

Optical studies of Cr³⁺-Cr²⁺ pair center in KZnF₃ crystal

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Abstract

The optical absorption spectra of Cr³⁺-Cr²⁺ pair centers in KZnF₃:Cr³⁺,Cr²⁺ crystals were investigated in a wide temperature range. A broad band at 30 800 cm⁻¹ is attributed to a cation-cation eg-electron transfer transition. Narrow lines with maxima at 16 720 and 19 880 cm⁻¹ have been assigned to purely electronic exchange-induced electric-dipole transitions from the ground (Cr³⁺,4A_{2g};Cr²⁺,5E_g) state to the excited (Cr³⁺,4A_{2g};Cr²⁺,3E_g a) and (Cr³⁺,4A_{2g};Cr²⁺,3E_g b) states, respectively. Its vibronic satellites corresponding to the a_{1g} local mode of the Cr³⁺ fluorine octahedron of the pair are also observed. The energy of the local mode for the ground and the mentioned excited states are 580, 540 and 530 cm⁻¹. The exchange integral $J = -14.9 \pm 0.4$ cm⁻¹ and the Jahn-Teller splitting $\Delta_{JT} = 340 \pm 40$ cm⁻¹ for the ground state of the pair were obtained by an analysis of the temperature dependence of the absorption lines. The important features of the crossover double exchange-ferromagnetic superexchange are discussed.

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