiley Interscience, 1986.) [Pp. 656.] £76·75. ISBN 0 47109 902 3.

This book is Volume 83 of a series devoted to techniques of chemical analysis. Although many of the nineteen chapters are concerned with analytical applications, the early ones are dedicated to developing the theoretical background of Fourier transform spectroscopy. The authors have achieved this with commendable thoroughness and in an interesting and novel way. While Chapter 1 itself is over fifty pages long it makes excellent reading with a useful combination of mathematical formulae linked to the necessary diagrams, essential for a full understanding of interferogram methods. The table at the end of this chapter listing the pros and cons of slow and fast-scan instruments is particularly useful.

The second and third chapters, 'Sampling the Interferogram' and 'Computing Techniques', are equally useful and essential reading for students beginning work in the FT area regardless of

whether they are pure spectroscopists or analytical chemists. To non-specialists, one of the mysteries of the FT method is the conversion of the interferogram to a spectrum, which is usually explained by extensive mathematics. At the end of Chapter 2 Griffiths and de Haseth appreciate this difficulty with their 'pictorial essay', a diagramatic stepwise account of how the interferogram is converted to a spectrum *via* either the Mertz or Forman methods. The sophistication of modern Fourier transform spectroscopy revealed in this way is truly impressive.

Another important subject, covered in Chapter 7, is the signal-to-noise ratio (SNR). This chapter begins with a consideration of theoretically predicted signal-to-noise ratios and how closely they might be approached in a real spectrometer. In reality there has to be a compromise embracing several factors, such as resolution or measurement time. These are the 'trading rules' which are also considered in this chapter. As in many fields of endeavour scientists are usually prejudiced in favour of their own chosen technique or method; Fourier transform spectroscopists are no exception in this regard. It is interesting to see therefore in Chapter 7 a balanced, quantitative comparison of FTIR versus grating instruments. The anticipated advantage of the former, due to Jacquinot and Fellgett's advantages, is partly offset by the lower sensitivity of the detectors on the FTIR instruments. The authors make the point that, particularly in the long-wavelength (far infrared) region, the advantage of the FTIR over the dispersion instrument may be only a factor of ten or lower.

The main areas of interest in the analytical uses of FTIR are well represented from Chapter 10 onwards. It would have been pleasing to see more about gas-phase applications, for example to plasma diagnostics where the work of Guelachvili and co-workers has made a considerable impact on the use of FTIR at very high resolution for studying transient species. Overall though there are very few blemishes and the text is remarkably free of misprints. Although the price will totally deter most scientists from obtaining a personal copy this is a very large book and, in terms of cost per page, good value for money. It is certainly important enough to be in any library serving good spectroscopic or analytical research.

In their introduction Griffiths and de Haseth describe the landmarks in the development of FTIR up to the advent of applicable microcomputer technology in the mid-seventies. Since then the technique has developed rapidly and this volume fulfils a real need in providing a comprehensive text on the fundamentals and applications of this important method of modern spectroscopy.

P. B. DAVIES
University Chemical Laboratory,
Cambridge