

The Creation of Inorganic-Organic Hybrid Materials Based on Polyoxometalate and Related Chemistry

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Abstract

In this article, two Polyoxometalate (POM)-based inorganic-organic hybrid materials $[(C_2H_6N_5)_2(C_9H_9N_4O)]$ and a copper (II) compound $[Cu(C_9H_7N_4O)_2]$ are presented. $[Cu(H_2O)_2(C_9H_8N_4O)]$. The coordination polymer Compound is based on the coordination complex $[Cu(C_9H_7N_4O)_2]$, with $C_9H_7N_4O$ serving as the ligand. The polyoxometalate of the phospho-tungstate type is also a component of compounds. The 1,4-diamino-4H-1,2,4-triazolium cation $[C_2H_6N_5]^{2+}$ which is generated in-situ from Hsaltz during the production of compound 2, is what makes compound 2 special. Notably, the 1, 4-diamino-4H-1, 2, 4-triazolium cation, which was generated in-situ, is recognised as a high-energy performance molecule. Regular spectrum analysis has been used to analyse the aforementioned compounds, as well as single crystal X-ray crystallography, which has allowed for their clear identification. To further understand the system, calculations based on density functional theory (DFT) were carried out on these three chemicals using the Gaussian 09 W programme.

Keywords: Polyoxometalates; Schiff base ligand; Copper coordination; complex 1; 4-Diamino-4H-1, 2, 4-triazolium cation

Introduction

Their numerous useful physical and chemical characteristics, such as their distinctive redox activity, polyoxometalates (POMs) are well-known metal oxide clusters that are actively researched. Also of great interest is the functionalization of polyoxometalate clusters by various chemical and inorganic moieties. Particularly, there has been a great deal of interest in the design and production of hybrid materials including transition metal functionalized polyoxometalates. Interesting features are produced by the synergistic interaction between POM anions and transition metal complexes. Various polyanion, transition metal, and organic ligand combinations have been used to create a variety of POM-based inorganic-organic hybrids. Masoud Mirzaei and colleagues have described a number of inorganic-organic hybrids based on lanthanides that may be produced utilising a variety of donor ligands that contain N and O, such as 1,10-phenanthroline,2,9-dicarboxylic acid, chelidamic acid, nicotinic acid, and 3,4-pyridinedicarboxylate. They emphasised the role of anion-anion interactions in maintaining these polyoxometalates based on lanthanides.

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These compounds exhibit intriguing features, such as single molecule magnetism and photochemical and electrochemical hydrogen evolution reactivity, as a result of interactions between multinuclear lanthanide clusters and polyoxometate anions. These multifunctional hybrids have highly intriguing single molecular magnetic behaviour, luminous qualities, and hydrogen evolution reactivity. For use in catalysis, Schiff's base coordination complexes have been the subject of in-depth research [1]. There are few reports of hybrid polyoxometalate and Schiff base transition metal complex compounds. Complex materials can be created by synthesising Schiff base ligands with several coordination sites included. Various coordination polymers, including metal organic framework materials, have been created using heterocyclic compounds, such as triazoles with multiple nitrogen coordination centres. Triazole-included Schiff base ligands, comprising nitrogen donor atoms from triazole, will be polydentate. Salicylaldehyde and 4-amino-4H-1, 2, 4-triazole are condensed to create the 4-salicylideneamino-1, 2, 4-triazole Schiff base ligand. The 4-salicylideneamino-1, 2, 4-triazole Schiff base ligand has the potential to be used in magnetic photo- and thermochromic applications due to its high solid state emission characteristics [2]. In this article, we present three copper complexes: (1) $[(C_2H_6N_5)_2(C_9H_9N_4O)_2]$ and (2) $Cu(H_2O)_2(C_9H_8N_4O)_2$. Additionally, $[Cu(C_9H_8N_4O)_6]$ [3]. The compounds 2 and 3 are hybrid polyoxometalate-based materials based on copper coordination complexes. It's interesting to note that the Schiff base ligand in compound 1, 4-salicylideneamino-1, 2, 4-triazole, behaves as a monodentate ligand while in complexes 2 and 3. Along with single crystal X-ray diffraction examinations, several spectroscopic methods are used to analyse all three molecules. While compounds 2 and 3 crystallise in the P-1 and R-3 space groups, respectively, the reddish-brown crystals of compound 1 crystallise in the space group. Additionally, we have emphasised how different topologies of the resultant compounds 1, 2, and 3 are influenced by ligand stoichiometry [4]. This approach might offer useful crystal engineering tools for designing and creating POM-based hybrid molecules.

By refluxing a reaction mixture of cupric chloride and the 4-(salicylideneamino)-1, 2, 4-triazole ligand, where the copper to ligand molar ratio is maintained at 1:1, reddish-brown crystals of compound 1 are produced. Solvothermal synthesis is used to create both molecules. The copper to ligand ratio is crucial [5]. While the copper to ligand molar ratio was kept at 1:1 during the synthesis of compound 2, it was kept at 1:10 during the synthesis of compound 3 [6]. Compound 3 is created by adding a heated methanol solution of the Hsaltrz ligand. Single crystal X-ray diffraction studies are used to describe the compounds. Compound 1 forms a monoclinic P21/c space group crystal. The asymmetrical component of substance. The N atom (imine nitrogen) and oxygen atom (salicylaldehyde) from a Hsaltrz ligand form the coordination ring around the copper atom. The octahedral geometry is completed by the four nitrogen donor and two oxygen donor atoms from the triazole unit of the Hsaltrz ligands that coordinate to the copper centre. According to the axial Cu-N bond distances of 2.707 and 2.707 and the basal plane distances of 1.887 and 2.010, the coordination surrounding Cu (II) is axially extended as a result of the Jahn-Teller effect. Two Hsaltrz ligands coordinate to the Cu (II) centre in the basal plane in a bidentate manner (O, N donors), and two distinct Hsaltrz ligands coordinate to the axial sites in a monodentate manner. Two different ligands at the basal plane, which coordinate to Cu (II) centres in a bidentate fashion using O, N donors, further coordinate to two different Cu (II) centres in a monodentate fashion. The monodentate ligands at the axial sites of the Cu (II) centre further coordinate to two different Cu (II) centres as bidentate fashion using O, N donors. A three-dimensional coordination polymer is created as a result of this intermolecular cooperation. The Schiff base ligand functions as a tridentate ligand to coordinate two distinct Cu (II) centres in the crystal structure of compound 1 [7]. Sinusoidal channels may be seen running along the crystallographic an axis in the packing. The Schiff's bases ligand (2.83) and intramolecular H-bonding have been to be strong. Between the two triazole rings and the phenyl rings of the Schiff base ligand, there are mild π -interactions (3.98) present [8].

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