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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Introduction -- Force field methods -- Hartree-Fock theory -- Electron correlation methods -- Basis sets -- Density functional methods -- Semi-empirical methods -- Valence bond methods -- Relativistic methods -- Wave function analysis -- Molecular properties -- Illustrating the concepts -- Optimization techniques -- Statistical mechanics and transition state theory -- Simulation techniques -- Qualitative theories -- Mathematical methods -- Statistics and QSAR -- Concluding remarks
Sommario/riassunto	"Introduction to Computational Chemistry 3rd Edition provides a comprehensive account of the fundamental principles underlying different computational methods. Fully revised and updated throughout to reflect important method developments and improvements since publication of the previous edition, this timely update includes the following significant revisions and new topics: Polarizable force fields; Tight-binding DFT; More extensive DFT functionals, excited states and time dependent molecular properties; Accelerated Molecular Dynamics methods; Tensor decomposition methods; Cluster analysis; Reduced scaling and reduced prefactor methods" -- From the publisher.