Analytical Investigations of Spin-Spin, Spin-Other-Orbit and Combined Mechanisms of Zero-Field Splitting for $3d^3$ Ions at Trigonal Symmetry

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A new method of obtaining approximate analytical expressions of zero-field splitting (ZFS) has been proposed. By analyzing the magnetic interaction mechanisms which affect the properties of ZFS of ground $^4A_2$ state for $3d^3$ ions at trigonal symmetry, and comparing with the calculated results of complete diagonalization method, the approximate analytical expressions of the contribution to zero-field splitting of $^4A_2$ state from spin-spin (SS), spin-other-orbit (SOO), and combined mechanisms have been obtained. Also the applicability of these approximate analytical expressions has been analyzed. It is shown that the approximate analytical expressions are suitable in a wide crystal field parameters range.

Key words: $3d^3$ Ions; Approximate Analytical Expression; Complete Diagonalization Method; Magnetic Interactions Mechanisms.