One-pot synthesis, crystal structure and theoretical calculations of a dinuclear Mn(III) complex with *in-situ* generated O,N,O- and O,N-donor dichelating hydrazone ligand.

Autorzy

Elaheh Pousaneh

Somayeh Sadighian

Rahman Bikas

Hassan Hosseini-Monfared

Ahmad Sousaraei

Miłosz Siczek

Tadeusz Lis

Rok wydania

2020

Czasopismo

Journal of Molecular Structure

Numer woluminu

1199

Strony

127023/1-127023/10

DOI

10.1016/j.molstruc.2019.127023

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

A new dinuclear Mn(III) complex, $[Mn_2(L)_2(CH_3OH)_2]$ (**1**), was synthesized by one-pot reaction of 2-aminobenzoylhydrazide, salicylaldehyde and $Mn(OAc)_2{\cdot}4H_2O$ in methanol (H_3L = (*E*)-*N'*-(2-hydroxybenzylidene)-2-((*E*)-(2-hydroxybenzylidene)amino)benzohydrazide). The obtained compound was characterized by elemental analysis, spectroscopic methods, thermogravimetric analysis (TGA) and single crystal X-ray studies. Structural studies indicated that a ditopic O,N,O- and O,N-dichelating hydrazone ligand is obtained by in-situ condensation of 2-aminobenzoylhydrazide with salicylaldehyde which simultaneously is coordinated to two manganese(III) ions as trianionic ligand, $(L)^{3-}$. During the formation of complex, Mn(II) is oxidized to Mn(III) by aerial oxygen and the Mn(III) ions have distorted octahedral geometry. The spectroscopic and structural properties of complex **1** were further studied by DFT calculations. DFT calculations on complex **1** indicated that the experimental geometric parameters and spectroscopic data are in the reasonable range obtained by theoretical studies.

Słowa kluczowe

Dinuclear manganese complex, In-situ reaction, crystal structure, DFT calculation, spectroscopic studies

Adres publiczny

http://dx.doi.org/10.1016/j.molstruc.2019.127023

Strona internetowa wydawcy

http://www.elsevier.com