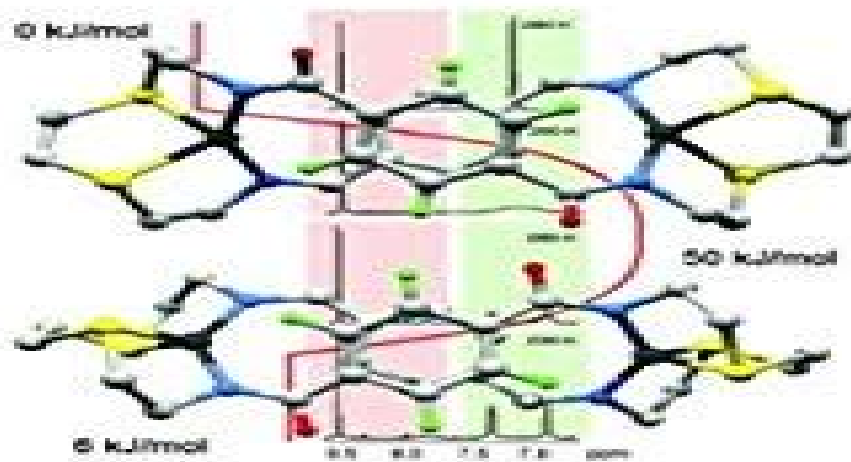


Peter Comba, Trevor W. Hambley

Molecular Modeling of Inorganic Compounds

Second, Completely Revised and Enlarged Edition



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Molecular Modeling of Inorganic Compounds Peter Comba, Trevor W. Hambley, Bodo Martin, 2009-07-10 After the second edition introduced first density functional theory aspects this third edition expands on this topic and offers unique practice in molecular mechanics calculations and DFT In addition the tutorial with its interactive exercises has been completely revised and uses the very latest software a full version of which is enclosed on CD allowing readers to carry out their own initial experiments with forcefield calculations in organometal and complex chemistry *Molecular Modeling of Inorganic Compounds* Peter Comba, Trevor W. Hambley, 2008-07-11 In many branches of chemistry Molecular Modeling is a well established and powerful tool for the investigation of complex structures The second completely revised and enlarged edition of this highly recognized book shows how this method can be successfully applied to inorganic and coordination compounds The first part of the book gives a general introduction to Molecular Modeling which will be of use for chemists in all areas The second part discusses numerous carefully selected examples chosen to illustrate the wide range of applicability of molecular modeling to metal complexes and the approaches being taken to dealing with some of the difficulties involved While the general outline is similar to that of the first edition many of the examples chosen for discussion reflect the changes of the past five years In the third part the reader learns how to apply Molecular Modeling to a new system and how to interpret the results The accompanying software features 20 tutorial lessons based on examples from the literature and the book itself The authors take special care to highlight possible pitfalls and offer advice on how to avoid them Therefore this book will be invaluable to everyone working in or entering the field *Bioinorganic Chemistry* Rosette M. Roat-Malone, 2007-10-05 An updated practical guide to bioinorganic chemistry *Bioinorganic Chemistry A Short Course* Second Edition provides the fundamentals of inorganic chemistry and biochemistry relevant to understanding bioinorganic topics Rather than striving to provide a broad overview of the whole rapidly expanding field this resource provides essential background material followed by detailed information on selected topics The goal is to give readers the background tools and skills to research and study bioinorganic topics of special interest to them This extensively updated premier reference and text Presents review chapters on the essentials of inorganic chemistry and biochemistry Includes up to date information on instrumental and analytical techniques and computer aided modeling and visualization programs Familiarizes readers with the primary literature sources and online resources Includes detailed coverage of Group 1 and 2 metal ions concentrating on biological molecules that feature sodium potassium magnesium and calcium ions Describes proteins and enzymes with iron containing porphyrin ligand systems myoglobin hemoglobin and the ubiquitous cytochrome metalloenzymes and the non heme iron containing proteins aconitase and methane monooxygenase Appropriate for one semester bioinorganic chemistry courses for chemistry biochemistry and biology majors this text is ideal for upper level undergraduate and beginning graduate students It is also a valuable reference for practitioners and researchers who need a general introduction to

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German Chemical Society The purpose of the conference was to bring together experts and an international professional audience to discuss and to further basic and applied research and development in the processing storage retrieval and use of chemical structures to focus international attention on the importance of chemical information and the vital research being carried out in chemical information science and to foster co operation among major chemical information organisations in North America and Europe Subjects covered included integrated in house databases substructure searching methodology spectral databanks new technologies microcomputers CD ROM parallel processing and expert systems and chemical reactions The keynote address was given by Mike Lynch of the University of Sheffield In this the opening chapter of the book Mike discusses progress made in chemical information science in the last fifteen years and describes his own approach to research In a plenary session Myra Williams of Merck Sharp and Dohme considered future trends from the point of view of the information manager and strategic planner in industry She emphasises the need for integration open architecture and a uniform user interface

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