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Theoretical Studies of Energy Spectra and g Factors of Cr^{3+}-Doped $YAl_3(BO_3)_4$

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Abstract: With the strong-field scheme and trigonal bases, by diagonalizing the complete d^3 energy matrix in a trigonally distorted cubic-field, the energy spectra and wavefunctions of $YAl_3(BO_3)_4:Cr^{3+}$ have been calculated. The rates of change of levels with respect to various parameters and the contributions to levels from various parameters are calculated, and the physical origins of various levels or splittings have been clearly and quantitatively shown. By using the wavefunctions obtained from diagonalizing the complete energy matrix, the g factors of the ground state of $YAl_3(BO_3)_4:Cr^{3+}$ have been evaluated. The calculated results are in good agreement with the optical-spectral and EPR experimental data. It is demonstrated that the bonding between Cr^{3+} and ligands (O^{2-}) is ionic.

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Key words: crystal fields, energy spectrum, g factor, electronic paramagnetic resonance

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