was published in 1936: it is the second of three to describe uranium(IV) oxide. The first (Supplement Volume C4; 1984) described the production, preparation and crystallographic properties of UO_2, whilst the third (Supplement Volume C6) will describe its chemical properties: the volume under consideration here (Supplement Volume C5) describes its physical properties and electrochemical behaviour. Specifically, this volume details the following properties of UO_2: density, thermal expansion, elastic properties, hardness, creep, plastic behaviour, volume changes under irradiation, phase relations and thermodynamic functions, transport phenomena (including self-diffusion and thermal conductivity), dielectric constant, electrical conductivity, the Hall effect, and magnetic susceptibility. Perhaps of more interest to the inorganic chemist, this book also discusses the electronic structure of UO_2, and studies of it by electronic spectroscopy (both transmission and reflectance) and photoelectron spectroscopy, the vibrational spectra of UO_2, the properties of the $[UO_2]$ molecule and the $[UO_2]^+$ ion, and the use of spectroscopy to determine and interpret the non-stoicheiometry of UO_{2+x}. Finally, the electrochemical behaviour of UO_2 is discussed in terms of potentials, electrokinetic phenomena, the properties of UO_2 anodes, electrolysis of UO_2 melts, polarography in melts, and electrodeposition.

The importance of UO_2 to nuclear technology (it is the fuel for all light and heavy water reactors, and is used in a mixed crystal with PuO_2 in fast breeder reactors) cannot be overstated, and it is not surprising that this single compound is the subject of three complete volumes of the Gmelin Handbook. It is clear that the prime users of this particular volume are envisaged as nuclear engineers, but the authors (V. Haase, H. Keller-Rudek, L. Manes, B. Schultz, G. Schumacher, D. Vollath and H. Zimmerman) are to be congratulated for making the text so readable by chemists. Indeed, the sections concerned with electronic structure and electrochemistry deal with mainstream inorganic chemistry. It is taken for granted that the volumes produced by the Gmelin Institute are models of excellent production, being pleasingly type-set and clearly illustrated, and this volume is no exception. This book, taken with its two companion volumes, is now clearly the definitive source for all data related to uranium(IV) oxide.

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Ab Initio Molecular Orbital Theory; by W.J. Hehre, L. Random, P.v. R. Schleyer and J.A. Pople, London, Wiley, 548 pages, £81.80, ISBN 0-421-812-412

This is an eagerly awaited book by members of one of the most active and influential groups in quantum chemistry. Over a period of nearly twenty years they have established some widely accepted techniques, have written and distributed computer programs to carry them out, and have applied these techniques to a very wide range of chemical problems. Perhaps the work of the group is most commonly associated with organic molecules, and indeed these occupy a large part of this book. However, the standard ab-initio method is equally applicable to molecules containing other Main Group elements and, with some reservations, to the lighter transition metals. Indeed organometallic compounds of the Main Group elements are some of the more novel systems to have been studied recently and they are prominently described in this book.

People will not buy this book just to learn the basic principles of the ab-initio molecular orbital method. There are five chapters which cover this topic and also describe the computational techniques which are needed and the structure of the computer programs. However, it is important to appreciate that the strategy developed by Professor Pople and his research group is not followed by all quantum chemists, and because of that the development of the theory given in the introductory chapters is important for an understanding of the rest of the book. In brief, their most important principle is that to make valid comparisons between molecules in the same class one must do calculations on all at the same level of accuracy; it is not a matter of doing the best calculation possible on individual members of the series. As a supplement to this they aim to have relative errors which increase roughly in proportion to the size of the molecule; this is extremely important for obtaining good dissociation energies.

Chapter Six is a very long chapter which examines the performance of the model. This covers equilibrium geometries, vibration frequencies, barriers to internal rotation, electron distributions and thermodynamic stabilities. It is often not too difficult to get good results for conventionally stable molecules; those, say, for which there is a normal valence structure. It is more difficult, to get good results for the unconventional, but such results are much more valuable to the experimentalist for they can turn out to be unexpected.

Broadly speaking the data presented make the case that the more you pay (computationally) the better the results. For example, in predicting the relative energies of structural isomers the cheapest calculations (so-called minimal basis) are quite unreliable, often giving an incorrect order of stabilities, and the most expensive are usually the best. However, the best occasionally performs less well than an intermediate level of calculation (split valence basis), and examples are given to illustrate this. The wealth of data in the book provides valuable guidance to those wishing to judge the predictive value of calculations.

The Final Chapter, also very long, describes a variety of applications of the method. Many of these are the striking results that have been produced by the group in recent years: the structures and energies of carbanions and carbocations, planar tetra-coordinated carbon, lithiocarbons and lithiated hydrocarbons, beryllium clusters, etc. A relatively small section deals with the potential energy surfaces for reactions, perhaps indicating that successes in this area are still rather sparse and where they exist have been extracted with much sweat; surely a most important field for future work.

There is no doubt that this book is a major contribution to the chemical literature not only for its pedagogic value but for the wealth of data it contains.

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