

Determination of crystal-field energy levels and temperature dependence of magnetic susceptibility for Dy^{3+} in $[\text{Dy}_2\text{Pd}]$ heterometallic complex.

Autorzy

Miroslaw Karbowski

Czesław Rudowicz

Takayuki Ishida

Rok wydania

2013

Czasopismo

Inorganic Chemistry

Numer woluminu

52

Strony

13199-13206

DOI

10.1021/ic4021542

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

This study is the first in a series of experimental and theoretical investigations of the crystal-field (CF) energy levels obtained from optical electronic spectra for selected heterometallic 4f-3d compounds intensively studied for the development of novel single-molecule magnets (SMMs). An intriguing question is why the $[\{\text{Dy}^{\text{III}}(\text{hfac})_3\}_2\text{Cu}^{\text{II}}(\text{dpk})_2]$ (abbreviated as $[\text{Dy}_2\text{Cu}]$; Hhfac = 1,1,1,5,5,5-hexafluoropentane-2,4-dione, Hdpk = di-2-pyridyl ketoxime) has antiferromagnetic coupling, whereas $[\text{Gd}_2\text{Cu}]$ and heavy $[\text{Ln}_2\text{Cu}]$ systems usually show ferromagnetic coupling. As the first step to explain this peculiarity, the recently synthesized complex, $[\text{Dy}_2\text{Pd}]$, is investigated. This complex is isostructural with $[\text{Dy}_2\text{Cu}]$ yet contains the diamagnetic Pd ion instead of the magnetic Cu(II) ion. Experimental energy levels of Dy^{3+} ions in the powder $[\text{Dy}_2\text{Pd}]$ sample were determined from the 4.2 K absorption spectra. CF analysis was performed yielding the fitted free ion and CF parameters. The number of freely varied parameters was restricted using the superposition model. The fittings yield very satisfactory agreement between the experimental and the calculated energy levels ($\text{rms} = 12.0 \text{ cm}^{-1}$). The energies and exact composition of the state vector for the ground multiplet $^6\text{H}_{15/2}$ of Dy^{3+} are determined. These results are used for the simulation of the temperature dependence of the magnetic susceptibility, which enables the theoretical interpretation of the experimentally measured magnetic susceptibility in the range 1.8–300 K for the $[\text{Dy}_2\text{Pd}]$ complex. This study provides background for the subsequent investigation of the magnetic exchange interactions in the pertinent heterometallic complexes.

Adres publiczny

<http://dx.doi.org/10.1021/ic4021542>

<https://www.acs.org/content/acs/en.html>

Plik został wygenerowany dnia 2026-08-25 14:23:04

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/MnU0hDv>.