1. Record Nr. UNINA9910830953803321

Autore	Nguyên Trong Anh <1935->
Titolo	Frontier orbitals : a practical manual / / Nguyen Trong Anh [[electronic resource]]
Pubbl/distr/stampa	Chichester, England ; ; Hoboken, NJ, : John Wiley & Sons Ltd, c2007
ISBN	0-470-06570-2
Descrizione fisica	1 online resource (xiv, 287 p.) : ill. ;
Disciplina	541/.224
Soggetti	Molecular orbitals Physical organic chemistry
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
Sommario/riassunto	"Frontier Orbitals is a practical manual intended for tutorial classes or 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 the intelligent use of the rules rather than their mathematical derivation. Written by one of the pioneers of the field, Frontier Orbitals is an essential practical guide to the successes and limitations of this theory."--Jacket.