1. Record Nr. UNINA9910463454003321 Autore Nakamura Hiroki Titolo Quantum mechanical tunneling in chemical physics / / Hiroki Nakamura, Gennady Mil'nikov Boca Raton:,: CRC Press, Taylor & Francis Group,, 2013 Pubbl/distr/stampa **ISBN** 0-429-08645-8 1-4665-0731-4 Descrizione fisica 1 online resource (225 p.) Disciplina 537.6/226 Soggetti Tunneling (Physics) Electronic books. Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Description based upon print version of record. Note generali Nota di bibliografia Includes bibliographical references. Front Cover: Quantum Mechanical Tunneling in Chemical Physics: Nota di contenuto Copyright; Table of Contents; Preface; 1. Introduction; 2. One-Dimensional Theory: 3. Two-Dimensional Theory: 4. Multidimensional Effects: Peculiar Phenomena; 5. Nonadiabatic Tunneling; 6. Multidimensional Theory of Tunneling Splitting; 7. Numerical Applications to Polyatomic Molecules; 8. Decay of Metastable States; 9. Tunneling in Chemical Reactions; 10. Concluding Remarks and Future Perspectives: Appendix A: Proofs of Equation (2.95) and Equation (2.110); Appendix B: Derivation of Equation (6.80) Appendix C: Herring Formula in Curved SpaceAppendix D: Derivation of Equation (6.97); Appendix E: Computer Code to Calculate Instanton Trajectory; Appendix F: Derivation of Some Equations in Section 6.4.2; Bibliography; Back Cover Sommario/riassunto This text explores methodologies that can be usefully applied to various realistic problems in molecular spectroscopy and chemical dynamics. It covers the direct evaluation of reaction rate constants for both electronically adiabatic chemical reactions on a single adiabatic potential energy surface and non-adiabatic chemical reactions in which

two or more adiabatic potential energy surfaces are involved. It also discusses the non-adiabatic tunneling phenomenon that represents one class of non-adiabatic transitions on which the authors have made