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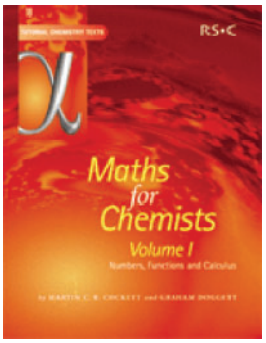
A Functional Introduction

*William S. Price**



Maths for Chemists, Vols. 1 (Numbers, Functions and Calculus) and 2 (Power Series, Complex Numbers and Linear Algebra)

by M. C. R. Cockett and G. Doggett
RSC 2003, 180 and 134 pp
ISBN 0-85404-677-1 and 0-85404-495-7
Softcover, £15 each

Over the past decade there has been a worrying trend involving the reduction in the mathematical content of chemistry courses. Thus, this two-volume set is a welcome addition to the literature and helps to reverse this trend. As stated in the preface '… in all branches of chemistry … mathematical tools are required to build models of varying degrees of complexity, in order to develop a language for providing insight and understanding together with some predictive capability', or, in other words, a decrease in mathematical ability and a reduced capability to see the inherent connections between mathematics and chemistry means chemists lose a prime research tool. These volumes attempt to fill the gap between high school and, say, upper undergraduate/graduate texts such as *Mathematics for Chemists* by Perrin and *The Mathematics of Physics and Chemistry* by Margenau and Murphy.

Volume 1 starts off at an extremely basic level with the first two chapters covering numbers, algebra, functions, and equations. The back covers of the volumes state that although the two volumes are intended to provide a resource for all undergraduate students, they are particularly focussed on students who may not have studied maths beyond the GCSE level (about year 10). Although these chapters are well done, it is nevertheless a sad comment on the secondary curriculum that a book for undergraduates needs to include such elementary concepts. On page 44, one hopes that the authors really meant to write 'to fit the model expression to the experimental data' and not vice versa. On page 56 many-to-one functions are introduced prior to introducing the concept of a one-to-one function on page 57. This is a small point, but the prior introduction of 'one-to-one' and 'onto' functions would have aided the understanding at this point. Further, in the discussion on polynomials on page 69, it would have been nice to introduce the concept of 'bisection' as a simple numerical means for root finding instead of just mentioning that one can turn to the programs *Maple* or *Mathematica*.

The subsequent four chapters of volume 1 introduce the concepts of limits, differentiation, differentials, integration, and differential equations. These chapters too are well done but they have their limitations. The concept of a limit is clearly introduced, but the standard rigorous techniques for finding limits should have been more clearly shown. The chapter on differentiation is quite lucid but more could have been made of the mathematical tools introduced here. One obvious example would have been to introduce the Newton–Raphson method, especially since the problems of finding roots to polynomials has already been mentioned. The chapter on integration explains the various standard techniques (necessarily excluding complex integration, since this chapter comes before the chapter on complex numbers) but curiously makes no mention that there exist books that tabulate virtually all of the definite and indefinite integrals that one is likely to encounter (e.g., *Table of Integrals, Series, and Products* by Gradshteyn and Ryzhik) or the applicability of symbolic algebra programs such as *Maple* and *Mathematica*. The final chapter gives a light-weight introduction to ordinary differential equations.

Volume 2 is significantly shorter than volume 1. The first chapter gives a good introduction to the concepts of series and convergence. Curiously, the formula for the binomial coefficient is given on page 6, but it is not stated as such. The final three chapters deal with determinants, matrices and matrix algebra, and vectors. The end of the chapter on matrices and matrix algebra gives an all-too-brief introduction to molecular symmetry and group theory—especially brief given that this book is meant for chemists.

Overall the two volumes are very good indeed and the authors strive hard to show the relevance of mathematics to chemistry. My reservations with these volumes lie in three areas: (1) ordering of the material, (2) topics that should not have been omitted (especially given the modest length of volume 2), and (3) that the books do not point the reader in the direction of further information. The ordering of the material in the two volumes, in my view, would have been improved if most of the chapter on vectors from volume 2 was moved to immediately after the chapter on differentiation in volume 1. The chapter on vectors should have contained some information on other coordinate systems apart from the Cartesian system and when it is more appropriate to use them. The chapters on integration and differential equations could have been moved to volume 2 after the chapters on matrices. This would have allowed complex integration to be included into the chapter on integration and the use of matrices and matrix exponentials as means for solving coupled differential equations to be covered in the chapter on differential equations. It also would have allowed some coverage on the method of Frobenius for solving differential equations and thus an introduction to the special functions (for example

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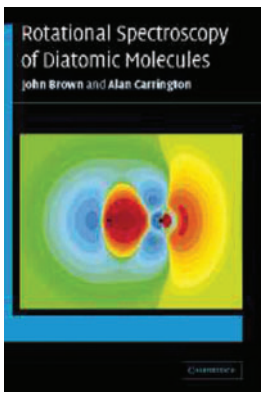
Bessel, Legendre, spherical harmonics, etc.) so commonly encountered in chemistry but yet entirely omitted in these volumes. Some discussion on partial differential equations would have been welcome too.

The argument in the preface concerning the omission of the statistical treatment of error analysis did not gel with me and, irrespective of what practical chemistry courses are provided by a chemistry department, the maths must be the same, and it would have been nice had this been included here. A final topic that should have been mentioned briefly was integral transform methods (for example Laplace and Fourier), not only because they are useful for solving differential equations, but because their understanding is so important for many forms of spectroscopy. It is unrealistic to expect too much to be crammed into two small volumes, but the usefulness of these volumes, especially as a resource, would have been greatly expanded had the authors chosen to include (annotated) bibliographies for further reading and more advanced methods.

*William S. Price is Professor of Nanotechnology at the University of Western Sydney. His research interests involve molecular dynamics in biological and chemical systems using NMR imaging, relaxation, and NMR diffusion measurements.

*Warren Lawrance**



Rotational Spectroscopy of Diatomic Molecules

by John Brown and Alan Carrington
CUP, Cambridge
2003, 1046 pp
ISBN 0-521-53078-4
Softcover, £43

To those in other fields of chemistry it may seem surprising that a book on the spectroscopy of diatomic molecules would fill 1000 pages, and even more surprising that a book focussing only on the rotational spectroscopy of these entities in the gas phase would do so. However, the book's size is a reflection of the authors' intended scope: Brown and Carrington have set out to produce the definitive text on this subject. They have, I believe, successfully met this objective.

Everyone has their prejudices for how such a work should be constructed, and I admit that my prejudice aligns with the approach taken by Brown and Carrington. The first third or so of the book is devoted to the quantum mechanics of the problem. The authors proceed from first principles to develop the Hamiltonian for the system and then relate this to what the spectroscopist measures, which is a set of constants for an effective Hamiltonian. Understanding how the effective Hamiltonian relates to the 'true' Hamiltonian is the key to extracting molecular behaviour from the measured constants. This section is well written and takes the reader through the complex interactions that are revealed by high-resolution rotational spectroscopy.

The second part of the book, which occupies about 60%, deals with various experimental techniques. A brief historical introduction to each technique is presented for each chapter and serves nicely to give the reader a sense of context. Each technique is discussed in detail as is its application to a variety of molecular systems. I liked the fact that the authors do not simply deal in the abstract here, but use liberal examples worked through in detail. In many ways this is the power of this book as a resource: the examples, with references to the original literature, provide the reader with a starting point for an analysis of other, related, systems. The book is comprehensive in its coverage of various techniques, and includes those that might now be considered almost obsolete, although I concur with the authors that their inclusion adds considerable value to the book as a definitive reference.

This is an excellent book and should be a widely used reference for those interested in molecular spectroscopy more generally and not just 'microwave' rotational spectroscopy of diatomic molecules. The interactions discussed can occur in larger molecular systems and in excited states and the discussion in this book serves as an excellent starting point for these cases. The spectroscopy of diatomic molecules is itself no longer a 'hot' topic and it is difficult to imagine getting funded for such work these days, although metal-containing species formed by laser ablation are a possible exception to this generalization. Nevertheless, an understanding of the behaviour of diatomic molecules, revealed by rotational spectroscopy, is an important starting point for understanding larger systems, both covalently and non-covalently bound. In my view the importance of this book will lie in its providing a comprehensive reference for the behaviour of diatomic molecules as a starting point for larger systems.

*Warren Lawrance is Professor of Chemistry at Flinders University, Adelaide. His research interests center on physical chemistry and molecular dynamics.

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