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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
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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