1.	Record Nr.	UNINA9910143194903321
	Autore	Young David C. <1964->
	Titolo	Computational chemistry [[electronic resource]] : a practical guide for applying techniques to real-world problems / / David C. Young
	Pubbl/distr/stampa	New York, : Wiley, c2001
	ISBN	1-280-54168-7
		9786610541683
		0-470-88008-2
		0-471-45843-0
		0-471-22065-5
	Descrizione fisica	1 online resource (408 p.)
	Disciplina	542.85
		542/.85
	Soggetti	Chemistry - Computer simulation
		Chemistry - Data processing
		Chemistry - Mathematics
		Electronic books.
	Lingua di pubblicazione	Inglese
	Formato	Materiale a stampa
	Livello bibliografico	Monografia
	Note generali	Includes glossary.
	Nota di bibliografia	Includes bibliographical references and index.
	Nota di contenuto	CONTENTS; PREFACE; ACKNOWLEDGMENTS; SYMBOLS USED IN THIS BOOK; 1. Introduction; 1.1 Models, Approximations, and Reality; 1.2 How Computational Chemistry Is Used; Bibliography; Part I. BASIC TOPICS; 2. Fundamental Principles; 2.1 Energy; 2.2 Electrostatics; 2.3 Atomic Units; 2.4 Thermodynamics; 2.5 Quantum Mechanics; 2.6 Statistical Mechanics; Bibliography; 3. Ab initio Methods; 3.1 Hartree-Fock Approximation; 3.2 Correlation; 3.3 Moller-Plesset Perturbation Theory; 3.4 Configuration Interaction; 3.5 Multi-configurational Self-consistent Field; 3.6 Multi-reference Configuration Interaction
		3.7 Coupled Cluster3.8 Quantum Monte Carlo Methods; 3.9 Natural Orbitals; 3.10 Conclusions; Bibliography; 4. Semiempirical Methods; 4.1 Huckel; 4.2 Extended Huckel; 4.3 PPP; 4.4 CNDO; 4.5 MINDO; 4.6 MNDO; 4.7 INDO; 4.8 ZINDO; 4.9 SINDO1; 4.10 PRDDO; 4.11 AMI; 4.12 PM3; 4.13 PM3/TM; 4.14 Fenske-Hall Method; 4.15 TNDO; 4.16 SAM1; 4.17 Gaussian Theory; 4.18 Recommendations; Bibliography; 5. Density

Sommario/riassunto	A practical, easily accessible guide for bench-top chemists, this book focuses on accurately applying computational chemistry techniques to everyday chemistry problems.Provides nonmathematical explanations of advanced topics in computational chemistry.Focuses on when and how to apply different computational techniques.Addresses computational chemistry connections to biochemical systems and polymers.Provides a prioritized list of methods for attacking difficult computational chemistry problems, and compares advantages and disadvantages of various approximation techniques.<li