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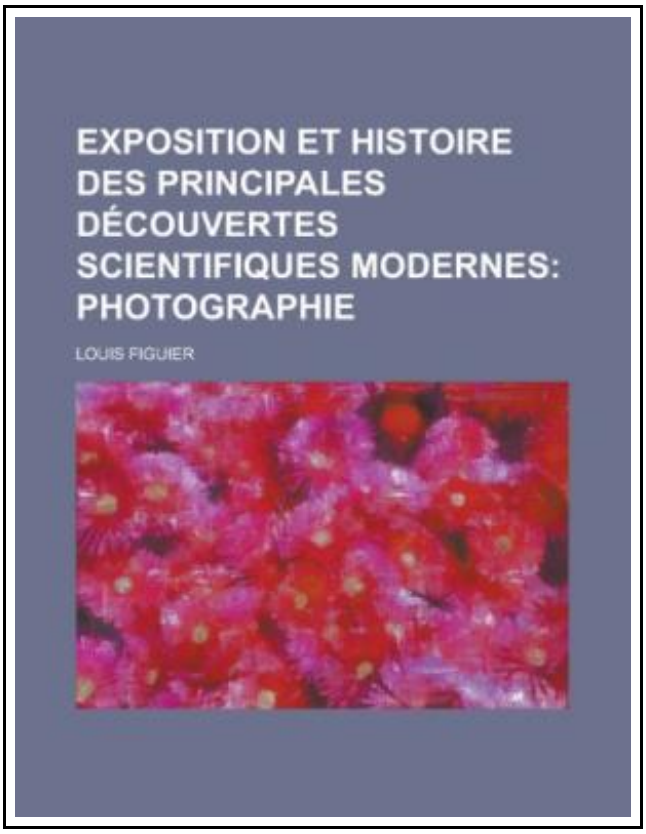

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RareBooksClub. Paperback. Book Condition: New. This item is printed on demand. Paperback. 114 pages. OCLC Number: (OCoLC)213370737 Subject: Hydrolysis. Excerpt: . . . The computational approaches in SPARC are a blending of conventional LFER 15-17 , Structure Activity Relations (SAR) 18, 19 and Perturbed Molecular Orbital (PMO) theory 20, 21 . In general, SPARC utilizes a classification scheme that defines the role of structural constituents in effecting or modifying reactivity, and quantifies the various mechanistic descriptions commonly utilized in physical analysis, such as resonance, electrostatic, induction and dipole effects, etc. SPARC uses LFER to compute thermodynamic or thermal properties and PMO theory to describe quantum effects such as delocalization energies or polarizabilities of electrons. In reality, every chemical property involves both quantum and thermal contributions and necessarily requires the use of both perturbation methods for prediction. A toolbox of mechanistic perturbation models has been developed that can be implemented where needed for a specific reactivity query. Resonance models were developed and calibrated on light absorption spectra 1, 22 , -whereas electrostatic models were developed and calibrated on ionization equilibrium constants 3, 4, 7-9 . Solvation models (e. g. , dispersion, induction, H-bonding, deipole-dipole) have been developed and calibrated on physical properties such as vapor pressure, solubility, distribution coefficient Henrys law constant and gas chromatographic retention time 4, 5, 11, 12 . 4. CHEMICAL HYDROLYSIS Hydrolysis is a chemical transformation process in which an organic compound, RX, reacts with water, forming a new carbon-oxygen bond and the cleaving of the carbon-X bond in the original molecule. The net reaction is most commonly a direct displacement of X by OH or: H O 2- H R-OH X R-X (1) 4 This item ships from La Vergne,TN. Paperback.

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