

1. Record Nr.	UNINA9910779784603321
Titolo	Quantum-chemical calculations of molecular systems as the basis of nanotechnologies in applied quantum chemistry [[electronic resource]] . Volume 3 Quantum chemical calculation of monomers of cationic polymerization and other unique molecular systems / / V.A. Babkin and G.E. Zaikov, editors
Pubbl/distr/stampa	New York, : Nova Science Publishers, c2012
ISBN	1-62417-398-5
Descrizione fisica	1 online resource (247 p.)
Collana	Nanotechnology science and technology Chemistry research and applications
Altri autori (Persone)	BabkinV. A (Vasilii Anatolevich) ZaikovG. E <1935-> (Gennadii Efremovich)
Disciplina	620/5
Soggetti	Nanotechnology Quantum chemistry - Data processing Molecular structure - Data processing
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 index.
Nota di contenuto	pt. I. Quantum-chemical calculation of chemical compounds, synthesized by laureates of Nobel Prize -- pt. II. Quantum-chemical calculation of cellulose -- pt. III. Quantum-chemical calculation of medical products -- pt. IV. Quantum-chemical calculation of jet engine fuels -- pt. V. Quantum-chemical calculation in biochemistry -- pt. VI. Quantum-chemical calculation of linear olefins of cationic polymerization by method ab initio -- pt. VII. Quantum-chemical calculation of linear olefins by method MNDO -- pt. VIII. Quantum-chemical calculation of linear olefins of cationic polymerization, branched out in A-position in relation to double bond by method ab initio -- pt. IX. Quantum-chemical calculation of linear monomers, branched out in A-position in relation to double bond by method MNDO -- pt. X. Quantum-chemical calculation of linear monomers, branched out in G-, D-, E-position in relation to double bond by ab initio -- pt. XI. Quantum-chemical calculation of isoolefins by method ab initio -- pt. XII. Quantum-chemical calculation of isoolefins by

method MNDO -- pt. XIII. Quantum-chemical calculation of dienes and trienes by method ab initio -- pt. XIV. Quantum-chemical calculation of dienes and trienes by method MNDO -- pt. XV. Styrene and its derivations -- pt. XVI. Indene and its EGO derivations -- pt. XVII. Bicyclic olefins -- pt. XVIII. Compound with small cycles.
