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Book Review

***Computational Organometallic Chemistry*. Edited by Thomas R. Cundari, Marcel Dekker, New York, 2001. ISBN 08247-0478-9; 448 pp.; US$185.**

Nowadays, barely a week goes by without one computer chip manufacturer or another announcing their latest, fastest processor. With all this computer power available, seemingly for only a few pence, it is inevitable that chemists will want to try and exploit these machines. Yet the very pace with which things computational move means that it is difficult to keep up and often we are left stranded under a mound of information. Therefore, a text which purports to summarise the current state-of-the-art is both timely and welcome.

Transition-metal (TM) systems in general and organometallics in particular have traditionally been deemed 'difficult' to model theoretically. Inevitably with a multi-author book with 15 chapters plus introduction, opinions differ about which is the best horse for a particular course, but what does come over strongly is the sense that enormous progress has been achieved especially over the previous few years, and while there may still be a long road ahead, computational chemistry for TM systems has established itself as a viable discipline.

Cundari sets himself and his co-authors up as both teachers and practitioners and, to a remarkable degree, the various chapters succeed in presenting 'something for everyone'. The largest number of chapters (nine) deals with quantum mechanical treatments of some kind. This reflects the growing significance of density functional theory (DFT) which has revolutionised the application of quantum chemistry to TM systems. At the same time, the book also compares and contrasts DFT with more traditional approaches based on the Hartree–Fock model and its many extensions. The only significant omission seems to the generalised valence bond approach championed by Goddard.

At the other end of the computational spectrum, four chapters describe the development and application of empirical molecular mechanics (MM). The contributions span the fundamentals of TM force-field parameter development, the use of MM to quantify those ubiquitous steric effects and even modelling transition states. In between the purely QM and the MM is a chapter describing hybrid QM/MM methods plus two chapters which discuss semi-empirical molecular orbital methods PM3(tm) and ZINDO.

The applications are as diverse as the computational methods and the reader will find, among others, information on simple binary carbonyls right through to the interactions between HIV integrase inhibitors with metal ions at the active site. There are also descriptions of Rh-mediated C–H insertion, oxidative addition of H_2 to Rh and Ir chlorophosphine complexes, d block and s block metallocenes, titanium hydrides, Group 13–15 ethene complexes, Re nitrides, Pt silyls and even a chapter on organoactinides. Mixed in with straight applications work are some interesting discussions of the theory behind nondynamic correlation and the consequences of spin state changes during a reaction.

In summary, Cundari sets himself an ambitious goal 'to combine instructional aspects with cutting-edge applications'. Overall, I think he succeeds pretty well and there is enough here to keep experimentalist, student and theoretician engaged. It will always be more challenging for the reader to dig out all the gems from a multi-author book of this sort but a little perseverance pays off handsomely. My copy is already well thumbed.

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