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Titolo	Solvent effects and chemical reactivity / / edited by Orlando Tapia and Juan Bertran
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Descrizione fisica	1 online resource (390 p.)
Collana	Understanding chemical reactivity ; ; v. 17
Altri autori (Persone)	TapiaOrlando <1938-> BertranJ <1931-> (Juan)
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Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Continuum Solvation Models -- Theoretical Basis for the Treatment of Solvent Effects in the Context of Density Functional Theory -- Monte Carlo Simulations of Chemical Reactions in Solution -- Computer Simulation for Chemical Systems: from Vacuum to Solution -- Crossing the Transition State in Solution -- Valence Bond Multistate Approach to Chemical Reactions in Solution -- Quantum Theory of Solvent Effects and Chemical Reactions.
Sommario/riassunto	This book gathers original contributions from a selected group of distinguished researchers that are actively working in the theory and practical applications of solvent effects and chemical reactions. The importance of getting a good understanding of surrounding media effects on chemical reacting system is difficult to overestimate. Applications go from condensed phase chemistry, biochemical reactions in vitro to biological systems in vivo. Catalysis is a phenomenon produced by a particular system interacting with the reacting subsystem. The result may be an increment of the chemical rate or sometimes a decreased one. At the bottom, catalytic sources

can be characterized as a special kind of surrounding medium effect. The materials involving in catalysis may range from inorganic components as in zeolites, homogenous components, enzymes, catalytic antibodies, and ceramic materials. . With the enormous progress achieved by computing technology, an increasing number of models and phenomenological approaches are being used to describe the effects of a given surrounding medium on the electronic properties of selected subsystem. A number of quantum chemical methods and programs, currently applied to calculate in vacuum systems, have been supplemented with a variety of model representations. With the increasing number of methodologies applied to this important field, it is becoming more and more difficult for non-specialist to cope with theoretical developments and extended applications. For this and other reasons, it is was deemed timely to produce a book where methodology and applications were analyzed and reviewed by leading experts in the field.