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Outlook on Electron Correlation Methods for Large SystemsLong-Range Behavior of Correlation Effects; Rigorous Selection of Transformed Products via Multipole-Based Integral Estimates (MBIE); Implications; Conclusions; References; 2. Conical Intersections in Molecular Systems; Introduction; General Theory; The Born-Oppenheimer Approximation and its Breakdown: Nonadiabatic Processes; Adiabatic-Diabatic Representation; The Noncrossing Rule; The Geometric Phase Effect; Conical Intersections and Symmetry; The Branching Plane; Characterizing Conical Intersections: Topography; Derivative Coupling Electronic Structure Methods for Excited StatesMulticonfiguration Self-Consistent Field (MCSCF); Multireference Configuration Interaction (MRCI); Complete Active Space Second-Order Perturbation Theory (CASPT2); Single Reference Methods; Choosing Electronic Structure Methods for Conical Intersections; Locating Conical Intersections; Dynamics; Applications; Conical Intersections in Biologically Relevant Systems; Beyond the Double Cone; Three-State Conical Intersections; Spin-Orbit Coupling and Conical Intersections; Conclusions and Future Directions; Acknowledgments; References

3. Variational Transition State Theory with Multidimensional TunnelingIntroduction; Variational Transition State Theory for Gas-Phase Reactions; Conventional Transition State Theory; Canonical Variational Transition State Theory; Other Variational Transition State Theories; Quantum Effects on the Reaction Coordinate; Practical Methods for Quantized VTST Calculations; The Reaction Path; Evaluation of Partition Functions; Harmonic and Anharmonic Vibrational Energy Levels; Calculations of Generalized Transition State Number of States; Quantum Effects on Reaction Coordinate Motion Multidimensional Tunneling Corrections Based on the Adiabatic Approximation

Sommario/riassunto

THIS VOLUME, LIKE THOSE PRIOR TO IT, FEATURES CHAPTERS BY EXPERTS IN VARIOUS FIELDS OF COMPUTATIONAL CHEMISTRY. Volume 23 COVERS LINEAR SCALING METHODS FOR QUANTUM CHEMISTRY, VARIATIONAL TRANSITION STATE THEORY, COARSE GRAIN MODELING OF POLYMERS, SUPPORT VECTOR MACHINES, CONICAL INTERSECTIONS, ANALYSIS OF INFORMATION CONTENT USING SHANNON ENTROPY, AND HISTORICAL INSIGHTS INTO HOW COMPUTING EVOLVED IN THE PHARMACEUTICAL INDUSTRY. FROM REVIEWS OF THE SERIES ""Reviews in Computational Chemistry remains the most valuable reference to methods and techniques in computational chemis