

## Contents

Preface	v
Atomic Static Dipole Polarizabilities <i>P. Schwerdtfeger</i>	1
First-Order ZPVA Correction to First Hyperpolarizabilities of Mono-Substituted Benzene Molecules <i>O. Quinet, B. Champagne and B. Kirtman</i>	33
Polarizability and Hyperpolarizability in Small Silicon Clusters <i>C. Pouchan, D. Y. Zhang and D. Bégué</i>	55
Theoretical Calculations of the Static Dipole Polarizability of Atoms and Small Atomic Clusters <i>P. Fuentealba</i>	75
Elongation Method for Polymers and Its Application to Nonlinear Optics <i>F. L. Gu, A. Imamura and Y. Aoki</i>	97
Responses of Molecular Vibrations to Intermolecular Electrostatic Interactions and their Effects on Vibrational Spectroscopic Features <i>H. Torii</i>	179
The (Hyper)polarizabilities of Liquid Water Modelled Using Coupled Cluster/Molecular Mechanics Response Theory Methods <i>J. Kongsted, A. Osted, K. V. Mikkelsen and O. Christiansen</i>	215
The Discrete Solvent Reaction Field Model: A Quantum Mechanics/Molecular Mechanics Model for Calculating Nonlinear Optical Properties of Molecules in Condensed Phase <i>L. Jensen and P. Th. van Duijnen</i>	283

Extraordinary First Hyperpolarizabilities from Loosely Bound Electron in Dipole-Bound Anions: $(\text{HF})_n^-$ ( $n = 2, 3, 4$ )	327
<i>D. Wu, Z. R. Li, Y. Li and C. C. Sun</i>	
Third-Order Nonlinear Optical Properties of Open-Shell and/or Charged Molecular Systems	337
<i>M. Nakano</i>	
Sequential Monte Carlo/Quantum Mechanics Study of the Dipole Polarizability of Atomic Liquids. The Argon Case	405
<i>K. Coutinho and S. Canuto</i>	
High Order Polarizabilities from Optical Interaction-Induced Spectroscopy	421
<i>T. Bancewicz, Y. Le Duff and J.-L. Godet</i>	
Polarizability Functions of Diatomic Molecules and their Dimers	455
<i>M. A. Buldakov and V. N. Cherepanov</i>	
Atomic Polarizabilities and Hyperpolarizabilities: A Critical Compilation	505
<i>A. J. Thakkar and C. Lupinetti</i>	
Polarizabilities of Few-Body Atomic and Molecular Systems	531
<i>Z. C. Yan, J. Y. Zhang and Y. Li</i>	
Nonlinear Optical Properties of Transition-Metal Clusters	565
<i>K. Wu</i>	
Interaction (Hyper)polarizability in $\text{N}_2\text{—He}$ , $\text{CO}_2\text{—He}$ , $\text{H}_2\text{O—He}$ , $(\text{H}_2\text{O})_2\text{—He}$ and $\text{O}_3\text{—He}$	605
<i>G. Maroulis and A. Haskopoulos</i>	
Theoretical Studies on Polarizability of Alkali Metal Clusters	625
<i>K. R. S. Chandrakumar, Tapan K. Ghanty and Swapan K. Ghosh</i>	
Charge Distribution and Polarizabilities of Water Clusters	657
<i>P. Senet, M. Yang and C. Van Alsenoy</i>	