Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Synthesis, structure, and characterizations of a new antiferromagnetic manganese(II) dichloro-bridged 1-D polymer decorated by 5-amino-1-H-tetrazole.

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Rok wydania

2015

Czasopismo

Journal of Coordination Chemistry

Numer woluminu

68

Strony

1261-1272

DOI

10.1080/00958972.2015.1019874

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

$[Mn(5\text{-}ATZ)_2Cl_2]_n$ (**1**) (5-ATZ – 5-amino-1-H-tetrazole) was synthesized from the reaction of 5-ATZ and manganese(II) chloride and isolated by solution evaporation at room temperature. **1** was characterized by elemental analysis, X-ray crystallography, infrared, and EPR spectroscopy as well as magnetic measurements. In the crystal structure, $[Mn(5\text{-}ATZ)_2Cl_2]$ units are linked by double μ_2-bridging chlorides to form 1-D chains parallel to the *a*-axis. The Mn sphere approximates to octahedral with the metal coordinated by four chlorides in the equatorial plane and two 5-ATZ molecules, bound through their ring nitrogens, in axial positions. The intramolecular N–H···Cl hydrogen bond between the 5-ATZ amino group and the adjacent coordinated Cl^- stabilizes the chain. N–H···N hydrogen bonds between adjacent chains form a 3-D supramolecular framework. No hyperfine coupling to the Mn nuclei (I = 5/2) is observed in the powdered EPR spectrum o f **1** at 77 K. The frozen solution EPR spectrum provides evidence of the mononuclearity of **1** in methanol. The magnetic properties have been analyzed using the Hamiltonian $H = -J\sum S_i \cdot S_{i+1}$ with $J = -1.38(3)$ cm^{-1} and g = 2.00(1). A small value of the exchange parameter is typical for 1-D six-coordinate bis(μ_2-chloro) Mn(II) polymers.

Słowa kluczowe

Manganese(II) polymer, 5-Amino-1-H-tetrazole, μ2-Bridging chloride, hydrogen bonding, EPR, Antiferromagnetic properties

Adres publiczny

http://dx.doi.org/10.1080/00958972.2015.1019874

Plik został wygenerowany dnia 2026-04-28 23:35:02
Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/rufRkIv.