

A lucid introduction to molecular spectroscopy

**The Spectra and Structures
of Simple Free Radicals:
An Introduction to
Molecular Spectroscopy**

By G. Herzberg

226 pp. Cornell U. P.,
Ithaca, N. Y., 1971. \$11.00

Reviewed by Edel Wasserman

This small volume provides a lucid and useful introduction to the field of molecular spectroscopy by one who has recently been cited for "his contributions to the knowledge of electronic structure and the geometry of molecules, particularly free radicals." The subject matter in the present work is broader than might appear from the main title, as the author uses "free radical" to refer to any transient species, including those in singlet states.

After an introduction discussing methods of observation and species identification, there are chapters on diatomics and linear and nonlinear polyatomics. Rotational and vibrational levels are discussed together with the electronic states. The book closes with a chapter on "Dissociation, Predissociation and Recombination." The argument concentrates on gas-phase electronic transitions. Occasional reference is made to the conclusions obtained from other spectroscopies, such as microwave and electron paramagnetic resonance.

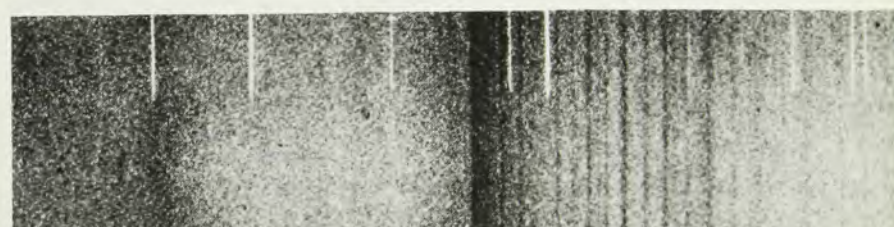
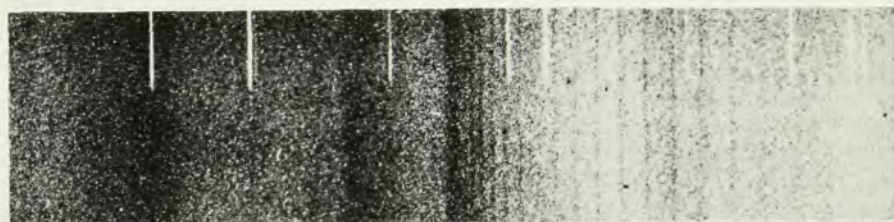
The contents are a distillation of the author's treatise, *Molecular Structure and Molecular Spectra*. Those three volumes have been the standard references in their fields since publication. In reducing the material by more than an order of magnitude the presentation here concentrates on fundamentals illustrated by selected examples. The informal, almost chatty, style of the early sections reflects the origin of the book in the series of Baker lectures given at Cornell in 1968 and makes for easy reading. As the complexities of polyatomic molecules are introduced the presentation becomes terser. The richness of the field is clearly presented in few pages. The reader's progress may well be slower here. Frequent

reference is made to the more complete discussions in the earlier volumes. The particular molecules discussed give a good view of recent interests in the field, with many examples coming appropriately, from the work of the author and his colleagues at the National Research Council of Canada. The publication schedule did not permit consideration of the latest conclusions as to the geometry of the ground state of CH_2 ;¹ some small changes in future editions will be desirable here.

In size and style the present volume is similar to the author's 35-year-old *Atomic Spectra and Atomic Structure*. That superb introduction to its field finds a molecular counterpart in many

sections of *Free Radicals*. I have no higher praise. The earlier work has an advantage in the comparative simplicity of atomic spectroscopy. The vibrational and rotational states involved in molecular spectra lead to greater complexity and a more rapidly paced presentation.

The two distinct levels of the book make it an unlikely choice as the sole text for a first course in molecular spectroscopy. It would appear particularly suitable as supplemental material for a senior or graduate student, perhaps as a reading period assignment. In addition, the material fills the very important need of an introduction and guide to *Molecular Structure and Mo-*



High-resolution absorption spectra of flash-photolyzed diazomethane and deuterated diazomethanes. The top spectrum shows diffuse lines due to CH_2 . The middle spectrum, taken with 50% deuterated diazomethane, prominently shows the absorption band of CHD. The bottom spectrum shows intensity alternation in the center band indicating that two D atoms are present in symmetrical positions. It was taken with CD_2 . From the book reviewed on this page.

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lecular Spectra. The reader can obtain an overall view of the field with much greater ease from the present work. The student beginning research in the area will gain much from it.

Reference

1. G. Herzberg, J. W. C. Johns, J. Chem. Phys. 54, 2276 (1971); E. Wasserman, W. A. Yager, V. J. Kuck, Chem. Phys. Lett. 7, 409 (1970).

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Edel Wasserman is a professor of chemistry at Rutgers University and a member of the technical staff at Bell Laboratories. He has studied the use of electron paramagnetic resonance in determining the structure of triplet states.

Mathematical Methods of Quantum Mechanics

By G. Fano. L. F. Landovitz,
ed. of English trans.

428 pp. McGraw-Hill, New York, 1971.
\$12.95

Our ideas about what constitutes an adequate mathematical preparation for graduate study in theoretical physics have changed markedly in recent years. Twenty years ago, the ability to solve the ordinary and partial differential equations arising from simple boundary value problems in the usual coordinate systems was considered the irreducible minimum.

Changes of taste, style and emphasis, as well as actual progress in our understanding of the physical universe require today's student to be conversant with functional analysis, analytic function theory, group theory and distribution theory in addition to the more classic topics mentioned above, merely to penetrate the current literature of theoretical physics.

An interesting parallel development is that the availability of large computers has altered our concepts of problem-solving, indeed, it has even changed our notions of what constitutes a solution. Efficient computer usage demands a reasonable acquaintance with computational mathematics—functional approximation, finite-difference methods, probability theory, optimization, and so on. By these standards, most entering graduate students are rather poorly prepared in both types of applied mathematics and require some form of remedial study in these areas.

How this should be administered is a problem, especially in view of the well-known reluctance of mathematics

departments to teach service courses in applied mathematics. One would think the times ripe for the applied-mathematics equivalent of the "Course Bourbaki" or the Landau and Lifshitz series. In its absence most physics departments try to cope with the situation by offering courses called "Mathematical Physics" in which smatterings of the above-mentioned subjects are taught at the level of "physical rigor." In due season these various courses give birth to a profusion of texts, each covering a subset of the necessary material, each having a decidedly parochial flavor reflecting the biases and special circumstances of the institution of its origin, and each entitled by some permutation of the words "mathematical," "theoretical," "methods" and "physics."

Mathematical Methods of Quantum Mechanics by Guido Fano is a pleasant departure from the norm in this field. Both in philosophy and content, its overlap with the standard texts described above is small. Moreover, rather than trying to be all things to all men, the subject matter of this book is unusually specific.

The first two chapters review the properties of complex, finite-dimensional linear vector space, while Chapters 3, 4 and 5 survey the ideas and results of functional analysis in Hilbert space. A sixth chapter dealing with the connection between Hilbert space and the axiomatics of quantum mechanics, as well as numerous useful exercises at the ends of the chapters have been added in the English-language edition. Advertised as "...written by a physicist for the physicist," the book is based on Fano's lectures at the University of Bologna, where he is Associate Professor of Mathematical Methods of Physics.

A more accurate description of the book might be that it is a mathematics text written for physicists, since the format is the usual one of definitions, lemmas, theorems, proofs and corollaries, all stated with mathematical rigor. However, the book departs from the ideal of extreme succinctness which unfortunately permeates so much of modern mathematical writing. The author is discursive, gives simple illustrations of important points and expresses himself with great clarity.

The major weakness of the book is the dearth of examples or exercises drawn from physical problems. For example, the theory of compact operators is developed at length and is essential in the theory of potential scattering, but no such application is given or mentioned. Again, one of the most useful and important applications of functional analysis in quantum mechanics is the establishment of variational principles and, thereby, bounds on quantities of physical interest. This subject is not touched upon in this