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4.5 Badger-type Relationships for Polyatomic Molecules4.6 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)