Record Nr. UNINA9911019111303321 The application of wave mechanical methods to the study of molecular **Titolo** properties / / edited by R. Daudel Pubbl/distr/stampa New York, : Interscience Publishers, 1965 **ISBN** 9786612347320 9781282347328 1282347322 9780470143544 0470143541 9780470143933 0470143932 Descrizione fisica 1 online resource (200 p.) Collana Advances in chemical physics: 8 Altri autori (Persone) DaudelRaymond Disciplina 627.042 Soggetti Wave mechanics Matter - Properties 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 ADVANCES IN CHEMICAL PHYSICS-VOLUME VIII; CONTENTS; PART I ELECTRONIC STRUCTURE AND SPECTRA; Some recent developments in the quantum theory of many-electron systems and the correlation problem.; Calculation of transition energies from the geometry of the system.; Optical absorptions and charge transfer states.; Model calculations in the theory of mixed-crystal spectra.; Applications of ligand-field theory to complexes.; PART II CHEMICAL AND BIOCHEMICAL ACTIVITY: Chemical reactivity.: A self-consistent field molecular orbital treatment of carbonyl base strength. Chemisorption of ethylene on metals and catalytic hydrogenation. Steroids, purine-pyrimidine pairs and polycyclic aromatic carcinogens.; Some aspects of the biological problems of heredity, mutations, aging, and tumours in view of the quantum theory of the DNA molecule.; Author index; Subject index Sommario/riassunto The Advances in Chemical Physics series provides the chemical physics and physical chemistry fields with a forum for critical, authoritative

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