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Altri autori (Persone)	MennucciBenedetta CammiRoberto
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Nota di contenuto	Continuum Solvation Models in Chemical Physics; Contents; Contributors; Preface; 1 Modern Theories of Continuum Models; 1.1 The Physical Model (Jacopo Tomasi); 1.2 Integral Equation Approaches for Continuum Models (Eric Cancès); 1.3 Cavity Surfaces and their Discretization (Christian Silvio Pomelli); 1.4 A Lagrangian Formulation for Continuum Models (Marco Caricato, Giovanni Scalmani and Michael J. Frisch); 1.5 The Quantum Mechanical Formulation of Continuum Models (Roberto Cammi); 1.6 Nonlocal Solvation Theories (Michail V. Basilevsky and Gennady N. Chuev) 1.7 Continuum Models for Excited States (Benedetta Mennucci)2 Properties and Spectroscopies; 2.1 Computational Modelling of the Solvent-Solute Effect on NMR Molecular Parameters by a Polarizable Continuum Model (Joanna Sadlej and Magdalena Pecul); 2.2 EPR Spectra of Organic Free Radicals in Solution from an Integrated Computational Approach (Vincenzo Barone, Paola Cimino and Michele Pavone); 2.3

Continuum Solvation Approaches to Vibrational Properties (Chiara Cappelli); 2.4 Vibrational Circular Dichroism (Philip J. Stephens and Frank J. Devlin)

2.5 Solvent Effects on Natural Optical Activity (Magdalena Pecul and Kenneth Ruud) 2.6 Raman Optical Activity (Werner Hug); 2.7 Macroscopic Nonlinear Optical Properties from Cavity Models (Roberto Cammi and Benedetta Mennucci); 2.8 Birefringences in Liquids (Antonio Rizzo); 2.9 Anisotropic Fluids (Alberta Ferrarini); 2.10 Homogeneous and Heterogeneous Solvent Models for Nonlinear Optical Properties (Hans Agren and Kurt V. Mikkelsen); 2.11 Molecules at Surfaces and Interfaces (Stefano Corni and Luca Frediani); 3 Chemical Reactivity in the Ground and the Excited State

3.1 First and Second Derivatives of the Free Energy in Solution (Maurizio Cossi and Nadia Rega) 3.2 Solvent Effects in Chemical Equilibria (Ignacio Soteras, Damian Blanco, Oscar Huertas, Axel Bidon-Chanal and F. Javier Luque); 3.3 Transition State Theory and Chemical Reaction Dynamics in Solution (Donald G. Truhlar and Josefredo R. Pliego Jr.); 3.4 Solvation Dynamics (Branka M. Ladanyi); 3.5 The Role of Solvation in Electron Transfer: Theoretical and Computational Aspects (Marshall D. Newton)

3.6 Electron-driven Proton Transfer Processes in the Solvation of Excited States (Wolfgang Domcke and Andrzej L. Sobolewski) 3.7 Nonequilibrium Solvation and Conical Intersections (Damien Laage, Irene Burghardt and James T. Hynes); 3.8 Photochemistry in Condensed Phase (Maurizio Persico and Giovanni Granucci); 3.9 Excitation Energy Transfer and the Role of the Refractive Index (Vanessa M. Huxter and Gregory D. Scholes); 3.10 Modelling Solvent Effects in Photoinduced Energy and Electron Transfers: the Electronic Coupling (Carles Curutchet); 4 Beyond the Continuum Approach

4.1 Conformational Sampling in Solution (Modesto Orozco, Ivan Marchan and Ignacio Soteras)

Sommario/riassunto

This book covers the theory and applications of continuum solvation models. The main focus is on the quantum-mechanical version of these models, but classical approaches and combined or hybrid techniques are also discussed. Devoted to solvation models in which reviews of the theory, the computational implementation Solvation continuum models are treated using the different points of view from experts belonging to different research fields Can be read at two levels: one, more introductory, and the other, more detailed (and more technical), on specific physical and numerical aspects
