

Structural, spectroscopic and magnetic properties of a novel copper(II) L-tyrosinato complex.

Autorzy

Agnieszka Wojciechowska

Anna Gągor

Julia Jezierska

Marek Duczmal

Rok wydania

2014

Czasopismo

RSC Advances

Numer woluminu

4

Strony

63150-63161

DOI

10.1039/c4ra10717a

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The complex $[\text{Cu}(\text{L-Tyr})_2(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}$ (**1**) (L-Tyr = L-tyrosine) was obtained as crystals and characterized by X-ray, spectroscopic (FT-IR, FT-Raman, NIR-vis-UV, and EPR) and magnetic methods. The monomeric complex crystallized in the monoclinic $P2_1$ symmetry with $a = 11.967(1) \text{ \AA}$, $b = 5.9986(4) \text{ \AA}$, $c = 14.936(1) \text{ \AA}$. The amino N and carboxylate O atoms of chelating L-tyrosinate anions together with the O atom of water molecules create a slightly distorted square pyramidal environment around the Cu(II) ions ($\tau = 0.11$). The distance of about $5.998(1) \text{ \AA}$ $[\text{Cu}(\text{L-Tyr})_2(\text{H}_2\text{O})]$ units is involved in a polymeric chain based on $\text{N}(1)\text{--H}\cdots\text{O}(4)^{\text{vi}}$ and $\text{N}(2)\text{--H}\cdots\text{O}(5)^{\text{vi}}$ hydrogen bonds. The d–d band found in the polycrystalline-reflectance spectrum at 15700 cm^{-1} is composed of three ${}^2\text{B}_1(\text{d}_{x^2-y^2}) \rightarrow {}^2\text{A}_1(\text{d}_{z^2})$, ${}^2\text{B}_1 \rightarrow {}^2\text{B}_2(\text{d}_{xy})$ and ${}^2\text{B}_1 \rightarrow {}^2\text{E}(\text{d}_{xz} \approx \text{d}_{yz})$ transitions with energies 14880 , 15800 and 19950 cm^{-1} , respectively. In DMSO solution the complex preserves its square pyramidal geometry as evidenced by an intensive band at ca. 16400 cm^{-1} . The EPR spectral parameters for powder ($g_{\parallel} = 2.236$ and $g_{\perp} = 2.063$) and DMSO frozen solution ($g_{\parallel} = 2.250$, $g_{\perp} = 2.055$, and $A_{\parallel} = 180 \text{ G}$) correspond to an axial symmetry of the Cu(II) coordination geometry with the $\text{d}_{x^2-y^2}$ orbital as a ground state of the unpaired electron. Furthermore, the frozen solution spectrum revealed signals corresponding to $S = 1$ spin states of Cu(II) ions coupled by dipole–dipole interactions with distinctly resolved hyperfine splitting due to two copper nuclei ($|D| = 0.0468 \text{ cm}^{-1}$, $g_{\parallel} = 2.238$, $g_{\perp} = 2.06$ and $A_{\parallel} = 85 \text{ G}$). The variable-temperature magnetic susceptibility measurements revealed the existence of a weak ferromagnetic interaction between neighboring copper(II) ions through the $\text{N--H}\cdots\text{O}$ hydrogen bonds.

Adres publiczny

<http://dx.doi.org/10.1039/c4ra10717a>

<https://www.rsc.org/>

Plik został wygenerowany dnia 2026-08-24 18:09:03

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