problem of the selection of basis sets and computational procedures generally. A reader prepared to put the effort into understanding this section will be well equipped to undertake DFT calculations with a feeling for the theory and the pitfalls.

The second part of the book, 'The performance of the model', describes the results of DFT calculations, successes and failures, for a variety of molecular systems of interest to the chemist; it covers structure, both Main Group and transition-metal compounds and organometallics, vibrational frequencies, energies and thermochemistry, population analysis, electric properties (dipole moments, polarizabilities, infrared intensities), magnetic properties, NMR chemical shifts and NMR coupling constants. There is a chapter on water and hydrogen-bonded systems and a final chapter on chemical reactivity: exploring potential energy surfaces. Throughout this section quantities and properties calculated at various levels of theory are compared with the experimental data to provide a basis for the critical assessment of computational procedures.

This is an important book. Although I have practised DFT for some years (and by no means as a black box) I found that reading the book provided many insights and clarified concepts that had been barely understood. It is a book for practising chemists, those who recognize the value of the computational opportunities provided by today's powerful computers and who seek and need a critical insight into what they might achieve via DFT calculations. It is strongly recommended.

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Activation and catalytic reactions of saturated hydrocarbons in the presence of metal complexes

A. E. Shilov and G. B. Shul'pin
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This book is essentially the second edition of Shilov's earlier book, *Activation of Saturated Hydrocarbons by Transition Metal Complexes*, published in 1984. The earlier book had 203 pages, so the present work is about two and a half times as long. While the majority of the references are later than 1983, the authors have generally given a balanced view of the topic which does not assume the reader is familiar with the previous work, and the principles are set out in the first chapter. The authors had already published a review of this area in 1997.[1]

The book contains an introduction, ten chapters and an index. Somewhat strangely, the list of abbreviations is at the back of the book, and even more surprisingly in the 21st century, the authors are still using kilocalories. The treatment of the subject is very thorough and the extremely extensive lists of references (an exceptionally high ratio of references to text is a feature of the book; even the introduction has nearly four pages) make this a valuable work of scholarship.

The authors concentrate on the subject described in the title, although Chapter 2 is concerned with 'Hydrocarbon transformations that do not involve metals or their compounds'. Anyone seeking enlightenment on heterogeneous catalysis involving saturated hydrocarbons will find a recent report[2] of the proceedings of a NATO conference to be complementary to the present work, which does, however, have a chapter entitled 'Heterogeneous hydrocarbon reactions with participation of solid metals and metal oxides' consisting of 34 pages of text and diagrams and 16 pages of references.

Shilov's work on activation of hydrocarbons using platinum complexes is very well known, and a chapter (58 pages including references) is devoted to this topic. We must, however, turn to the chapter on 'Hydrocarbon reactions with high valent metal complexes' for a discussion of the work by Periana *et al.* on the conversion of methane to methanol involving a platinum complex in sulfuric acid.

A welcome feature of this edition is the inclusion of a chapter (55 pages) on 'Oxidation in living cells and its chemical models'. Cytochrome P450, methane monooxygenase and metalloenzymes containing copper, molybdenum and manganese are described here, along with synthetic models which attempt to mimic the activity of the metalloenzymes.

Another chapter is concerned with 'Homogeneous catalytic oxidation of hydrocarbons by molecular oxygen'. This covers both the commercial cobalt-catalysed oxidation of cyclohexane, and Barton's Gif systems, which usually contain iron.

Perhaps the chapter of most interest to organometallic chemists is the account of 'Activation of C–H bonds by low valent complexes' (73 pages). This chapter describes the oxidative addition of C–H bonds to low-oxidation-state complexes, but mechanisms are carried over to another chapter (40 pages). In these two chapters, and indeed throughout the book, the authors focus predominantly on alkanes with some digressions into unsaturated hydrocarbons, so that the fact that the choice of metal complex for activation of a C–H bond adjacent to a functional group is dependent on the nature of the functional group is not covered here.

To summarize, this is a scholarly account of recent research on the activation of alkanes by metal complexes. It can be recommended to researchers working in the area, and as supplementary reading for advanced courses on organometallic chemistry and catalysis.

REFERENCES

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