

Optics and Spectroscopy (English translation of Optika i Spektroskopiya) 2011 vol.111 N3, pages 393-396

Energy level diagram, wavefunctions, and probabilities of optical transitions in KCuF 3

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Abstract

Using modern concepts of the crystal field in ion-covalent compounds, we calculate the energy level diagram, wavefunctions, and probabilities of optical transitions in the orbital ordering phase of KCuF 3. On this basis, we discuss the possible mechanisms by which an optical absorption sideband structure forms, accompanied by the creation of magnons. © Pleiades Publishing, Ltd., 2011.

<http://dx.doi.org/10.1134/S0030400X11090062>
