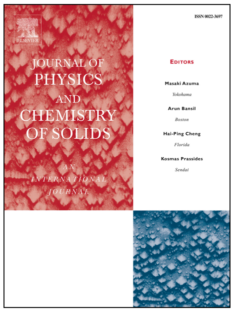

Manifestation of phase transitions in the crystal field spectra of $[(CH_3)_2CHNH_3]_4Cd_3Cl_{10}$:Cu crystals

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Manifestation of Phase Transitions in the Crystal Field Spectra of $[(CH_3)_2CHNH_3]_4Cd_3Cl_{10}$:Cu Crystals

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On the basis of absorption spectroscopy data the temperature evolution of the Cu^{2+} ion environment in the crystal of $[(CH_3)_2CHNH_3]_4Cd_3Cl_{10}$ doped with Cu^{2+} (IPACC:Cu**)** was studied. As it follows from the temperature dependences of heat capacity and absorption coefficient at a constant wavelength IPACC:Cu crystals are characterised by I order phase transitions at $T_1 = 358$ K and $T_3 = 253$ K whereas the continuous changes observed at $T_2 = 293$ K would be related to the first order phase transition close to the second order. For the detailed analysis of the crystal field spectra in the temperature range from T_3 till T_1 the special program package *Crys Tool* 2.0 based on the quantum mechanical models first of all on the model of normalized spherical harmonics (NSH) has been employed. It has been found that similarly to the crystal of $((CH_3)_2CHNH_3)_4Cd_3Cl_{10}$ (IPACC**)** the investigated doped crystal contains the distorted octahedral metal-halogen complexes of two types and the degree of their distortion is considerable changed in vicinity of the phase transition at $T_2 = 293$ K. The phase transitions at T_2 and T_3 were found to be shifted toward the low temperatures in comparison with initial IPACC crystal whereas the high temperature transition at T_1 is shifted to the higher temperatures.

Keywords: Transition metal alloys and compounds; Optical materials; Optical spectroscopy; Crystal and ligand fields; Phase transitions.

1 Introduction

Unusual structural architectures are formed in halogeno-cadmate (II) compounds. Owing to the chemical flexibility (the flexibility which accommodates different organic counterions as well as inorganic components) of these hybrid organic-inorganic materials, it