Theoretical Study of the Local Lattice Distortion at the Trigonal Cr\(^{3+}\) Center in BiI\(_3\)

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The local lattice distortion at the trigonal Cr\(^{3+}\) center in BiI\(_3\) is theoretically studied by the perturbation formulas of the EPR parameters for a 3d\(^3\) ion in trigonal symmetry, based on the cluster approach. In these formulas the contributions from the s-orbitals of the ligands, which were often ignored, are taken into account. It is found that the local angle \(\beta\) (between the direction of the impurity-ligand bonding \(R\) and the \(C_3\) axis) in the impurity center is smaller than the host angle \(\beta_H\) in the pure crystal. The calculated EPR parameters are improved compared to those in absence of the ligand s-orbital contributions. The local lattice distortion obtained in this work is discussed.

Key words: Electron Paramagnetic Resonance; Crystal- and Ligand-Field Theory; Cr\(^{3+}\); BiI\(_3\).