Book Reviews

Synthetic Methods of Organometallic and Inorganic Chemistry: Transition Metals Parts 1 and 2. Edited by W. A. Herrmann (Anorganisch-chemisches Institute der Technischen Universität München). Thieme: Stuttgart and New York. 1997. xii + 294 pp (Part 1), xii + 254 pp (Part 2). DM185.00 (Parts 1 and 2). ISBN 3-13-103081-X (Part 1), 3-13-103091-7 (Part 2).

These volumes complete an eight-volume set on the title subject. They provide an extensive collection of synthetic procedures of organometallic and inorganic complexes of transition metals. Every element from groups 6−12 and Au is covered. Part 1 (Volume 7) consists of five chapters and focuses on transition metal complexes containing noncyclic ligands such as carbon monoxide, alkyl, olefin, carbene, carbyne, and alkyne ligands. The collection of carbene, carbyne, and rhenium complexes is particularly strong. Part 2 covers, in two chapters, the synthesis of cyclopentadienyl complexes and to a lesser degree arene and cycloheptatrienyl complexes. Additional ligands such as nitrosyl, hydride, halide, and sulfur-containing ligands are also included. A third chapter entitled Miscellaneous Complexes includes complexes with weakly bonded anionic ligands, heterobimetallic complexes, and a variety of group 6−10 complexes containing (in part) acetato, acetonitrile, amino, imido, oxo, dihydrido, and perfluorophenyl ligands. In addition, each volume includes an index with multiple listings for each complex organized by name, metal, and ligand. Not including intermediates, ligand syntheses, and simple derivatives, the editor has gracefully organized a collection of approximately 350 synthetic procedures in these two volumes.

There are many exciting compounds chosen on the basis of their general applicability as starting materials and synthetic intermediates in inorganic and organometallic synthesis. In addition, numerous compounds are included with applications in organic synthesis and catalysis. These include reagents for stoichiometric transformations such as in the Dotz reaction, and catalysts for olefin polymerization, Heck coupling, hydrogenation, and olefin metathesis/ROMP (Mo(N-2,6-*i*-$Pr_2C_6H_3$)($CHCMe_2Ph$)[$OCMe(CF_3)_2$]$_2$). In some cases, procedures for the organic reactions are also given. The collection includes a fair selection of compounds that are commercially available ($Cr(CO)_6$, ferrocene, $Rh(PPh_3)_3Cl$) or have appeared in previous "recipe" books. However, the majority of procedures make their appearance for the first time in a recipe book.

The procedures are said to be "well-proven"; however, since they have not been independently checked, it is difficult to comment on their general reliability. The more interesting syntheses to read are those given with an informative introduction about the synthetic method and utility of the compound. Unfortunately, the majority of preparations merely list the procedure, leaving one wanting for more information about the history and (potential) utility. In addition, several procedures fail to cite recent references (e.g., an improved preparation of Vaska's complex previously appeared in *Inorg. Synth.* **1990**, *28*, 92) or adequately indicate the source of uncommon starting materials or ligands. Although most procedures are easy to follow, a few are not. For example, the synthesis of Ti(η^5-C_5H_5)$_2X_2$ complexes by metathesis with BX_3 does not give quantities of reagents or reaction times. The preparation of $Na_2[Cr(CO)_5]$ was difficult to follow. The caution statement for the preparation of $Tc_2(CO)_{10}$ indicated milligram quantities of ^{99}Tc "do not present a serious health hazard", but the procedure used gram quantities.

Since this collection completes the "Herrmann/Brauer" series of *Synthetic Methods of Organometallic Chemistry*, it is recommended for libraries and persons who have the previous volumes. In addition, because the collection is so extensive and easy to browse through, individual laboratories practicing primarily in organometallic synthesis will also find these two volumes very useful to have around. Purchasers should also consult Volume 1 of this series which presents additional transition metal complexes which are only cross-referenced in Volumes 7 and 8.

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Advances in Molecular Similarity Volume 1. Edited by Ramon Carbó-Dorca (University of Girona) and Paul G. Mezey (University of Saskatchewan). JAI Press: London. 1996. xxi + 287 pp. $112.50. ISBN 0-76230-131-7.

Molecular similarity has always been a part of mechanistic chemistry even if the name was not used. What aspects of a molecular's structure give it certain physical properties, cause it to take part in some reactions and not others, and cause it to follow one reaction pathway more than another? Some aspects of similarity can be recognized by undergraduate students. They can differentiate an ester from an ether, an alcohol from a carboxylic acid, and an alicyclic ring from an aromatic ring. What can be more difficult is identifying similarities when multifunctional molecules and, to add to the complexity, flexible multifunctional molecules are compared. More subtle, but more profound, are the electronic similarities and dissimilarities. These are not easily recognizable by visual inspection but require computer-intensive computations.

Advances in Molecular Similarity is the first volume in a series that promises to provide chapters showing how molecular similarity can identify physical properties and their underlying molecular properties. Molecular similarity has applications ranging from drug design to molecular engineering. The first book in this series consists of 11 chapters.

With any attempt at describing molecules in order to carry out comparisons, questions that must be answered include the following: What descriptors are appropriate? How accurate are the descriptors? Are they easily measurable? How are the descriptors selected in order to avoid bias? With so many descriptors available, how is or should the multidimensional space be reduced? Will use of the descriptors provide statistically valid conclusions? Will the results provide a means to design new molecules, or will it only provide an explanation of why an already existing set of molecules behave in a certain way?

Several chapters describe quantum chemical based descriptors. Of course, as the molecule becomes larger and more complex in terms of atomic diversity and conformational flexibility, the computational requirements increase. For quantum chemical based similarity studies to be practical in terms of computer time, procedures have to be simplified. Readers will have to decide if the assumptions described in the chapters have broad applications or are limited to the molecules in the data sets. The first chapters describe various quantum molecular similarity measures (QMSM). The first chapter gives a good overview of this approach and discusses the development of quantum molecular similarity indices (QMSI). The authors provide wide-ranging examples showing how their indices will predict both physical and biological properties.

The second chapter uses quantum chemical approaches to measure the similarity of atoms in molecules, producing an atomic similarity index. The third chapter's descriptor describes quantum chemistry based momentum-space similarity and dissimilarity indices and describes the use of cluster analysis to aid in the analysis of similarities. Biological data sets are used. Six chapters describe newer approaches at calculating indices and either do not show how well the approach will work in similarity analysis or use very limited examples.

The latter three chapters describe other methods to carry out molecular similarity studies. These include substructure similarity, topological analysis, spatial matching in three-dimensional space, and molecular connectivity.

As computer power at the desktop increases, it will become easier for the chemist to carry out similarity analysis. For people unfamiliar with the molecular similarity literature, *Advances in Molecular Similarity* brings the leading authors together in one volume. It is a well-written multi-authored book. Each chapter has an abstract and follows a standard outline. There is a good index. Because the chapters are well-referenced, each chapter provides an entry to the literature of the field. Chemists interested in the field should consider purchasing the book for their personal libraries.

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