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6 Responses of Molecular Vibrations to Intermolecular Electrostatic Interactions and their Effects on Vibrational Spectroscopic Features1 Introduction; 2 Basic Formulas; 3 Structural Changes Induced by Electric Field and Their Consequences in Vibrational Properties; 4 Modulation of the Electric Fields in Liquids: Field-Modulating Modes (FMMs); 5 Effect of Electrostatic Interactions on the Low-Frequency Vibrational Spectra of Liquids; 6 How to Recognize the Vibrational Modes with Large Effects of Electrostatic Interactions: Intensity-Carrying Modes (ICMs)
7 Electrostatic Vibrational Coupling between Molecules: Transition Dipole Coupling (TDC)8 Conclusions; Acknowledgments; References; 7 The (Hyper)polarizabilities of Liquid Water Modeled Using Coupled Cluster/Molecular Mechanics Response Theory Methods; 1 Introduction; 2 Coupled Cluster Theory for States in Vacuum; 3 Solvent Models; 4 Response Theory and Molecular Properties for Solvated Molecules; 5 Electric Properties of Molecules in Condensed Phases; 6 Conclusions; Acknowledgments; References
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10 Third-Order Nonlinear Optical Properties of Open-Shell and/or Charged Molecular Systems

Sommario/riassunto

With the central importance of electric polarizability and hyperpolarizability for a wide spectrum of activities, this book charts the trends in the accurate theoretical determination of these properties in specialized fields. The contributions include reviews and original papers that extend from methodology to applications in specific areas of primary importance such as cluster science and organic synthesis of molecules with specific properties.