IR and Raman spectroscopic analysis, DFT modeling, and magnetic properties of a nickel(II) complex, $[Ni(succ)(H_2O)_4]_n$

Autorzy

Dariusz Bieńko

Magdalena Malik-Gajewska

Paulina Walencik

Michalina Kaj

Wiktor Zierkiewicz

Ghulam Murtaza

Tobias Ruffer

Saeed Ahmad

Rok wydania

2019

Czasopismo

Journal of Coordination Chemistry

Numer woluminu

72

Strony

2215-2232

DOI

10.1080/00958972.2019.1650351

Kolekcja

Naukowa

Język

Angielski

Streszczenie

A nickel(II) coordination polymer of succinic acid (1,4-butanedioic acid, H_2succ), $[Ni(succ)(H_2O)_4]_n$ (**1**), was prepared and characterized in depth using IR and Raman spectroscopic methods and theoretical (DFT) calculations. The magnetic properties of **1** were investigated to explain the magneto-structural correlation. The experimental vibrational spectroscopic studies combined with the DFT calculations are indispensable to elucidate the molecular structures of such complexes. A complete assignment of the IR and Raman spectra was made on the basis of the calculated potential energy distribution (PED). The structures of two analogues, monomer $[Ni(succ)(H_2O)_4]$ (**2**) and dimer $[Ni(succ)(H_2O)_4]_2$ (**3**), were modeled by DFT calculations in good agreement with the experiment. The atomic charges and spin densities for the model complexes were calculated with natural bond orbital analysis. Magnetic susceptibility measurements for **1** indicated that Ni(II) paramagnetic centers bridged by succinic ligand in the 1 D chain are almost insolated, and also a great impact of zero-field splitting effect of the Ni(II) ions is visible.

Słowa kluczowe

Nickel(II), coordination polymer, succinic acid, DFT calculations, magnetic susceptibility

Adres publiczny

http://dx.doi.org/10.1080/00958972.2019.1650351

Typ publikacji

Artykuł