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Synthesis and crystal structure of poly{bis-(3-nitro-2,4-pentanediono)-copper(II)}, [Cu(NO₂-acac)₂]_n

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ABSTRACT

The organo-inorganic polymer, poly{[Cu(NO₂-acac)₂]₃}_n, has been prepared and its crystal structure was determined. The structure consists of a trimeric unit in which, acetylacetone ligated symmetrically to copper atoms that pose in the center of octahedrons. The three octahedral fragments of the trimer are linked to each other through nitro group. Crystal Data: C₁₀H₁₂CuN₂O₈, M_r = 351.76, triclinic, P-1 (No. 2), a = 5.8237(2) Å, b = 7.7963(3) Å, c = 7.8847(3) Å, α = 81.988(2)°, β = 75.294(2)°, γ = 72.217(2)°, V = 328.98(2) Å³, T = 143(2) K, Z = 1, Z' = 0.5, μ(Mo Kα) = 1.703, 3021 reflections measured, 1421 unique (R_{int} = 0.0156) which were used in all calculations. The final wR₂ was 0.0686 (all data) and R₁ was 0.0217 (I > 2σ(I)).

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1. Introduction

Coordination polymers are a class of polymers whose repeated units are coordination complexes. A subclass of these is the metal-organic frameworks that are coordinated with organic ligands containing potential voids [1]. Coordination polymers are relevant to many fields such as organic, inorganic, bio-, electro-chemistry; material science and pharmacology. Many potential applications led to extensive studies in the past few decades [2,3].

Coordination polymers have many applications such as dyes [4], molecular storages [5], catalysts, ion exchange, electrical conductors [6-10], bioactive molecules, sensors, and single molecule magnet [11]. Also, they can be used in the fields of molecular electronics, medicine, luminescence and optics [12].

The identity and oxidation state of metal [13], the length and geometry of the organic ligand [14] and the relative orientation of the ligand donor group [15,16] are the fundamental aspects to direct the overall architecture. Also, the coordination geometry of the metal ion, the coordination site and the flexibility of the pre-organized ligand donor show the same effects.

Transition metals are commonly used as nodes or hubs and the electronic structure of these partially filled d-orbitals causes some of them to exhibit multiple coordination geometries particularly copper ion. Thus, the synthetic study of the ternary Cu(II)/malemate (-I)/1,10-phenanthroline reaction system showed: mononuclear, binuclear and polymeric complexes [11].

The family of organic ligands used many at times in combination with terminal N-donors for the construction of metal-organic clusters and coordination polymers consist of various types of dicarboxylates which are capable of bridging metal ion at different distances [17]. Baker *et al.* synthesized 2,2'-bipyrimidine adducts of the β-diketones complexes of lanthanides metal-ion. Thus the 2,2'-bipyrimidine has been used as a bridging moiety and as a channel for energy and electron transfer [18].

Herein, we report the synthesis of the poly{bis-(3-nitro-2,4-pentanediono)-copper(II)} linked via nitro group as bridging agent. Thus, we believe that this moiety can be functioned as a channel for energy and electron transference, presenting the X-ray single crystal structure of [Cu{Cu(NO₂-acac)₂]₃}]_n.