Synthesis, crystal structure, spectroscopic, magnetic, theoretical and microbiological studies of a nickel(II) complex l-tyrosine and imidazole, $[Ni(Im)_2(l\text{-}tyr)_2]\cdot 4H_2O$.

Autorzy

Agnieszka Wojciechowska

M. Daszkiewicz

Zbigniew Staszak

Agnieszka Trusz-Zdybek

Alina Bieńko

Andrew Ozarowski

Rok wydania

2011

Czasopismo

Inorganic Chemistry

Numer woluminu

50

Strony

11532-11542

DOI

10.1021/ic201471f

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The $[Ni(Im)_2(l\text{-}tyr)_2]\cdot 4H_2O$ (**1**) complex was obtained in crystalline form as a product of interaction of l-tyrosine sodium salt, imidazole, and $NiSO_4$. The X-ray structure was determined, and the spectral (IR, FIR, NIR–vis–UV, HF EPR) and magnetic properties were studied. The Ni^{2+} ion is hexacoordinated by the N and O atoms from two l-tyrosine molecules and by two N atoms of imidazole, resulting in a slightly distorted octahedral $[NiN_2N_2'O_2]$ geometry with a tetragonality parameter T = 0.995. The bands observed in the electronic spectra were ascribed to the six spin-allowed electronic transitions $^3B_{1g} \rightarrow {}^3E_g$ and $^3B_{2g}$, $^3B_{1g} \rightarrow {}^3A_{2g}$ and ^3E_g, and $^3B_{1g} \rightarrow {}^3A_{2g}$ and ^3E_g. The spin Hamiltonian parameters g, D, and E, which were determined from high-field HF EPR spectra, excellently reproduced the magnetic properties of the complex. Calculation of the zero-field splitting in the S = 1 state of nickel(II) using DFT and UHF was attempted. The biological activity of the complexes has been tested for antifungal and antibacterial effects against *Aspergillus flavus*, *Fusarium solani*, *Penicillium verrucosu*, *Bacillus subtilis*, *Serratia marcescens*, *Pseudomonas fluorescens*, and *Escherichia coli*.

Adres publiczny

https://doi.org/10.1021/ic201471f

Strona internetowa wydawcy

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