Spin-lattice Coupling Coefficient *G*₄₄ of KMgF₃:Mn²⁺ Calculated from Two Cases

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The high (fourth) order perturbation formulas based on the dominant spin-orbit coupling mechanism for the zero-field splittings D_{tri} of a ⁶S-state ion in trigonal symmetry and E_{tho} in rhombic symmetry are derived from the strong field scheme. Two analytic expressions of the spin-lattice coupling coefficient G_{44} obtained from the formulas of D_{tri} and E_{tho} are established by using a simple and uniform method. Based on the two expressions, the coefficients G_{44} for KMgF₃:Mn²⁺ are calculated in two cases. The results show that the lowest (third) order perturbation formulas of $D_{tri}^{(3)}$ and $E_{tho}^{(3)}$ are too simple and too approximate to give reasonable and consistent values of G_{44} , whereas when the fourth-order perturbation terms $D_{tri}^{(4)}$ and $E_{tho}^{(4)}$ are considered, the calculated values of G_{44} (= $G_{44}^{(3)} + G_{44}^{(4)}$) in both cases are not only close to each other, but also in agreement with the observed value. So, the fourth-order perturbation terms cannot be neglected.

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