The divine dice keep rolling

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Molecular Quantum Mechanics, 2nd Edn.
By P. W. Atkins.
Oxford University Press: 1983. Pp.471. Hbk £29.50, $45; pbk £14.95, $27.95.

Quantum Chemistry.
By Donald A. McQuarrie.
University Science Books/Oxford University Press: 1983. Pp.517. $29, £22.50.

Problems in Quantum Chemistry.
By Poul Jørgensen and Jens Oddershede.
Addison-Wesley: 1983. Pp.286. $26.95, £24.30.

OVERHEARD in the corridor of Ancient Languages: "What's new in Classics then, Robin?". "Good Lord, nothing, I hope!". No such exchange about quantum mechanics seems conceivable, yet five decades of elaboration since Pauling and Wilson (four since Eyring, Walter and Kimball) do not obscure the distinct lineage to the three books reviewed here.

Novelty is most evident in the second edition of Atkins's *Molecular Quantum Mechanics,* which is likely to exceed the first in popularity. Most chemistry lecturers (but this is not a book for chemists alone) would probably choose to introduce non-particulate mechanics via Schrödinger rather than Heisenberg, although this may well be out of tune with the customers — students — who these days seem to prefer matrices to differential equations. In accord, Atkins's matrix-based introduction is developed in terms of the powerful operator and group theory methods towards approximate techniques and applications. Here it is that we expect new books to be different, and justice is done to ligand field theory, Hückel's method, bonding, and spectroscopy generally, and much else of what can be treated quantum mechanically. However, Atkins notably omits solids and reaction mechanism. Of the latter he says (*pace* the first edition) "No attention is paid to the theory of chemical reactions which, however fascinating, is still an infant subject". Well, well: theoreticians have a special view of things but such austerity could yet find mitigation in edition three, where adiabatic and nonadiabatic electron transfer might be nominated for honourable mention.

Atkins's book is also of spectacularly fine appearance, with wide margins providing locations for diagrams which thus do not interrupt the text. The separate litho typescript of solutions to the many problems (about 20 at the end of each of the 14 chapters) is by contrast quite acceptable in a companion workbook.

To quote Pauling and Wilson, "A book written for the reader not adept at mathematics [should] be richer in equations than one intended for the mathematician . . . who can follow a sketchy derivation with ease". By this criterion, all three books are suitable for moderate algebraists, being certainly rich in equations. But McQuarrie has set himself the goal of humanizing the story (as indeed does Atkins, but differently) by the inclusion of brief biographies of the *eminenti,* complete with photographs. The omission of Einstein from this stellar gallery precludes mention of his distaste for a merely probable universe, governed by the deity's dice. Chapter sub-headings tell a story of their own — "Pertubation Theory Expresses the Solution to One Problem in Terms of Another Problem That Has Been Solved Previously"; "Valence-Bond Theory Plus Ionic Terms Are Formally Identical to Molecular-Orbital Theory with Configuration Interaction" — and the whole vehicle of exposition has an attractive facility to it. Matrices only appear halfway through the book, indicative of the level of treatment. The depictions of orbitals are quite nicely illustrative, except for the cotton-wool museum pieces which date back to White in the 1920s. However, omission in the 1980s of ligand fields, even in an introductory text, does seem either too far ahead of or too far behind fashion to be comforting.

Neither Atkins nor McQuarrie uses Coulson's description of the electron as cloud. It is of course formally a probability density, but if the particle is deemed wave- or cloud-like in some aspects, it must be conceptually congruent to believe in a cloud which appears particulate in some of its aspects; the tradition as it has grown derives historically from the greater body of knowledge of particle behaviour than of clouds, and Kimball's notable efforts in the 1950s to restore some even-handedness perhaps deserve perpetuation.

The title of Jørgensen and Oddershede's book, *Problems in Quantum Chemistry,* might excite expectations. It is in fact a misnomer: these are *Student Calculations in a Quantum Mechanics Course,* to be used in conjunction with texts such as the other two reviewed here. Since most student textbooks, in particular Atkins, already contain numerous exercises, the value of such a compendium is to some extent in question; but then the authors do include the transition state, and the case is made. The solutions are well presented and provide a useful educational course not confined to the philosophy of a single text.

The books reviewed here afford the contemporary scientific tyro an access to intellectual avenues which will be invaluable, especially in view of the challenge arising from the present rate and extent of factual accumulation and theoretical development. □

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Rates of exchange

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Basic Chemical Thermodynamics, 3rd Edn.
By E. Brian Smith.
Oxford University Press: 1982. Pp.160. Hbk £9.50, $21.95; pbk £4.95, $9.95.

Chemical Thermodynamics.
By Peter A. Rock.
University Science Books/Oxford University Press: 1983. Pp.548. $29, £22.50.

Three Phases of Matter, 2nd Edn.
By Alan J. Walton.
Oxford University Press: 1983. Pp.482. Hbk £25, $49.50; pbk £10.95, $24.95.

IF CHEMISTRY is about systems in which the composition changes (whether because of "mixing" or of "reaction" is for real systems entirely a matter of convention), and physics is about systems in which the composition is constant, then the first two of these textbooks are of chemistry, and the third is of physics. While Smith and Rock restrict themselves to discussions of equilibrium ("thermodynamic") states, Walton deals not only with equilibrium states but also with the rates of approach to them. All three books are modern in attitude and scope, have been written with modern terminology and symbols, and — at least for the most part — consistently use SI units and the algebra of quantities.

Basic Chemical Thermodynamics is a short, readable well-established introductory textbook suitable for undergraduates during the first half of a degree course. If inevitably it tells much less than the whole of the truth, it manages to avoid telling more than a very few lies. The main change in this third edition is a new final chapter called "The Molecular Basis of Thermodynamics", a concise and welcome addition except for the false implication of its title which ought to have been something more like "The Molecular Basis of that Highly Specialized Small Part of Thermodynamics Concerned with Perfect Gases". It is a pity that Dr Smith did not find a few pages to make it plain, by talking more about real experiments with real apparatus, that thermodynamics is essentially an experimental subject. It is unfortunate, too, that he mars his modern exposition in a few places: by using the same symbol (*P*) sometimes for pressure and sometimes for the ratio (a number) of

Textbook supplement — prices

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