

MAGNETIC INTERACTIONS AMONG f ELECTRONS

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Abstract

Dependence of properties at nano scale offers an opportunity to experiment with materials. The fullerene molecule, C_{60} , has just the right size and chemical stability to host a large variety of atoms. Endohedrally doped fullerenes has been synthesized in the past. These structures are important to understand the behavior of atoms with unfilled f -shell. A systematic theoretical study of behavior of rare earth ions should serve as a guideline to experimentalists and theoreticians as well. A rare earth doped endohedral fullerene shows an icosahedral symmetry. A group theoretic treatment of f -electrons in a strong icosahedral crystal field has been discussed in the present study. A many body perturbation theory has been used to calculate the exchange interactions among the pairs of rare earth ions with $2f$ -electrons. It

is found that the doping of rare earth in fullerenes favors the emergence of magnetic order. The ground multiplet of pairs are found to be non magnetic. The exchange coupled electronic states of these pairs are found to be non magnetic. The exchange coupled electronic states of these pairs provide a chance to understand the optical behavior of these systems. The coupling of vibrational and electronic states provides the possibilities of Raman spectra. The existence of an accidental doublet in the ground multiplet suggests a reduction in symmetry from icosahedral to a lower group with two dimensional irreducible representations. It is believed that these studies will lead to a better understanding of optical and magnetic behavior of endohedral fullerenes.