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SYNTHESIS OF MIXED-LIGAND COMPLEX COMPOUNDS BASED ON MANGANESE(II) METAGYDROXIBENZOATE AND NICOTINAMIDE AND STUDY OF THE CORRELATIONS BETWEEN THEIR COMPOSITION AND STRUCTURE

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Abstract

In this article, the synthesis, structure, and physicochemical properties of complex compounds formed with nicotinamide in the presence of the divalent manganese ion were studied in detail. m-Hydroxybenzoic acid was used as the primary ligand. The elemental analysis method was employed to determine the composition of the synthesized complex compounds. The optimized geometric structure, molecular electrostatic potential (MEP), frontier molecular orbitals (HOMO–LUMO), and global chemical reactivity parameters were analyzed based on density functional theory (DFT) quantum chemical calculations.

Keywords: *Nicotinamide, Mn(II) m-hydroxybenzoate, complex compound, elemental analysis, DFT, HOMO–LUMO, X-ray phase analysis*

Introduction

Meta-hydroxybenzoic acid (m-hydroxybenzoic acid) is one of the bioactive compounds that has a phenolic structure and a carboxyl group. It is used in medicine mainly due to its antibacterial, antifungal, and antioxidant properties (Salgado, 2020). The phenolic structure of meta-hydroxybenzoic acid helps neutralize reactive oxygen species, which plays an important role as a protective agent against cellular oxidative stress. Additionally, its derivatives are widely used as intermediates in the synthesis of pharmaceuticals. For example, parabens (methylparaben, propylparaben) used as certain antiseptics and preservatives (Beppu et al., 2019; Karakaya, 2018) is a key component in production. Manganese compounds are diverse in composition and structure, forming various compounds depending on the ligand and synthesis conditions. For manganese, as for Fe and Cr, the presence of an Mn3O skeleton in its complexes with carboxylic acids is most characteristic (Migwi, Nyamato, Ojwach, Darkwa, 2025).

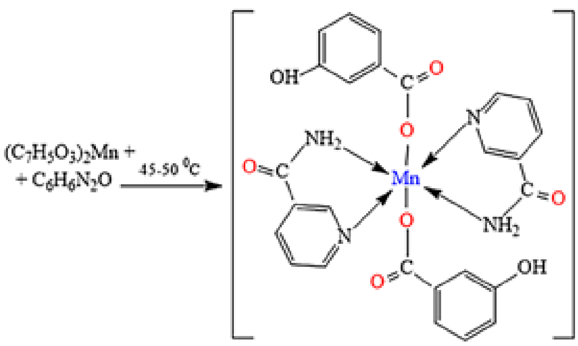
Among the polynuclear manganese compounds, the twelve-nuclear complex occupies a special position. $[Mn_{12}O_{12}(O_2CR)_{16}(H_2O)x]^n$ (n=0–2) compounds have been found to exhibit unusual magnetic properties. As an example of a twelve-nuclear complex, $[Mn_{12}O_{12}(O_2CPh)_{16}(H_2O)_4]$ was obtained from the solid oxidation of a manganese acetate mixture. Benzoic acid was introduced into pyridine, and then the compound was isolated with ethanol (Christou G., 2005). In our subsequent study, $[Mn_3(HL)_2(H_2O)_6]$ n (I) (H_4L = 3-(2,4-dicarboxyphenyl)-2,6-dicarboxypyridine) was synthesized and characterized by IR, elemental analysis, and single-crystal X-ray diffraction. (CIF CCDC No.1915189). The complex crystallizes in the monoclinic C2/c space group with Z=4, a=20.6597(11) Å, *b*=9.0949(5) Å, c=20.6041(12) Å, and β =110.056 (6)°. The crystal consists of $\{Mn_3\}$ clusters of three-nuclear Mn (II) ions, each coordinated by four independent HL^3 ligands, with these trimer units linked into a 2D structure via the pentadentate HL^3 ligand in alternating bis(bridging) and chelate coordination modes. Thermogravimetry, powder X-ray diffraction, and magnetic measurement experiments are also performed to determine thermal stability, phase purity, and magnetism. The results show that weak antiferromagnetic interactions occur between the Mn(II) centers in the bridged three-nuclear $\{Mn_3\}$ cluster (Liu, Ma, Feng, 2020). In a subsequent study, Mn(II) and Zn(II) complexes of a Schiff ligand derived from ethylenediamine and 4-chloro(N-phenyl)formamide were synthesized and characterized by various analytical, spectral, and magnetic methods. The antioxidant potential of the prepared compounds was evaluated by DPPH radical scavenging activity analysis and the FRAP method, and the following general trend was identified: BHT > ligand ~ Zn(II) complex > Mn(II) complex > ligand precursor. Subsequently, the antibacterial efficacy of all synthesized compounds was evaluated against two Gram-negative and two Gram-positive bacteria (Juyal, Thakuri, Panwar, Rashmi, Bukhari, Nand, 2024). The Mn(II) complex exhibited better bactericidal properties than the other compounds, which was confirmed by studying the molecular docking interactions. In studies conducted with the S. typhi cell membrane protein OmpF complex and S. aureus tyrosyl-tRNA synthetase, the Mn(II) complex, followed by the ligand and the Zn(II) complex, showed the highest binding affinity (Osman, et al., 2020; Matmurodova, Xudoyberganov, Hasanov, Taxirov, 2023).

Research method

In this study, in addition to the Mn(II) ion and nicotinamide complex, m-hydroxybenzoic acid was also synthesized. Preparation of manganese(II) m-hydroxybenzoate: Initially, 0.1 g of m-hydroxybenzoic acid was mixed in 30 ml of distilled water and gradually heated. After the acid had completely dissolved, 5 ml of a 0.1 N KOH solution was added to the mixture to create an alkaline environment. Then, 0.8 grams of $MnSO_4 \cdot 5H_2O$ was dissolved in 10 ml of distilled water, added to the solution, and transferred into a 50 ml beaker.

$$\mathbf{2C_7H_6O_3 + 2KOH + MnSO_4{\cdot}5H_2O \rightarrow}$$
$$\mathbf{\rightarrow [MnC_7H_5O_3)_2] + K_2SO_4 + 8H_2O}$$

0.22 grams of nicotinamide was completely dissolved in 8 ml of distilled water and slowly added to the solution of manganese(II) m-hydroxybenzoate.



Typically, manganese sulfate appears colorless in solution, but during the experiment the solution turned light brown, indicating that Mn(II) ions had formed a complex. Upon the addition of nicotinamide, the solution became more stable, indicating that it acted as a secondary ligand in the formation of the complex structure. This suggests the formation of a mixed-ligand coordination complex.

Results analysis

An elemental analysis was conducted to determine the composition of the obtained compound, and the product's yield was 88% (Table 1).

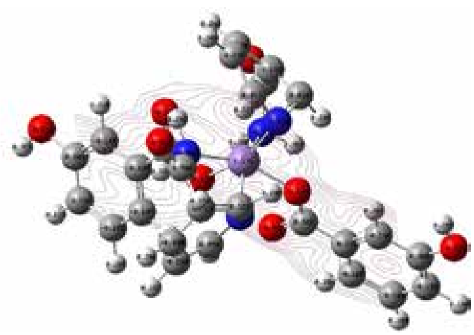
Table 1. *Results of the elemental analysis of the obtained complex compound*

Compounds		$[Mn(C_7H_5O_3)_2(C_6H_6N_2O)_2]$
Mn	Calculated	10.08
	Determined	10.01
N	Calculated	9.65
	Determined	9.55
C	Calculated	54.02
	Determined	53.05
O	Calculated	21.08
	Determined	20.10
Compound color		Light brown

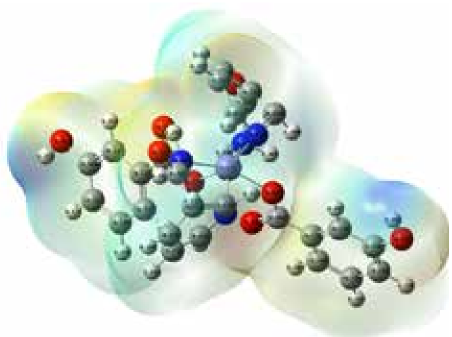
A quantum chemical analysis was performed on the coordination compound based on Mn(II) meta-droxibenzoate and nicotinamide to determine the spatial structure of the central atom, its energetic parameters, and the upper- and lower-lying vacant molecular orbitals. The resulting complex compound was optimized using the 3–21G B3LYP method within the DFT framework of Gaussian 9.0 software. The total electronic energy of the system was calculated to be −2960 Hartree, which confirms the stability of the optimized electronic structure. The absence of imaginary frequencies (NImag=0) indicates that the obtained geometry corresponds to a true minimum on the potential energy surface. The calculated Debye dipolar moment of 3.267651 indicates an intrinsically polar molecular system.

Figure 1. *Electrostatic potential (ESP) map (a), Molecular electron density model (b), Geometric structure and bond lengths (c), Molecular orbitals and electron distribution (HOMO–LUMO) (d)*

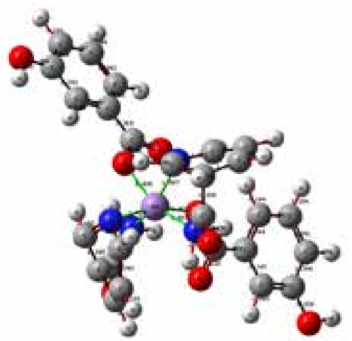
a)



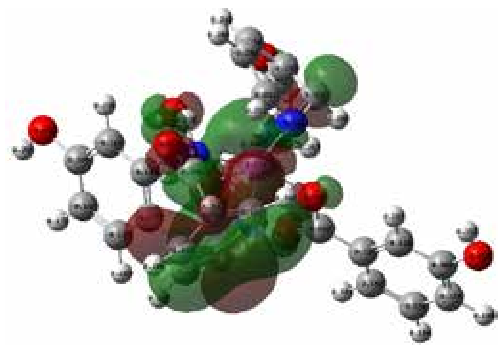
b)



c)

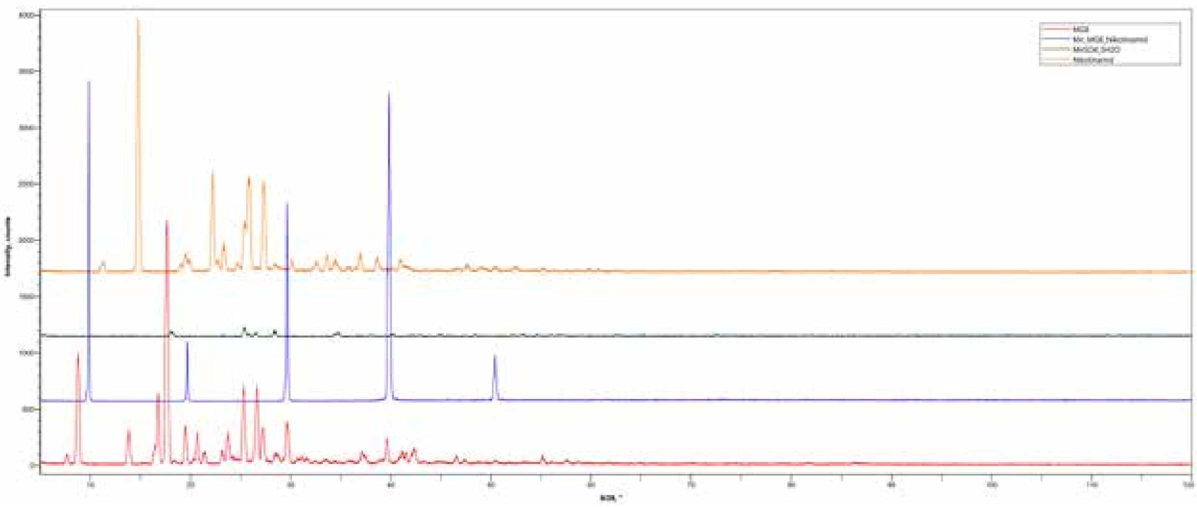


d)



The electrostatic potential distribution of the complex, with red and blue contours, depicts the distribution of electrostatic charge in different parts of the molecule. Red regions have high electron density and typically indicate sites that interact with electrophilic reagents. The molecular electron density model reflects the overall electron distribution and electron density clouds of the molecule. The blue and green regions represent areas of high electron density, while the yellow and reddish regions indicate areas of relatively low electron density. The geometric structure and bond lengths are shown, along with the bonds between the complex's atoms and their lengths. Mn(II) and amid ions are located in the coordination environment. Oxygen (O) and nitrogen (N) atoms are shown by their interatomic bond lengths. Molecular orbitals and electron distribution of the molecule's highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are depicted. The red and green orbitals illustrate the electron motion in the molecule and its propensity for potential chemical reactions. HOMO is the highest-energy orbital capable of donating electrons. LUMO is the lowest vacant orbital prone to accepting electrons. The red and blue contours depict the electrostatic charge distribution in different parts of the molecule. The red regions have high electron density and typically indicate the sites where electrophilic reagents interact.

Figure 2. *X-ray diffraction patterns of marganese(II) hydroxybenzoate and nicotinamide and of the complex compound derived from them*



The X-ray diffraction pattern of the complex compound differs from those of the starting materials (nicotinamide and meta-hydroxybenzoic acid). The appearance of new peaks and the disappearance of earlier ones indicate the formation of a new crystal phase. This confirms the synthesis of the complex compound by X-ray phase analysis. According to the X-ray diffraction analysis and phase formation, the nicotinamide diffraction pattern exhibits medium-intensity but characteristic peaks (in the 15°–30° range). The high- or medium-intensity peaks do not correspond to metagidroxybenzoic acid. In the complex compound, however, new high-intensity peaks appear (for example, at ~20°, ~30°, and ~40°). Some peaks have disappeared or shifted. This is not a simple sum of the initial substances, indicating the formation of a new crystal phase.

Conclusion

According to the research results, it was determined that a successful complex is formed with nicotinamide and Mn(II) ions, and that these complexes have an octahedral structure. Nicotinamide is a strong ligand, and the resulting manganese(II) complexes are highly stable, possess a strong coordination sphere, and exhibit distinct spectroscopic changes. According to X-ray diffraction pattern comparison and phase formation analysis, manganese sulfate produced lower-intensity and fewer peaks. The degree of crystallinity is lower. The peaks differ significantly from those of nicotinamide and m-hydroxybenzoic acid, indicating their distinctiveness. The X-ray diffraction pattern of the new $[Mn(C_7H_5O_3)_2(C_6H_6N_2O)_2]$ complex compound shows new, high-intensity peaks. Some peaks have disappeared or changed, while others have shifted. This indicates the formation of a new crystal phase. The X-ray diffraction pattern of the complex compound does not directly match those of the other two substances, which proves that the compound is not a simple mixture but a true complex.

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