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Molecular Orbital Theory In Drug Research (Medicinal chemistry)

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Medicinal Chemistry, Volume 10: Molecular Orbital Theory in Drug Research is a 12-chapter text that emerged from a series of lectures presented to graduate students in medicinal chemistry at the University of Michigan.
After dealing with the general considerations of drug phenomena and quantum theory, this book goes on exploring the various molecular orbital calculation methods and the significance of molecular orbital indices. The subsequent chapters on the applications of molecular orbital theory are organized on the basis of physical chemical phenomena concluded from the studies described to be involved in the biological activity. These chapters also look into the correlations between indices reflecting covalent bond formation and biological activity. This text further examines the charge transfer mechanisms of several drug classes. The remaining chapters are devoted to the use of molecular orbital theory in several aspects of drug research, including molecular conformation, acid-base phenomena, hydrogen bonding, and dispersion forces.
This work is directed to the advanced undergraduate or graduate students in medicinal chemistry or pharmacology, as well as to the practicing scientists interested in acquiring some understanding of molecular orbital theory. Theoretical chemists seeking information on biological phenomena amenable to semiempirical molecular orbital study will find this book invaluable.

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