

Frontier Orbitals: A Practical Manual - Nguyen Trong Trong Anh

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Written by one of the pioneers of the field, Frontier Orbitals is an essential practical guide to the successes and limitations of this theory. Applications are classified by chemical criteria: competition between reagents, sites or reaction trajectories. The steps involved in solving each problem, such as the choice of model, the calculation of molecular orbitals, and the interpretation of results, are explained. Numerous exercises are found throughout the text, and the full solution and references are given in each case. An extensive listing of MOs is also given to allow those without access to a computer to work out the exercises. Practical advice is given for those wishing to do their own calculations. Frontier Orbitals is aimed at experimentalists who are well versed in organic chemistry but have little or no understanding of quantum mechanics. A greater emphasis is put on chemistry than on quantum mechanics, and the intelligent use of the rules rather than their mathematical derivation. Author: Anh, Nguyen Trong Trong Publisher: Wiley Illustration: N Language: ENG Title: Frontier Orbitals: A Practical Manual Pages: 00304 (Encrypted PDF) On Sale: 2007-04-30 SKU-13/ISBN: 9780471973591 Category: Science : Chemistry - Physical & Theoretical

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