Preface

The last decade has seen an explosive increase in the use of computers in all aspects of life. It is now common to find computers in the home, the school, in work and in the laboratory. For many years computers were the prerogative of large institutions but all that has been changed by the emergence of the ubiquitous 'micro'. The ready availability of cheap computing power that, only a few years ago, would have cost many thousands of pounds, has created the need for a new type of textbook—one that utilizes this new-found computer power to extend and enlarge upon the more traditional methods of teaching scientific material.

This book has the aim of providing an introduction to molecular spectroscopy whilst making extensive use of computer programs written in BASIC to provide practical examples and illustrations of the topics under consideration. The book is primarily aimed at first- and second-year undergraduates in Chemistry and Physics taking an introductory course in molecular spectroscopy, however, it should also serve as a source book for more advanced undergraduates and those who use molecular spectroscopy as a practical tool.

The book contains a large number of well-documented BASIC programs which form the basis for a library of practical problem-solving routines. BASIC was chosen as the language for this book, and indeed for this whole series, since it is simple to write, easy to use and almost universally available on microcomputers. A further important consideration is the ease with which programs can be written, tested, modified and run in an *interactive* mode. This results in much faster program development—albeit at the cost of less elegance—than is possible with computer languages such as FORTRAN or PASCAL.

It is expected that readers will want to modify the programs presented here to suit their own particular needs and, indeed, each chapter is accompanied by a number of problems designed to explore spectroscopic and computational aspects of the material in more depth. Although the majority of problems are closely related to the programs and text itself, some are given that provide the student with

more challenging material and the chance to develop certain aspects of the subject to a higher level. To this end the reader is also referred to other books in the series, such as *BASIC Numerical Mathematics* and *BASIC Matrix Methods*, for more advanced numerical techniques.

In a subject as large as molecular spectroscopy, a book of this length presents the author with a difficult dilemma. One can either attempt to treat all areas equally, albeit at a superficial level, or one is forced to restrict the scope so as to achieve a reasonable coverage of selected topics. The second approach has been adopted here for two reasons; first, it provides for greater coherence and a more satisfying level of exposition. Secondly, the tremendous strides in instrumentation and the advent of lasers in particular, has meant that high resolution spectroscopy is now the norm rather than the exception. It thus becomes imperative that any discussion of modern spectroscopy should concern itself with the finer molecular interactions that are responsible for the complex spectra revealed at high resolution.

The contents of this book are concerned solely with spectra arising from the interaction of the electric field component of light with molecular or electronic motions. The chapters deal successively with programming, fundamentals of molecular quantum mechanics and light absorption, rotational spectroscopy, vibrational spectroscopy, and finally Raman and electronic spectroscopy. The lack of space has precluded a discussion of molecular symmetry or magnetic phenomena and, although this is to be regretted, it is hoped that the greater detail afforded to the other topics will more than compensate.

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