CF calculation, optical and magnetic characteristics of lanthanide chelate dimer systems.

Autorzy

Małgorzata Puchalska

P. Porcher

Vera I. Tsaryuk

Marcin Sobczyk

Janina Legendziewicz

Rok wydania

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Streszczenie

The lanthanide chelates with two types of ligands are the subject of wide research because of their relevance in solid-state technology. They can be applied in synthesis of nanosize systems and can be used in technology of electroluminescence diodes [1], [2].The single crystals of dimeric compounds: $Ln(C_5H_{11}COO)_3Phen$, where Ln = Nd^{3+}, Eu^{3+} and Phen = 1,10 phenanthroline, were synthesized. The neodymium complex crystallizes in monoclinic system, space group $P2_1/n$ with lattice parameters: a = 15.975(2) Å, b = 12.714(2) Å, c = 16.539(2) Å, β = 110.76° and Z = 4 [M.A. Porai-Koshits, A.S. Antsyshkina, G.G. Sadikov, E.N. Lebedeva, S.S. Korovin, R.N. Shchlelokov, V.G. Lebedev, Z. Neorgan. Khimii 40 (1999) 748]. The $Eu(C_5H_{11}COO)_3Phen$ is isotypic with neodymium one. The lanthanide ion occupies one symmetry site in centrosymmetric dimeric unit. The metal ion is coordinated by seven oxygen atoms of carboxyl groups and two nitrogen atoms of phenanthroline forming a distorted monocapped antiprism. High resolution absorption and luminescence spectra at 298, 77 and 4 K were measured. The role of ligand singlet and triplet states and charge-transfer (C-T) states on efficiency of lanthanide emission have been discussed. The set of the crystal field (CF) Stark components were used in the CF calculations. The energy levels scheme was determined and satisfactory correlation between experimental and calculated levels was found. On the basis of obtained results the magnetic susceptibility were calculated for europium(III) and neodymium(III) systems. The calculated results quite good reproduce observed experimental values. The changes of magnetic susceptibility and magnetic moment with temperature are analyzed in the frame of weak metal–metal (M–M) interaction scheme.