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### Book Reviews

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## BOOK REVIEWS

P. Arrighini. *Lecture Notes in Chemistry, Vol. 25, Intermolecular Forces and Their Evaluation by Perturbation Theory*, Springer-Verlag, 1981. 243 pp. \$17. ISBN 0 387 10866 1.

The theory of intermolecular forces has its origins in the early days of quantum mechanics through the work on dispersion forces by F. London and others and the conceptual framework was largely established at that time. In contrast it is still a difficult task to calculate the intermolecular potential between molecules from first principles with the accuracy needed to interpret the best experimental data.

Intermolecular energies are a very small part of the total energy and the 'state' of the molecule, i.e. its geometry, electron distribution, force field, etc., is very little affected by the interaction with other molecules. A benzene molecule is clearly recognizable as benzene whether in the gas, liquid or solid states. For this reason an approach to intermolecular energies through perturbation theory is attractive, and was the favoured route for qualitative theories from the early days. Again there is a contrast with the currently most favoured approach to quantitative calculations which is the variation method; this is frequently used for intermolecular as well as intramolecular interactions.

The most important development of the past 20 years in the theory of intermolecular forces has been to put quantitative muscle into the qualitative perturbation theories and this book deals largely with this theme. The problem that has to be faced is that at van der Waals distances there is a balance between forces that are long range and do not depend on the overlap of electrons of the interacting systems, and forces that are short range that do depend on this overlap. The extension of perturbation theories into this overlap region leads to difficulties in specifying the zeroth-order Hamiltonian and with over-completeness of basis functions. There have been several suggestions on how to overcome these and this book gives an excellent review.

The chapter titles show the importance of symmetry in the field. After a brief introduction we have:

Chapter 2. Symmetry: an excursion through its formal apparatus.

Chapter 3. Symmetry-adapted perturbation theory: a general approach.

Chapter 4. Why symmetry-adapted perturbation theories are needed.

Chapter 5. Symmetry-adapted perturbation theories at low orders: from  $H_2^+$  to the general case.

There then follow two chapters dealing with the specific problems of calculating first and second order energies.

I found the book very satisfactory in its balance: a little heavier to read but more comprehensive than the excellent review article by Claverie in *Intermolecular Interactions from Diatomics to Biopolymers* (Ed. B. Pullman, Wiley, 1978) which covers very similar ground. Given the current state of the subject it is a very fair coverage. However, one must say that the subject still has some way to go. This book is still dominated by atom-atom interactions, particularly  $H_2^+$  and  $H_2$ , with only brief mention of such important systems as  $(H_2O)_2$ . It is a very analytical book—for

theoreticians rather than experimentalists I think. I liked it very much and can recommend it for specialists in the field.

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H. F. Hameka. *Quantum Mechanics*. New York: Wiley-Interscience, 1981. pp. 387. £24. ISBN 0-471-09223-1.

This book is based in part on an earlier book by the same author, *Introduction to Quantum Theory* (1967). It is intended for a two-semester course, and in particular for 'junior and senior physics courses and senior and first-year graduate chemistry courses'.

The approach is mathematical and historical, rather than physical or chemical. There are eleven chapters with the following titles: preliminaries; matrix mechanics, matrices and determinants; wave mechanics and the Schrödinger equation; some properties and simple applications of the Schrödinger equation; differential equations and the Schrödinger equation; the hydrogen atom; approximate methods in quantum mechanics; time-dependent perturbation theory; interactions between radiation and matter; electron spin and the helium atom; atomic structure. At the conclusion of each chapter there are a number of problems, and a recommended reading list.

Mathematical and quantum-mechanical developments are successfully brought into contact, but this approach is unlikely to suit the more 'physically' oriented student. Thus the confluent hypergeometric functions will deter some before they have reached the harmonic oscillator and rigid rotor. The approach is not particularly even—thus there is an account of Brillouin-Wigner perturbation theory and Green function methods, but no mention of nuclear spin.

There are some mistakes, as in the spelling of Clebsch-Gordan, and in the first equation of page 267 for the Dirac  $\delta$  function, where the limit should be  $\alpha \rightarrow \infty$  rather than  $\alpha \rightarrow 0$ . SI units are not used, and the fundamental constants given in Appendix D are out of date.

The book lacks the clarity and authority of a great exposition, but it is a useful addition to the large number of good books in this field. It will be particularly helpful to mathematically gifted undergraduates in physics and chemistry.

A. D. Buckingham.