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BOOK REVIEWS

Gold Chemistry: Applications and Future Directions in the Life Sciences. Edited by Fabian Mohr (Bergische Universität Wuppertal, Germany). WILEY-VCH Verlag GmbH & Co. KGaA: Weinheim.2009. xvi + 408 pp. $215. ISBN: 978-3-527-32086-8.

The purported purpose of this book is to cover new "directions and to update and highlight important applications of gold complexes." To achieve this purpose, advances in three distinct areas of gold chemistry are presented: coordination chemistry, understanding of properties, and applications.

The first three chapters cover aspects related to coordination chemistry. Chapter 1 is an examination of recently published gold(I) compounds with a focus toward amidinate, pyrazolate, and guanidinate ligand sets. Chapter 2 complements the first by providing synthetic and structural details of gold(III) complexes containing *N*- and *O*-donors, and Chapter 3, the most detailed of the three, is a lengthy review of pentafluorophenyl gold chemistry. Notably, this chapter provides a significant amount of detail outlining the chemistry of these complexes as well as a description of potential applications.

Chapters 4 and 5 may be linked through their description of the properties of gold complexes. In Chapter 4, the theoretical chemistry of gold—ranging in scale from atoms to the bulk—is adequately described. The authors note that this area has been heavily reviewed within the past few years, but their rendition is done fairly well and serves to enhance the quality of the overall monograph. Chapter 5 is a surprisingly brief overview of gold(I) and gold(III) luminescence. The majority of the references are out-of-date (more than 5 years old) and do not serve to provide the reader with a recent outlook on advances in this important field.

The applications of gold chemistry are discussed in the final three chapters. The authors of Chapter 6 describe the role of gold in medicine, although the references here are a bit dated. However, the organization and material covered in this chapter should help the novice understand the principles of medicinally important gold complexes. Conversely, the remaining two chapters, on nanoscience and liquid crystals, respectively, are shorter and the topics are generally more thoroughly covered by other recent reviews and monographs.

In conclusion, I have rather mixed impressions of this book. On a positive note, the chapter on pentafluorophenyl gold chemistry reports on research in which the authors, Luquin et al., have made numerous contributions. The reader can find insights and helpful comments here, especially on synthetic considerations and potential applications. The chapter on the applications of gold in medicine also provides valuable discussion of the role of gold in various biological processes. On the other hand, there are some negative aspects to the book. As already pointed out, some of the most important recent results are omitted from several chapters. In addition, most of the "new directions" discussed in this monograph have been previously reviewed in detail. Overall, this book is suggested for individuals with a specific interest in gold chemistry and for those interested in becoming more involved in the field but who do not require detailed reviews of a specific area. The material is logically organized and is therefore also recommended for purchase by academic libraries.

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Hybrid Methods of Molecular Modeling. By Andrei L. Tchougréeff (Lomonosov Moscow State University). From the series, Progress in Theoretical Chemistry and Physics. Edited by W. N. Lipscomb and Y. Chauvin (Honorary Editors) and J. Maruani and S. Wilson (Editors-in-Chief). Springer Science + Business Media B.V.: New York.2008. xvii + 344 pp. $449.00. ISBN 978-1-4020-8188-0.

This book is an advanced treatise on hybrid methods of molecular modeling. It provides a thorough and relatively self-contained presentation of the theoretical foundations of hybrid modeling with detailed derivations of the key equations and discussion of approximations for their solution. Its contents provide a clear overview of hybrid methods that is appropriate for readers who have a basic knowledge of computational chemistry and a year of upper-level undergraduate or graduate-level physical chemistry. Many of the methods described in the book have been implemented into FORTRAN programs and are available through the Net Laboratory access system. As such, this is a very useful reference for graduate students, practicing experts, and developers alike.

The first chapter opens by framing the molecular modeling problem and introducing relevant background for later development. It is well presented, beginning with a discussion of the motivation for addressing molecular modeling and transitioning to the problem of representing the quantum-mechanical potential energy. Basic quantum-mechanical principles are then described, such as variational approaches and perturbation theory. Many-electron wave functions are discussed as well as standard methods for their solution, including introduction of atomic orbital basis sets, single determinants, full configuration interaction, Hartree−Fock theory, second quantization, unitary group formalism, and group function approximation. A particularly useful aspect of this text is the integration of more advanced concepts, such as alternate representations of quantum mechanics (QM)—e.g., projection operators, resolvent of the Hamiltonian, wave operator, and Van-Vleck transformation—and nonstandard quantum chemistry tools, such as reduced density matrices and Green's functions. The chapter concludes with general schemes for separating electronic variables to break down the many-body problem.

The second chapter launches into an analysis of current hybrid methods from the author's personal perspective and presents suggestions for their improvement. Here Tchougréeff takes a quantum-mechanical approach, beginning with a discussion of methods in ab initio quantum chemistry and then describing approximate methods, such as pseudopotential and various traditional Hartree−Fock-based semiempirical methods. Only

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brief mention is made of more modern semiempirical methods in a section called "Miscellanea. Further Development". There is also a list of unsolved problems or "Holy Grails" of the HFR-based semiempirics, some of which have now been solved or greatly advanced. The chapter proceeds with a discussion of methods that go beyond Hartree−Fock in terms of treatment of nontrivial electron correlation, including the strictly local geminal (SLG) wave function method and a lengthy and interesting review of methods for transition metal complexes with open d-shells. Only a short section is devoted to molecular mechanics (MM) methods, which more or less takes the tone of an incomplete survey. A few of the basic functional forms are mentioned, but there is relatively little coverage of next-generation polarizable force fields, such as AMOEBA, SIBFA, GEM, and Drude oscillator models. The author concludes with an overview of conventional hybrid methods that couple QM and MM parts of the system.

The next chapter delves into bridging quantum and classical models of molecular structure through so-called "deductive molecular mechanics" (DMM). Tchougréeff outlines a series of sequential steps intended to traverse the landscape between approximate quantum-mechanical description of electronic structure and a classical representation of the potential energy surface, with emphasis on organic compounds. This construct, dubbed DMM, is appealing in that each of its components can be traced to a specific quantum-mechanical counterpart. The author begins by characterizing features of molecular electronic structure within the SLG approximation and then introduces a family of sequential approximations ranging from fixed amplitudes and fixed orbitals (FAFO) to tuned amplitudes and tuned orbitals (TATO). The relationship between these models and conventional MM methods is discussed and placed within the context of DMM. Before concluding, the author focuses on the boundary between QM and MM regions within the TATO−DMM model.

The fourth and final chapter builds on the previous ones and focuses on the methods that have been so far developed on the problem of coordination compounds both with and without transition metals. These systems are poorly described by MM methods due to the nondirectional and often unsaturated character of the bonds and, in some cases, open d-shells that require consideration of correlation between multiple electronic states. The chapter addresses these two challenges together with the generalized hybrid methodology to develop a QM/MM scheme for coordination compounds that includes sufficient quantum representation of subsystems with d-shell character embedded in a general classical MM environment. The book concludes with the identification of remaining problems and directions for future research.

Overall, this book is a novel contribution to the field of hybrid modeling that lays the foundation for formulating a useful general QM/MM modeling approach. The text is self-contained in this regard and is presented clearly, with helpful discussions that make connections with other methods in common use in the field. It is not a comprehensive review of the most common state-of-the-art QM/MM modeling methods currently used in practice. In this sense, hybrid methods that go beyond molecular mechanics, such as methods for solvation, continuum electrostatics, integral equations, and course grained methods, are missing from the book. The book does not delve comprehensively into the molecular mechanics side, and the many modern methods that strive to integrate quantum many-body effects through use of electron density, electronic response models, orbital free methods, and reactive force fields are not discussed. There is relatively little discussion of density-functional theory and related methodological developments, such as tight-binding models and orbital-free methods, and there is only sparse discussion on linear-scaling methods in general. What the book does and does very well is provide a general theoretical foundation of hybrid modeling that is capable of attacking challenging problems ranging from organic systems to coordination compounds with open d-shells.

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