1. Record Nr. UNINA9911020166203321

Titolo	New methods in computational quantum mechanics / / edited by I. Prigogine and Stuart A. Rice
Pubbl/distr/stampa	New York, : J. Wiley, c1996
ISBN	9786612682049 9781282682047 1282682040 9780470141526 0470141522 9780470142059 0470142057
Descrizione fisica	1 online resource (829 p.)
Collana	Advances in chemical physics ; ; v. 93
Altri autori (Persone)	PrigogineI (Ilya) RiceStuart Alan <1932-2024.>
Disciplina	539 541.305 541/.08
Soggetti	Chemistry - Mathematics Quantum chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and indexes.
Nota di contenuto	Advances in CHEMICAL PHYSICS; CONTENTS; QUANTUM MONTE CARLO METHODS IN CHEMISTRY; MONTE CARL0 METHODS FOR REAL-TIME PATH INTEGRATION; THE REDFIELD EQUATION IN CONDENSED-PHASE QUANTUM DYNAMICS; PATH-INTEGRAL CENTROID METHODS IN QUANTUM STATISTICAL MECHANICS AND DYNAMICS; MULTICONFIGURATIONAL PERTURBATION THEORY : APPLICATIONS IN ELECTRONIC SPECTROSCOPY; ELECTRONIC STRUCTURE CALCULATIONS FOR MOLECULES CONTAINING TRANSITION METALS; THE INTERFACE BETWEEN ELECTRONIC STRUCTURE THEORY AND REACTION DYNAMICS BY REACTION PATH METHODS; ALGEBRAIC MODELS IN MOLECULAR SPECTROSCOPY TIGHT-BINDING MOLECULAR DYNAMICS STUDIES OF COVALENT

	SYSTEMSPERSPECTIVES ON: SEMIEMPIRICAL MOLECULAR ORBITAL THEORY; AUTHOR INDEX; SUBJECT INDEX
Sommario/riassunto	The use of quantum chemistry for the quantitative prediction of molecular properties has long been frustrated by the technical difficulty of carrying out the needed computations. In the last decade there have been substantial advances in the formalism and computer hardware needed to carry out accurate calculations of molecular properties efficiently. These advances have been sufficient to make quantum chemical calculations a reliable tool for the quantitative interpretation of chemical phenomena and a guide to laboratory experiments. However, the success of these recent developments in computa