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Structure and Bonding

Aims and Scope

The series *Structure and Bonding* publishes critical reviews on topics of research concerned with chemical structure and bonding. The scope of the series spans the entire Periodic Table and addresses structure and bonding issues associated with all of the elements. It also focuses attention on new and developing areas of modern structural and theoretical chemistry such as nanostructures, molecular electronics, designed molecular solids, surfaces, metal clusters and supramolecular structures. Physical and spectroscopic techniques used to determine, examine and model structures fall within the purview of *Structure and Bonding* to the extent that the focus is on the scientific results obtained and not on specialist information concerning the techniques themselves. Issues associated with the development of bonding models and generalizations that illuminate the reactivity pathways and rates of chemical processes are also relevant

The individual volumes in the series are thematic. The goal of each volume is to give the reader, whether at a university or in industry, a comprehensive overview of an area where new insights are emerging that are of interest to a larger scientific audience. Thus each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole. The most significant developments of the last 5 to 10 years should be presented using selected examples to illustrate the principles discussed. A description of the physical basis of the experimental techniques that have been used to provide the primary data may also be appropriate, if it has not been covered in detail elsewhere. The coverage need not be exhaustive in data, but should rather be conceptual, concentrating on the new principles being developed that will allow the reader, who is not a specialist in the area covered, to understand the data presented. Discussion of possible future research directions in the area is welcomed.

Review articles for the individual volumes are invited by the volume editors.

In references *Structure and Bonding* is abbreviated *Struct Bond* and is cited as a journal.

More information about this series at http://www.springer.com/series/430

Stuart A. Macgregor • Odile Eisenstein
Editors

Computational Studies in Organometallic Chemistry

With contributions by

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Preface

In compiling this volume *Computational Studies in Organometallic Chemistry*, we have invited seven contributions that showcase how state-of-the-art quantum methods can address practical problems in molecular inorganic chemistry and provide insights into the factors that underpin the behaviour of these systems. In the first chapter Perrin, Carr, McKay, McMullin, Macgregor and Eisenstein present a description of current practices for the exploration of reaction mechanisms. This is further illustrated by Lin's chapter on the structure and reactivity of boryl complexes. Jover and Maseras then describe the use of QM/MM methods in modelling selectivity, and Vidossich, Lledós and Ujaque detail how molecular dynamic simulations have been applied in this area. Almeida, McKinlay and Paterson describe what is now possible in modelling excited states and associated reactivity. Tools to understand the origin of energy barriers are the focus of the chapters presented by Wolters and Bickelhaupt who outline the energy decomposition analysis (EDA) approach, while King, Gustafon and Ess apply this technique to the topic of C–H activation.

As well as thanking all the contributing authors, the editors would like to dedicate this volume to the memory of Tom Ziegler, a true pioneer in the development of methods and their applications in inorganic chemistry.

Stockholm, Sweden
4 September 2015

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