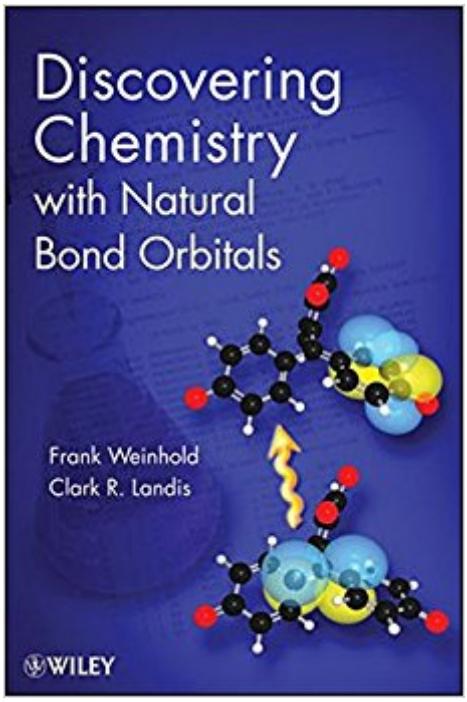
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Discovering Chemistry With Natural Bond Orbitals



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Synopsis

This book explores chemical bonds, their intrinsic energies, and the corresponding dissociation energies which are relevant in reactivity problems. It offers the first book on conceptual quantum chemistry, a key area for understanding chemical principles and predicting chemical properties. It presents NBO mathematical algorithms embedded in a well-tested and widely used computer program (currently, NBO 5.9). While encouraging a "look under the hood" (Appendix A), this book mainly enables students to gain proficiency in using the NBO program to re-express complex wavefunctions in terms of intuitive chemical concepts and orbital imagery.

Book Information

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Customer Reviews

Ã¢â ¬Å“Following this textÃ¢â ¬â„¢s clear explanations, even readers with limited backgrounds in quantum mechanics will learn how to perform sophisticated explorations of modern bonding and valency concepts.Ã¢â ¬Â•Ã Â (Chimie Nouvelle, 1 March 2013)

Learn how to investigate chemical bonding questions using modern NBO computational methods Using the latest computational technology, this practical how-to guide to chemical discovery introduces readers to natural bond orbital (NBO) concepts, strategies, and practical implementations. Without resorting to complex mathematics and programming, readers will learn how to fully leverage the NBO 5.9 computer program to re-express complex multi-electron wave functions in terms of intuitive chemical concepts and orbital imagery. Discovering Chemistry with

Natural Bond Orbitals begins with an introductory chapter that sets forth the basics, including how to produce orbital imagery. Next, the authors cover such critical topics as: Electrons in atoms Hybrids and bonds in molecules Steric and electrostatic effects Atoms in molecules Resonance delocalization corrections Nuclear and electronic spin effects Each chapter ends with problems and exercises that enable readers to apply NBO methods to investigate chemical bonds, their intrinsic energies, and the corresponding dissociation energies that are relevant in reactivity problems. There are also worked-out examples and sample input and output throughout the text to help guide and support readers in their own investigations. In addition, the text features numerous sidebars and links to websites and other texts where more in-depth information can be found on individual topics. There are five appendices at the end of the text filled with useful supplementary material, including Appendix D, "What if Something Goes Wrong?", to help readers solve common problems that arise in NBO investigations. Following this text's clear explanations, even readers with limited backgrounds in quantum mechanics will learn how to perform sophisticated explorations of modern bonding and valency concepts.

While I teach molecular modeling at the undergraduate and graduate level, I am far from a card carrying theorist or computational chemist. My need for computational chemistry is highly applied. Hence I really need books which provide examples and detail about how to set up and interpret, not those packed with equations.This book meets my needs. My opinion is this book is an excellent introduction and companion to the current standard NBO6 manual and online NBO6 tutorials and website; note that the book primarily concerns up to NBO5, but I didnÃƒÂ¢Ã â ¬Ã â„¢t see much difference from NBO6. The content does a good job of bridging from novice to intermediate level, with elements of some advanced (for me) treatment here and there. Most of the very well illustrated examples are for use with Gaussian 09 with significant detail on specifying parameterization for both G09 and NBO. This G09/NBO parameterization detail takes away a lot of guesswork for those relatively new to NBO.I recommend this book to graduate students, faculty and researchers getting started with NBO, and those who have some experience, but desire additional tips and insights.

This book is excessively basic. It dit not meet my expectations.

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