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The Polar C-Li Electron Pair Bond in Tetrameric CH3LiAnalysis of the Charge Distributions in CH3Li Oligomers; Summary; Conclusions and Outlook; Acknowledgments; References; A Computational Strategy for Organic Photochemistry; Introduction; Modeling Photochemical Reactions; Aims and Objectives; Characterization of Conical Intersections; "Noncrossing Rule" and Conical Intersections; Conical Intersection Structure; An Example: The S,/So Conical Intersection of Benzene; Practical Computation of Photochemical Reaction Paths Quantum Chemical Methods and Software for Excited State Energy and Gradient ComputationsConical Intersection Optimization; Locating Decay Paths from a Conical Intersection; Semiclassical Trajectories; Mechanistic Organic Photochemistry: Some Case Studies; Three-Electron Conical Intersections of Conjugated Hydrocarbons; Conical Intersections of n--7t"" Excited States; The S1/S0 Conical Intersection of Protonated Schiff Bases; Competitive Ground State Relaxation Paths from Conical Intersection; Competitive Excited State Photoisomerization Paths; Conclusions; Acknowledgments; References
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The Development of Computational Chemistry in Canada

Sommario/riassunto

THIS VOLUME, WHICH IS DESIGNED FOR STAND-ALONE USE IN TEACHING AND RESEARCH, FOCUSES ON QUANTUM CHEMISTRY, AN AREA OF SCIENCE THAT MANY CONSIDER TO BE THE CENTRAL CORE OF COMPUTATIONAL CHEMISTRY. TUTORIALS AND REVIEWS COVER* HOW TO OBTAIN SIMPLE CHEMICAL INSIGHT AND CONCEPTS FROM DENSITY FUNCTIONAL THEORY CALCULATIONS,* HOW TO MODEL PHOTOCHEMICAL REACTIONS AND EXCITED STATES, AND* HOW TO COMPUTE ENTHALPIES OF FORMATION OF MOLECULES.A FOURTH CHAPTER TRACES CANADIAN RESEARCH IN THE EVOLUTION OF COMPUTATIONAL CHEMISTRY. ALSO INCLUDED WITH THIS VOLUME IS A SPECIAL TRIBUTE TO QC