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 β (between the direction of the impurity-ligand bonding R and the C_3 axis) in the impurity center is smaller than the host angle β_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.