

Nickel(II) based homo- vs heterometallic 1D coordination polymers derived from a novel 6-aminouracil building block: structures, topologies, non-covalent interactions, magnetism, and antibacterial activity.

Autorzy

Atanu Purkayastha

Diptanu Debnath

Moumita Majumder

Joaquín Ortega-Castro

Alexander M. Kirillov

Rakesh Ganguly

Julia Kłak

Antonio Frontera

Tarun Kumar Misra

Rok wydania

2018

Czasopismo

Inorganica Chimica Acta

Numer woluminu

482

Strony

384-394

DOI

10.1016/j.ica.2018.06.037

Kolekcja

Naukowa

Język

Angielski

A new azo-ligand, 1,3-dimethyl-5-(p-carboxy-phenylazo)-6-aminouracil (H3L) containing 6-aminouracil (a biomolecule) and a carboxylic function (a potential linker) was synthesized. This ligand was then employed for complexation with Ni(II), resulting in the Ni(II)/Na(I) heterometallic $\{[\text{NiNa}_2(\mu\text{-HL})_2(\mu\text{-H}_2\text{O})_2(\text{H}_2\text{O})_6]\cdot 6\text{H}_2\text{O}\}_n(1)$ and Ni(II) homometallic $\{[\text{Ni}_2(\mu\text{-HL})_2(\text{H}_2\text{O})_4]\cdot 5\cdot 5\text{H}_2\text{O}\}_n(2)$ 1D coordination polymers. These were obtained from similar reaction mixtures and conditions, except the type of the base (NaOH for 1 or KOH/Et3N for 2). Compounds 1 and 2 were characterized by single-crystal X-ray diffraction, UV-vis, NMR, and IR spectroscopy. Both the coordination polymers 1 and 2 show resembling zigzag chains that are topologically classified as 2-connected underlying nets with the 2C1 topology. In 1, the 1D metal-organic chains are further extended by intermolecular H-bonds, giving rise to a 3D H-bonded net; it is topologically described as a uninodal 6-connected net with the pcu topology. In solution, the 1D polymeric structures of both compounds disaggregate into monomeric Ni(II)-square-planar complex units $[\text{Ni}(\text{HL})_2]^{2-}$, as evidenced by NMR and UV-vis spectroscopy studies. The magnetic properties of 2 were also investigated, indicating a dominant zero field splitting parameter D of the Ni(II) center. The type of the base is important for tuning the selective formation of the desired product 1 or 2. Density functional theory (DFT) study justifies the experimental findings for a base-assisted selectivity between the compounds 1 or 2 by optimizing their structures at the PBE-D/DNP level of theory. The existence of agostic interactions between the CH bonds of the methyl groups of the coordinated HL_2^- moieties and the Ni centers in both structures is suggested by natural bond orbital (NBO) calculations at the M06-2X/6-31+G* level of theory. The compound 1 proves to be a potential inhibitor of a bacterial virulence factor, pyocyanin.

Słowa kluczowe

coordination polymers, crystal structure, agostic Interaction, topology, magnetism, pyocyanin

Adres publiczny

<https://doi.org/10.1016/j.ica.2018.06.037>

Plik został wygenerowany dnia 2026-10-03 08:16:58

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/3SACYZD>.