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Nota di contenuto	Title Page; Copyright Page; Contents; Contributors; Preface; Chapter 1 Relativistic Configuration Interaction Calculations for Lanthanide and Actinide Anions; 1.1 Introduction; 1.2 Bound Rare Earth Anion States; 1.3 Lanthanide and Actinide Anion Survey; 1.3.1 Prior Results and Motivation for the Survey; 1.3.2 Techniques for Basis Set Construction and Analysis; 1.3.3 Discussion of Results; 1.4 Resonance and Photodetachment Cross Section of Anions; 1.4.1 The Configuration Interaction in the Continuum Formalism; 1.4.2 Calculation of the Final State Wavefunctions; Acknowledgments; References Chapter 2 Study of Actinides by Relativistic Coupled Cluster Methods2. 1 Introduction; 2.2 Methodology; 2.2.1 The Relativistic Hamiltonian; 2.2.2 Fock-Space Coupled Cluster Approach; 2.2.3 The Intermediate Hamiltonian CC method; 2.3 Applications to Actinides; 2.3.1 Actinium and Its Homologues: Interplay of Relativity and Correlation; 2.3.2 Thorium and Eka-thorium: Different Level Structure; 2.3.3 Rn-like actinide ions; 2.3.4 Electronic Spectrum of Superheavy Elements Nobelium (Z=102) and Lawrencium (Z=103); 2.3.5 The Levels of U4+

Sommario/riassunto

The f-elements and their compounds often possess an unusually complex electronic structure, governed by the high number of electronic states arising from open f-shells as well as large relativistic and electron correlation effects. A correct theoretical description of these elements poses the highest challenges to theory. Computational Methods in Lanthanide and Actinide Chemistry summarizes state-of-the-art electronic structure methods applicable for quantum chemical calculations of lanthanide and actinide systems and presents a broad overview of their most recent applications to