Frontier Orbitals. A Practical Manual

Description: Many Chemical phenomena cannot be explained by classical physics and need quantum mechanics for a full understanding. However these calculations are complicated and their results are not always easily translated into chemical language. For most practical purposes chemists need simple "Chemically transparent" methods which allow them to make qualitative general predictions. Frontier Orbitals introduces the most valuable of these methods, the frontier orbital approximation, and shows how it can be used for treating structural and reactivity problems in organic chemistry.

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, and 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 he 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.

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