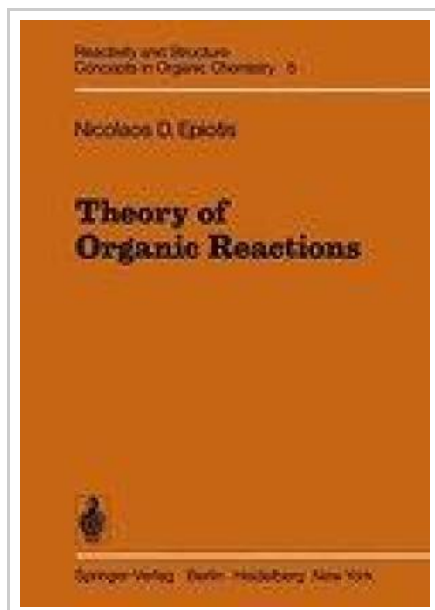




Theory of Organic Reactions

By N. D. Epiotis

Springer Okt 2011, 2011. Taschenbuch. Book Condition: Neu. 244x170x16 mm. This item is printed on demand - Print on Demand Neuware - Inhaltsangabe1. One-Determinantal Theory of Chemical Reactivity.- 1.1 General Principles and Computational Schemes.- 1.2 Qualitative One-Determinantal Models of Chemical Reactivity.- 1.3 The Static One Electron Molecular Orbital Model.- 1.4 Orbital Energies. The Donor-Acceptor Classification of Molecules and the Concept of Reaction Polarity.- 1.5 One Electron Interaction Matrix Elements and Overlap Integrals.- 1.6 The Woodward-Hoffmann Molecular Orbital Correlation Diagram.- 2. Configuration Interaction Overview of Chemical Reactivity.- 2.1 General Principles.- 2.2 Qualitative Configuration Interaction Models of Chemical Reactivity.- 2.3 The Static Linear Combination of Fragment Configurations Method.- 2.4 The Static Delocalized Configuration Interaction Method.- 2.5 The Dynamic Delocalized Configuration Interaction Method.- 3. The Dynamic Linear Combination of Fragment Configurations Method.- 3.1 Definitions.- 3.2 General Theoretical Considerations.- 3.3 The Interaction of Diabatic Surfaces.- 3.4 Polarity Control of Barrier Heights and Decay Efficiencies.- 3.5 The Effect of Excitation Energy on Photochemical Barrier Height.- 3.6 Diabatic Surface Interrelationships. A Classification of Chemical Reactions.- 4. Even-Even Intermodular Multicentric Reactions.- 4.1 Potential Energy Surfaces for 2 +2 Cycloadditions.- 4.2 The Effect of Polarity. Potential Energy Surfaces for Nonionic and Ionic In 2 +2 Cycloadditions.- 4.3 Pericyclic,...



READ ONLINE

Reviews

These kinds of pdf is the best publication readily available. This is for anyone who statte there had not been a well worth reading through. You wont truly feel monotony at at any moment of your own time (that's what catalogs are for relating to if you ask me).

-- **Neil Halvorson**

A brand new eBook with an all new point of view. I could possibly comprehended every little thing using this written e publication. Your life span is going to be change once you comprehensive looking at this publication.

-- **Sabina Waelchi**