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Properties of Chemically Interesting Potential Energy Surfaces

Series: Lecture Notes in Chemistry

Contemporary chemical reaction theory is the characterization of Potential Energy Hypersurfaces (PES). The authors critically analyze chemically and mathematically suitable reaction path definitions. The book presents a simple mathematical analysis of stationary and critical points of the PES. It provides tools for studying chemical reactions by calculating reaction paths and related curves. A further aspect of the book is the dependence of PES properties on approximations used for the analysis. Recent quantum chemical calculations, particularly of single proton transfer processes, and experimental data are compared. The book addresses students and researchers in Theoretical Chemistry, Chemical Kinetics and related fields.

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