Conical Intersections: Theory, Computation and Experiment (Advanced Series in Physical Chemistry)

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The concept of adiabatic electronic potential-energy surfaces, defined by the Born-Oppenheimer approximation, is fundamental to our thinking about chemical processes. Recent computational as well as experimental studies have produced ample evidence that the so-called conical intersections of electronic energy surfaces, predicted by von Neumann and Wigner in 1929, are the rule rather than the exception in polyatomic molecules. It is nowadays increasingly recognized that conical intersections play a key mechanistic role in chemical reaction dynamics. This volume provides an up-to-date overview of the multi-faceted research on the role of conical intersections in photochemistry and photobiology, including basic theoretical concepts, novel computational strategies as well as innovative experiments. The contents and discussions will be of value to advanced students and researchers in photochemistry, molecular spectroscopy and related areas.

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