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Isaac B. Bersuker

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Electronic Structure and Properties of Transition Metal Compounds Isaac B. Bersuker, 1996-03-28 Covering all the latest developments and applying the theory of electronic structure to problem solving at every opportunity Electronic Structure and Properties of Transition Metal Compounds places the reader at the cutting edge of this important field of research The book focuses on the electronic structure and related properties of coordination compounds essentially treating chemical bonding as an electronic phenomenon It also covers the central concepts of quantum chemistry and atomic states examines theories of electronic structure and vibronic coupling and explores physical methods of investigation. The applications of the theory to stereochemistry and crystal chemistry electron transfer and electron conformational effects and reactivity and catalytic action are also discussed Introduction to Stereochemistry Kurt Mislow, 2012-06-11 Molecular shape form and symmetry play a central role in organic chemistry and this text presents a brief introduction to the conceptual basis of stereochemistry. Its focus lies in the fundamentals of structural stereochemistry rather than the dynamic aspects that are more relevant to reaction mechanisms. The three part treatment deals with structure and symmetry stereoisomerism and the separation and configuration of stereoisomers. The first section reviews molecular architecture relating empirical bonding geometries to the hybridization of the central carbon atom Students receive a nonrigorous treatment of symmetry elements and point groups with particular focus on the presence or absence of reflection symmetry. The second section classifies stereoisomers according to symmetry properties and to the nature of their barriers it also discusses the dependence of optical activity on structure and concludes with an examination of topological isomerism. The third and final section explores the conceptual basis of asymmetric syntheses and kinetic resolutions Each of the major sections features a series of exercises that reinforce and extend the preceding material and answers are provided Preface to the Dover edition Answers to Exercises Bibliography Index Bibliography of Mass Spectroscopy Literature for 1971, 1973 Stereochemistry of **Organometallic and Inorganic Compounds** Bozzano G Luisa, 2012-12-02 The authors of this fourth volume in the series have reviewed the making and breaking of chemical bonds in a sophisticated manner In particular new pressures brought about by environmental concerns larger demands for the medical and pharmaceutical sectors and economics of the market place are forcing us into demanding greater stereochemical control and better product yields for chemical reactions capable of producing useful products The chapters are written by leading experts in this area and give excellent overviews of the strengths and weaknesses of the various methodologies In Chapter 1 newer discoveries in such tried and true methods of C C bond formation as alkylations and aldol reactions of metal enolates are reviewed The author of Chapter 2 discusses the ability of ab initio methods to justify the results of empirical observations in the field of transition metal derivatives of small molecules such as N2 CO2 and similar small molecules Having established the strengths and weaknesses of the various approaches to such theoretical calculations a more interesting approach to these methods is pursued namely their ability to

predict in those areas in which they are particularly strong and reliable chemical and stereochemical events and or results in advance of experiments later carried out in the laboratory Finally Chapter 3 reviews the stereochemical results of electron transfer reactions in mononuclear copper compounds The Chemical Bond I D. Michael P. Mingos, 2016-09-09 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 **Atomic Clusters with Unusual Structure, Bonding and** Reactivity Pratim Kumar Chattaraj, Sudip Pan, Gabriel Merino, 2022-10-06 Atomic Clusters with Unusual Structure Bonding and Reactivity Theoretical Approaches Computational Assessment and Applications reviews the latest computational tools and approaches available for accurately assessing the properties of a cluster while also highlighting how such clusters can be adapted and utilized for the development of novel materials and applications Sections provide an introduction to the computational methods used to obtain global minima for clusters and effectively analyze bonds outline experimental approaches to produce clusters discuss specific applications and explore cluster reactivity and usage across a number of fields Drawing on the knowledge of its expert editors and contributors this book provides a detailed guide to ascertaining the stability bonding and properties of atomic clusters Atomic clusters which exhibit unusual properties offer huge potential as building blocks for new materials and novel applications but understanding their properties stability and bonding is essential in order to accurately understand characterize and manipulate them for further use Searching for the most stable geometry

of a given cluster is difficult and becomes even more so for clusters of medium and large sizes where the number of possible isomers sharply increase hence this book provides a unique and comprehensive approach to the topic and available techniques and applications Introduces readers to the vast structural and bonding diversity that clusters show and reflects on their potential for novel application and material development Highlights the latest computational methods and theoretical tools available for identification of the most stable isomers and accurate analysis of bonding in the clusters Focuses on clusters which violate the rules established in traditional chemistry and exhibit unusual structure bonding and reactivity

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