1. Record Nr. UNINA9910144320903321 Autore Nguyên Trong Anh <1935-> Titolo Frontier orbitals: a practical manual / / Nguyen Trong Anh [[electronic resource]] Chichester, England;; Hoboken, NJ,: John Wiley & Sons Ltd, c2007 Pubbl/distr/stampa **ISBN** 0-470-06570-2 Descrizione fisica 1 online resource (xiv, 287 p.): ill.; Disciplina 541/.224 Soggetti Molecular orbitals Physical organic chemistry Electronic books Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Nota di bibliografia Includes bibliographical references and index. Nota di contenuto CHAPTER I. What can we do with Frontier Orbitals? -- CHAPTER II. Atomic and molecular orbitals -- CHAPTER III. The perturbation method -- CHAPTER IV. Absolute and relative reactivities -- CHAPTER V. Regioselectivity -- CHAPTER VI. Stereoselectivity -- CHAPTER VII. Some structural problems -- CHAPTER VIII. Going further "Frontier Orbitals is a practical manual intended for tutorial classes or Sommario/riassunto self-studies. Applications are classified by chemical criteria: competition between reagents (relative reactivity, including chemoselectivity), sites (regioselectivity) or reaction trajectories (stereoselectivity). 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 solutions 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

derivation. Written by one of the pioneers of the field, Frontier Orbitals is an essential practical guide to the successes and limitations of this

the intelligent use of the rules rather than their mathematical