

Bond-order and Magnetic Behavior of Diatomic Species without Molecular Orbital Theory

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Abstract In this chapter text based learning approaches has been highlighted by innovative and time economic way to enhance interest of students' who belong to paranoia zone in Electronic Structure of Atoms and Molecules beneath Inorganic Chemistry of chemical science. In this pedagogical survey, I have tried to hub two (02) time economic pedagogies by including seven (07) new formulae in the field of chemical education. This chapter explores the results and gives implications for context based teaching, learning and assessment.

Keywords: general public, high school, graduate student, chemical bonding, bond order, paramagnetic, diamagnetic, molecular orbital theory

Cite This Article: Arijit Das, "Bond-order and Magnetic Behavior of Diatomic Species without Molecular Orbital Theory," World Journal of Chemical Education, vol. 5, no. 4 (2017): 128-131, doi: 10.12691/wjce-5-4-2.

1. Introduction

The conventional methods [1-5] for prediction of bond order and magnetic properties of diatomic species having (1-20)e's using molecular orbital theory is time consuming. Keeping this in mind, I have introduced some innovative methods [6-12] in this book chapter to make chemistry metabolic, time economic and interesting.

2. Bond-Order of Diatomic Species without MOT

Bond-order usually predicted from the Molecular Orbital Theory. Molecular Orbital Theory (M.O.T.) was first proposed by Friedrich Hund and Robert Mulliken in 1933. They developed an approach to covalent bond formation which is based upon the effects of the various electron fields upon each other and which employs molecular orbital rather than atomic orbital. Each such orbital characterizing the molecule as a whole is described by a definite combination of quantum numbers and possesses relative energy value.

For homo and hetero nuclear diatomic molecules or ions having (1-20)e's.

The graphical representation presented in Figure 1 shows that bond-order gradually increases to 1 in the range (0-2) electrons then falls to zero in the range (2-4) electrons then it further rises to 1 for (4-6) electrons and once again falls to zero for (6-8) electrons then again rises to 3 in the range (8-14) electrons and then finally falls to zero for (14-20) electrons. For total no of electrons 2, 6 and 14, we may use multiple formulae, because they fall in the overlapping region in which they intersect with each other.



Figure 1. (B.O. vs number of electrons)

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Evgeny Y. Tsymbal, Igor Žutić

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spin dependent tunneling control of spin and magnetism in semiconductors and spin based applications Features Presents the most comprehensive reference text for the overlapping fields of spintronics spin transport and magnetism Covers the full spectrum of materials and structures from silicon and organic semiconductors to carbon nanotubes graphene and engineered nanostructures Extends coverage of two dimensional materials beyond graphene including molybdenum disulfide and study of their spin relaxation mechanisms Includes new dedicated chapters on cutting edge topics such as spin orbit torques topological insulators half metals complex oxide materials and skyrmions Discusses important emerging areas of spintronics with superconductors spin wave spintronics benchmarking of spintronics devices and theory and experimental approaches to molecular spintronics Evgeny Tsymbal's research is focused on computational materials science aiming at the understanding of fundamental properties of advanced ferromagnetic and ferroelectric nanostructures and materials relevant to nanoelectronics and spintronics He is a George Holmes University Distinguished Professor at the Department of Physics and Astronomy of the University of Nebraska Lincoln UNL Director of the UNL's Materials Research Science and Engineering Center MRSEC and Director of the multi institutional Center for NanoFerroic Devices CNFD Igor uti received his Ph D in theoretical physics at the University of Minnesota His work spans a range of topics from high temperature superconductors and ferromagnetism that can get stronger as the temperature is increased to prediction of various spin based devices He is a recipient of 2006 National Science Foundation CAREER Award 2005 National Research Council American Society for Engineering Education Postdoctoral Research Award and the National Research Council Fellowship 2003 2005 His research is supported by the National Science Foundation the Office of Naval Research the Department of Energy and the Airforce Office of Scientific Research Littell's Living Age ,1868 New views of matter, life, motion, and resistance: also an enquiry into the materiality of electricity, heat, light, colours, and sound Joseph Hands, 1879

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 - The Rise of Digital Reading Magnetic Bond A World Without Bias
 - Advantages of eBooks Over Traditional Books
- 2. Identifying Magnetic Bond A World Without Bias
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
- 3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Magnetic Bond A World Without Bias
 - User-Friendly Interface
- 4. Exploring eBook Recommendations from Magnetic Bond A World Without Bias
 - Personalized Recommendations
 - Magnetic Bond A World Without Bias User Reviews and Ratings
 - Magnetic Bond A World Without Bias and Bestseller Lists
- 5. Accessing Magnetic Bond A World Without Bias Free and Paid eBooks

- Magnetic Bond A World Without Bias Public Domain eBooks
- Magnetic Bond A World Without Bias eBook Subscription Services
- Magnetic Bond A World Without Bias Budget-Friendly Options
- 6. Navigating Magnetic Bond A World Without Bias eBook Formats
 - o ePub, PDF, MOBI, and More
 - Magnetic Bond A World Without Bias Compatibility with Devices
 - Magnetic Bond A World Without Bias Enhanced eBook Features
- 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Magnetic Bond A World Without Bias
 - Highlighting and Note-Taking Magnetic Bond A World Without Bias
 - Interactive Elements Magnetic Bond A World Without Bias
- 8. Staying Engaged with Magnetic Bond A World Without Bias
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Magnetic Bond A World Without Bias
- 9. Balancing eBooks and Physical Books Magnetic Bond A World Without Bias
 - Benefits of a Digital Library
 - $\circ\,$ Creating a Diverse Reading Collection Magnetic Bond A World Without Bias
- 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
- 11. Cultivating a Reading Routine Magnetic Bond A World Without Bias
 - Setting Reading Goals Magnetic Bond A World Without Bias
 - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Magnetic Bond A World Without Bias
 - Fact-Checking eBook Content of Magnetic Bond A World Without Bias
 - Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development

- Exploring Educational eBooks
- 14. Embracing eBook Trends
 - Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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