Record Nr. UNINA9910814073003321 Computational strategies for spectroscopy: from small molecules to **Titolo** nano systems / / edited by Vincenzo Barone Pubbl/distr/stampa Hoboken, N.J., : Wiley, c2012 **ISBN** 9786613331960 9781283331968 1283331969 9781118008713 1118008715 9781118008720 1118008723 9781118008706 1118008707 Edizione [1st ed.] Descrizione fisica 1 online resource (594 p.) Altri autori (Persone) BaroneVincenzo, Dr. Disciplina 543/.50285 Soggetti Spectrum analysis - Data processing Lingua di pubblicazione Inglese Formato Materiale a stampa Livello bibliografico Monografia Note generali Bibliographic Level Mode of Issuance: Monograph Nota di bibliografia Includes bibliographical references and index. Nota di contenuto pt. 1. Electronic and spin states -- pt. 2A. Effects related to nuclear motions: time-independent models -- pt. 2B. Effects related to nuclear motions: time-dependent models. Computational spectroscopy is a rapidly evolving field that is becoming Sommario/riassunto a versatile and widespread tool for the assignment of experimental spectra and their interpretation as related to chemical physical effects. This book is devoted to the most significant methodological contributions in the field, and to the computation of IR, UV-VIS, NMR and EPR spectral parameters with reference to the underlying vibronic and environmental effects. Each section starts with a chapter written by an experimental spectroscopist dealing with present challenges in the different fields; comprehensive coverage of conventional and advanced spectroscopic techniques is provided by means of dedicated chapters

written by experts. Computational chemists, analytical chemists and

spectroscopists, physicists, materials scientists, and graduate students will benefit from this thorough resource.