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Problem of the Error in Theoretical Calculations of Chemical Shifts and Coupling Constants; References; 3 Calculation of Magnetic Tensors and EPR Spectra for Free Radicals in Different Environments; 3.1 Introduction; 3.2 The General Model; 3.3 Spin Hamiltonian, g-Tensor, Hyperfine Coupling Constants, and Zero-Field Splitting; 3.3.1 The Spin Hamiltonian; 3.3.2 Electronic Structure Theory 3.3.3 Additional Terms in the Hamiltonian 3.3.4 Linear Response Theory; 3.3.5 Linear Response Equations for Spin Hamiltonian Parameters; 3.3.6 Computational Aspects: Functionals and Basis Sets; 3.4 Stereoelectronic, Environmental, and Dynamical Effects; 3.4.1 Structures and Magnetic Parameters; 3.4.2 Environmental Effects; 3.4.3 Short-Time Dynamical Effects; 3.5 Line Shapes; 3.6 Concluding Remarks; References; 4 Generalization of the Badger Rule Based on the Use of Adiabatic Vibrational Modes; 4.1 Introduction; 4.2 Applicability of Badger-Type Relationships in the Case of Diatomic Molecules 4.3 Dissection of a Polyatomic Molecule into a Collection of Quasi-Diatomic Molecules: Local Vibrational Modes 4.3.1 Localized Vibrational Modes; 4.3.2 The Adiabatic Internal Coordinate Modes; 4.3.3 Properties of Adiabatic Internal Coordinate Modes; 4.3.4 Characterization of Normal Modes in Terms of AICoMs; 4.3.5 Advantages of AICoMs; 4.4 Local Mode Properties Obtained from Experiment; 4.4.1 Isolated Stretching Modes; 4.4.2 Local Mode Frequencies from Overtone Spectroscopy; 4.4.3 Local Mode Information via an Averaging of Frequencies: Intrinsic Frequencies; 4.4.4 Compliance Force Constants 4.5 Badger-type Relationships for Polyatomic Molecules 4.6 Conclusions; References; 5 The Simulation of UV-Vis Spectroscopy with Computational Methods; 5.1 Introduction; 5.2 Quantum Mechanical Methods; 5.3 Modeling Solvent Effects; 5.4 Toward the Simulation of UV-Vis Spectra; 5.5 Some Numerical Examples; 5.6 Conclusions and Perspectives; References; 6 Nonadiabatic Calculation of Dipole Moments; 6.1 Introduction; 6.2 The Molecular Hamiltonian; 6.3 Symmetry; 6.4 The Hellmann-Feynman Theorem; 6.5 The Born-Oppenheimer Approximation; 6.6 Interaction between a Molecule and an External Field 6.7 Experimental Measurements of Dipole Moments

Sommario/riassunto

Unique in its comprehensive coverage of not only theoretical methods but also applications in computational spectroscopy, this ready reference and handbook compiles the developments made over the last few years, from single molecule studies to the simulation of clusters and the solid state, from organic molecules to complex inorganic systems and from basic research to commercial applications in the area of environment relevance. In so doing, it covers a multitude of apparatus-driven technologies, starting with the common and traditional spectroscopic methods, more recent developments (THz)
