## **Choices for courses**

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Inorganic Chemistry, 2nd Edn. By A.G. Sharpe. Longman:1986. Pp.696. Hbk £25; pbk £12.95.

ONE can regard the arrival of a new or revised textbook very much in the way one anticipates a full-course dinner. One knows it is likely to be filling, maybe nourishing, but will it be interesting, attractively presented, even memorable? Sharpe's second edition provides a repast very similar to his first, but with some refinement of selected courses.

The text is aimed at the early years of an undergraduate course in inorganic chemistry, and nearly everything of importance is included in some measure. The preliminaries deal with nuclear, electronic structure and theory, and physical properties of molecules. Solid state chemistry and the behaviour of inorganic compounds in aqueous and non-aqueous media are dealt with in three chapters. Altogether, one can regard the first eight chapters as a condensed diet of basic physical/"general" chemistry with heavy inorganic seasoning.

The main meal is structured around nine chapters dealing with the s- and pblock elements, presented in their vertical groups, and ten chapters on the d- and fblock elements. This second section is based mainly on a topic approach, for example, electronic structure and the consequences for bonding, and thermo-

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dynamics, kinetics, metal carbonyls and organometallics. The d- and f-block elements are discussed in a limited way systematically, according to "tradition" (1st, 2nd/3rd row, lanthanides and actinides). In relation to the previous edition, there are additions to the discussions of donor-acceptor interactions, of the transition between non-metals and metals, and of aspects of polymer and bio-inorganic chemistry. Each chapter is referenced to general, more advanced, texts or specialist articles, and there are questions provided with numerical answers (where appropriate).

So what sort of rating does one give to this meal? In itself, it is satisfying dietarily and contains little extraneous or indigestible matter. When compared with other offerings, however, the rating is equivocal. Huheey, Mellor and Porterfield all use the same ingredients, but present them in different ways. There is a difference in philosophy in Sharpe's treatment - he deliberately accentuates thermodynamics rather than the symmetry, structure and bonding approach more common in the United States. Neither is preferable over the other, but in books of this size and price it is not possible to do justice to both. As far as presentation is concerned, the American texts look tastier. Sharpe's book is, however, interesting and memorable — anyone using this book in depth will find it clear and easy to read, if a trifle dull visually.

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## Chemistry in theory

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**The Chemical Bond, 2nd Edn.** By J.N. Murrell, S.F.A. Kettle and J.M. Tedder. *Wiley:1985. Pp.333. Hbk £19.95, \$31.85; pbk £8.95, \$14.30.* 

**Structure and Spectra of Molecules.** By W.G. Richards and P.R. Scott. *Wiley:* 1985. *Pp.172. Hbk £14.75, \$23.55; pbk £6.95, \$11.10.* 

**Potential Energy Surfaces: Molecular Structure and Reaction Dynamics.** By David M. Hirst. *Taylor & Francis:1985. Pp.234. £19, \$38.* 

"MURRELL, Kettle and Tedder" has been a popular textbook for 20 years, in its first incarnation as Valence Theory and latterly as The Chemical Bond. The first edition of Valence Theory appeared in 1965, at a time when it was still a common belief that most chemists had no need of quantum mechanics, but being intended for theoretical specialists at the graduate level the book did not need to avoid mathematics. By the time the first edition of The Chem*ical Bond* appeared in 1978, it was usual for undergraduate chemistry courses to contain material on quantum mechanics and its application to chemical bonding. Regrettably, however, chemistry was then still widely thought to be a suitable subject for the semi-numerate, and many of the mathematical details had to be omitted.

For some years this deficiency could be made good by turning to Valence Theory. That is now out of print and is not even mentioned in the new edition of The Chemical Bond, which nevertheless remains very much the plain chemist's guide to the theory of chemical bonding; much of the mathematics is left out, although there is in the new edition a chapter on methods of ab initio calculation, introduced in the knowledge that programs to perform such calculations are now widely available.

It is a pity that in protecting the reader from the complications the authors have allowed some misleading material to remain, as for instance in the account of group theory. The treatment assumes that everything is real (without, as far as I can see, actually saying so). Unfortunately several of the statements of grouptheoretical results are incorrect in the complex case. It is possible, too, to disagree with the presentation in places. For example the discussion of Walsh diagrams is essentially an *explanation* of the behaviour of the calculated orbital energies of  $H_2O$  as the bond angle is varied, and the reader is not shown how to use the insights in Walsh's famous series of papers to understand and predict bond-angle relationships *without* performing elaborate calculations, or how to use descent of symmetry to identify the significant effects.

However these are minor criticisms of a wide-ranging, thorough and useful text. Richards and Scott's book Structure and Spectra of Molecules suffers from much greater deficiencies. It aims to emphasize the relationship between molecular structure and spectra, but cannot be said to succeed. The trouble is in part that a full appreciation of this relationship requires first a good understanding of the principles of molecular structure on the one hand and of spectroscopy on the other. However the account given here is extremely superficial. Formulae are plucked out of the air, without derivation; explanations are sketchy or entirely absent; and a sprinkling of typographical errors adds to the confusion.

It is notable that many important and valuable concepts have no objective reality. For example, we are accustomed to thinking of electronic structure in terms of molecular orbitals, but they are no more than theoretical constructs arising from a particular approximation. The same is true of the "potential energy surface" governing the motion of nuclei in molecules. Lying behind this idea, however, is the Born-Oppenheimer approximation, arguably the most successful approximation in molecular quantum mechanics. In much of chemical physics the potential energy surface provides the common ground between theory and experiment; it is a readily understandable concept which summarizes the results of ab initio calculations and provides the basis for the interpretation of experiments.

In his book, Hirst has sought to provide an introduction to the use of this fundamental idea and has succeeded rather well. He deals with the calculation of potential energy surfaces by both accurate and approximate methods, and their relationship to vibrational spectroscopy and reactive molecular beam scattering. As always in an introductory text one could wish for more detail in places; for instance, there is no quantitative discussion of the accuracy of the Born-Oppenheimer approximation away from intersections. On the whole, however, this is a careful account of an important topic. 

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