1. Record Nr. UNINA9910828693003321

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Titolo	The effective crystal field potential / / Jacek Mulak and Zbigniew Gajek
Pubbl/distr/stampa	New York ; ; Amsterdam, : Elsevier, 2000
ISBN	1-281-18640-6 9786611186401 0-08-053071-0
Edizione	[1st ed.]
Descrizione fisica	1 online resource (319 p.)
Altri autori (Persone)	GajekZbigniew
Disciplina	538/.43
Soggetti	Complex compounds Crystal field theory
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 (p. 263-286) and indexes.
Nota di contenuto	Front Cover; The Effective Crystal Field Potential; Copyright Page; Contents; Chapter 1. Introduction; Chapter 2. Parameterization of crystal field Hamiltonian; 2.1. Operators and parameters of the crystal field Hamiltonian; 2.2. Basic parameterizations; 2.3. Symmetry transformations of the operators; 2.4. The number of independent crystal field parameters; 2.5. Standardization of the crystal field Hamiltonian; 2.6. Final remark; Chapter 3. The effective crystal field potential. Chronological development of crystal field models Chapter 4. Ionic complex or quasi-molecular cluster. Generalized product function4.1 Concept of the generalized product function; 4.2 The density functions and the transition density functions; 4.3 Model of the generalized product functions; 4.4 Crystal field effect in the product function model; Chapter 5. Point charge model (PCM); 5.1 PCM potential and its parameters; 5.2 Simple partial PCM potentials; 5.3 Extension of PCM-higher point multipole contribution; Chapter 6. One-configurational model with neglecting the non-orthogonality. The charge penetration and exchange effects 6.1 Classical electrostatic potential produced by the ligand charge distribution6.2 The charge penetration effect and the exchange interaction in the generalized product function model; 6.3 The weight of the penetration and exchange effects in the crystal field potential;

6.4 Calculation of the two-centre integrals; 6.5 Final remarks; Chapter 7. The exclusion model. One-configurational approach with regard to non-orthogonality of the wave functions; 7.1 Three types of the non-orthogonality
7.2 The renormalization of the open-shell Hamiltonian Ha owing to the non-orthogonality of the one-electron functions7.3 The contact-covalency-the main component of the crystal field potential; 7.4 The contact-shielding; 7.5 The contact-polarization; 7.6 Mechanisms of the contact-shielding and contact-polarization in terms of the exchange charge notion; Chapter 8. Covalency contribution, i.e. the charge transfer effect; 8.1 The one-electron excitations. Group product function for the excited state; 8.2 The renormalization of the open-shell Hamiltonian due to the covalency effect
8.3 Basic approximations8.4 The one-electron covalency potential Vcov; 8.5 The one-electron covalency potential V cov in the molecular-orbital formalism; 8.6 Remarks on the covalency mechanism; Chapter 9. Schielding and antishielding effect: contributions from closed electron shells; 9.1 Phenomenological quantification of the screening effect; 9.2 Microscopic model of the screening effect; 9.3 General expressions for the screening factors; 9.4 The screening factors; Chapter 10. Electrostatic crystal field contributions with consistent multipolar effects. Polarization
10.1 Expansion of the electrostatic potential of point charge system into the multipole series

Sommario/riassunto

As it results from the very nature of things, the spherical symmetry of the surrounding of a site in a crystal lattice or an atom in a molecule can never occur. Therefore, the eigenfunctions and eigenvalues of any bound ion or atom have to differ from those of spherically symmetric respective free ions. In this way, the most simplified concept of the crystal field effect or ligand field effect in the case of individual molecules can be introduced. The conventional notion of the crystal field potential is narrowed to its non-spherical part only through ignoring the dominating spherical part