CHEMISTRY JOURNAL OF MOLDOVA. General, Industrial and Ecological Chemistry. 2025, 20(2), 101-103
ISSN (p) 1857-1727 ISSN (e) 2345-1688
http://cjm.ichem.md
https://doi.org/10.19261/cjm.2025.1382

ELECTRONIC STRUCTURE AND PROPERTIES OF TRANSITION METAL COMPOUNDS. THEORY AND APPLICATIONS, THIRD EDITION BY ISAAC B. BERSUKER, YANG LIU John Wiley & Sons, Hoboken, NJ, 2025, 889 p. ISBN 978-1-394-17889-6.

Introduction

The volume *Electronic Structure and Properties of Transition Metal Compounds. Theory and Applications*, now in its third edition, is one of the most comprehensive and modern works dedicated to the theory of the electronic structure of transition metal compounds. The lead author, Acad. Isaac B. Bersuker, renowned for his contributions to the theory of the Jahn–Teller effect and vibronics, collaborated in this edition with Dr. Yang Liu, a specialist from the Harbin Institute of Technology, China, thus adding an updated and international perspective to the field.

Structure and Content

The book consists of 11 chapters, preceded by prefaces and an extensive set of tables, abbreviations, and symbols. Each chapter concludes with summary notes, questions, and problems, supplemented by solutions and mathematical appendices. This pedagogical structure makes it valuable both as a textbook and as a reference treatise.

- **Chapters 1–3** establish the fundamentals, defining chemical bonding and coordination systems, introducing the Schrödinger equation and the role of approximations, as well as a rigorous presentation of molecular symmetry and group theory.
- **Chapters 4–6** address crystal field and ligand field theories, develop the molecular orbital method (LCAO, DFT, QM/MM methods), and discuss the classification of chemical bonds. Applications to CO, NO, N_2, ethylene complexes, and metal–metal bonding are presented.
- **Chapter 7** introduces vibronics and the Jahn–Teller effects (classical, pseudo, and hidden), highlighting their role in nuclear configuration instability and chemical transformations.
- **Chapter 8** is dedicated to spectroscopic methods (UV–Vis, Raman, IR, photoelectron, EXAFS, Mössbauer, ESR), with examples of interpreting d–d transitions, spectrochemical series, and electron density.
- **Chapters 9–11** deal with stereochemistry, charge-transfer and redox phenomena, as well as reactivity and catalysis. Fundamental processes are discussed, such as the activation of small molecules (CO, H_2, N_2, O_2), substitution and insertion mechanisms, and photocatalytic reactions on Ru(II) complexes.

Innovations and Contributions

This edition brings several significant updates:

1. **Integration of the latest computational methods**: modern density functional theory (DFT), QM/MM, fragmentation methods, and the recent introduction of machine-learning-based force fields (MLFF).
2. **Focus on electron–nuclear interactions**: the authors demonstrate that structural instabilities and molecular transformations are controlled by the mixing of excited and ground electronic states, constituting a new paradigm in theoretical chemistry.
3. **Interdisciplinary applicability**: from catalysis and magnetic materials to biochemistry (haemoproteins, redox enzymes), the book presents examples that bridge theory with experimental applications.

Style and Accessibility

Despite the complexity of the subject, the authors maintain a clear and didactic style, avoiding excessive mathematical developments and prioritizing physico-chemical explanations. The numerous examples, exercises, and solved problems make the book a learning tool accessible to graduate and doctoral students, as well as researchers in chemistry and condensed matter physics.

Target Audience and Relevance

The work is aimed at a broad audience:

- Advanced students and PhD candidates, who can use it as a textbook in courses on theoretical inorganic chemistry, coordination chemistry, or advanced spectroscopy;

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- Researchers and professors interested in modern computational methodologies and the interpretation of electronic phenomena;
- Interdisciplinary specialists in materials science, catalysis, or biochemistry, for whom understanding electronic interactions is essential.

Electronic Structure and Properties of Transition Metal Compounds. Theory and Applications remains a landmark in the field, consolidating Isaac B. Bersuker's fundamental contribution to vibronic chemistry and the Jahn–Teller effect. This expanded and modernized edition provides not only theoretical updates but also relevant applied examples for contemporary research.

The volume is recommended to all those seeking to deepen their understanding of the relationship between electronic structure and the properties of transition metal compounds, being indispensable in 21st-century specialized bibliographies.

Importance of the Work and International Recognition

Isaac B. Bersuker's contributions, brought together in *Electronic Structure and Properties of Transition Metal Compounds*, transcend the framework of a simple academic textbook. The work synthesizes over six decades of fundamental research on the electronic structure of transition metal compounds, becoming a landmark in the literature.

A central aspect of this book is the integration of vibronic effects and Jahn–Teller theory in explaining chemical and physical phenomena. While classical theories—such as crystal field theory or the molecular orbital model—provided a solid basis for understanding coordination compounds, Bersuker elevated this understanding to a new level, showing that structural instabilities, stereochemistry, crystalline phases, and even catalytic reactivity are profoundly influenced by the mixing of ground and excited electronic states. This vision represents a paradigm shift in modern chemistry, comparable to the introduction of quantum mechanics into chemistry in the mid-20th century.

Moreover, Bersuker successfully connected pure theory with interdisciplinary applications:

- **In biochemistry**, explaining mechanisms such as haemoglobin oxygenation or metalloenzyme activity;
- **In catalysis**, by elucidating the activation of small molecules (H_2, O_2, N_2, CO) at metal centres;
- **In materials science**, through the application of Jahn–Teller effects to magnetic properties, crystalline phases, and electrical conductivity phenomena;
- **In emerging technologies**, where his models have been adopted in the design of materials for energy conversion and photocatalysis.

Thus, the book not only summarizes an entire school of thought but also lays the foundation for entire research domains.

Arguments for the Nobel Prize

According to the Nobel Committee's criteria, the prize is awarded for discoveries or innovations that have had a lasting impact on the progress of science and humanity. Analysing Isaac B. Bersuker's contributions and the relevance of his volume, several arguments can be made:

1. **Discovery and development of the modern concept of the Jahn–Teller effect and vibronics.**

- Bersuker was among the first scientists to demonstrate that geometric distortions in molecules and crystals are governed by vibronic interaction, not merely by electrostatic factors.
- The concept of the "vibronic constant orbital" introduced by him is now an essential tool in interpreting spectra and reaction mechanisms.

2. **Integration of electronic theory with chemical and biological applications.**

- The book demonstrates how theory explains complex phenomena: stereochemistry, crystalline phases, catalytic reactivity, biochemical mechanisms.
- This bridge between theory and application is comparable to major discoveries recognized by the Nobel Prize in theoretical chemistry (e.g., John Pople for computational methods, 1998).

3. **Educational impact and the formation of an international research school.**

- The volume, used as a textbook in numerous universities, has trained entire generations of chemists and physicists.
- Bersuker created a scientific tradition that has influenced chemistry schools in the USA, Europe, China, and the former USSR.

4. **Contemporary relevance.**

- In the context of the energy transition, the understanding of transition-metal-based catalysis and multifunctional materials (magnetic, superconducting, photocatalytic) relies largely on the principles presented in this book.
- Thus, his work has not only theoretical value but also direct impact on the development of green and sustainable technologies.

Conclusion

Through this third edition, *Electronic Structure and Properties of Transition Metal Compounds* becomes not only an academic synthesis but also a historical reference work encapsulating a lifetime of research. Isaac B. Bersuker's contributions to the development of vibronic theory and the explanation of coordination phenomena deserve recognition at the highest international level.

Given the Nobel Committee's criteria and the lasting impact of his discoveries, there are strong arguments for this work and the associated studies to be considered worthy of the Nobel Prize in Chemistry, as they have fundamentally changed the way we understand the electronic structure and reactivity of transition metal compounds.

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