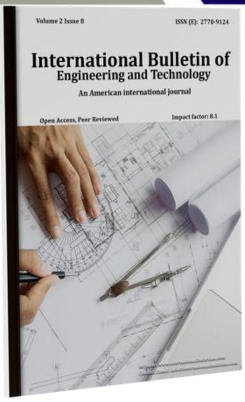

SYNTHESIS AND PHYSICOCHEMICAL ANALYSIS OF A MANGANESE-BASED METAL COMPLEX DERIVED FROM A PIPERIDINE DERIVATIVE

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Annotation. The study focuses on the physicochemical properties of metal complexes synthesized based on piperidine derivatives. Infrared (IR) spectroscopy was used to investigate the vibrational characteristics of the main functional groups and the metal-ligand interactions. Ultraviolet (UV) spectral analysis enabled the identification of electronic transitions and ligand field splitting. The compound's microstructure and morphology were examined using electron microscopy, revealing a uniform nanocrystalline structure. Quantum chemical calculations described the electronic structure, optimal geometry, and thermodynamic stability of the complex.The findings contribute to a deeper understanding of the properties of metal complexes, enhancing their potential in drug development, catalysis, and the design of novel functional materials.

Keywords: Piperidine, piperidine betaine, manganese (II) chloride, IR spectroscopy, vibration, carboxylate anion, MolView, spatial structure, BioBlue BB4253 digital microscope, ligand.

Annotatsiya: Maqolada piperidin xosilalari asosida sintez qilingan metall kompleks birikmalarning fizik-kimyoviy xossalari tadqiq qilingan. Infraqizil (IK) spektroskopiya orqali asosiy funksional guruhlarning vibratsion xususiyatlari va metall-ligand bogʻlanishlari oʻrganilgan. Ultrabinafsha (UF) spektral tahlil esa elektron o'tish jarayonlarini va ligand maydoni ajralishlarini aniqlashga imkon berdi. Elektron mikroskop yordamida birikmaning mikrostruktura va morfologiyasi oʻrganilib, bir xil nanokristall struktura kuzatildi. Kvant-kimyoviy hisoblashlar asosida kompleksning elektron tuzilishi, optimal geometriyasi va termodinamik barqarorligi tavsiflandi.Tadqiqot natijalari metall komplekslarining xossalarini chuqur anglashga, ularning dori vositalari, katalizatorlar va yangi funksional materiallar yaratishdagi potensialini oshirishga xizmat qiladi.

Kalit so'zlar: Piperidin, piperidinobetain, marganes (II) xlorid, IQ spektroskopiya, tebranish, karboksilat anioni, MolView, fazoviy tuzilma, BioBlue BB4253 raqamli mikroskop, ligant.

Аннотация. Исследование посвящено изучению физико-химических свойств металлических комплексов, синтезированных на основе производных пиперидина. С помощью инфракрасной (ИК) спектроскопии изучены вибрационные характеристики основных функциональных групп и взаимодействия металл-лиганд. Ультрафиолетовый (УФ) спектральный анализ позволил выявить электронные переходы и расщепление в лигандном поле.Микроструктура и морфология соединения были исследованы с использованием электронной микроскопии, что показало однородную нанокристаллическую структуру. Квантово-химические расчёты

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охарактеризовали электронное строение, оптимальную геометрию и термодинамическую устойчивость комплекса. Результаты исследования углубляют понимание свойств металлических комплексов и повышают их потенциал в разработке лекарственных препаратов, катализаторов и создании новых функциональных материалов.

Ключевые слова: Пиперидин, пиперидинбетаин, хлорид марганца (II), ИК-спектроскопия, вибрация, карбоксилатный анион, MolView, пространственная структура, цифровой микроскоп BioBlue BB4253, лиганд.

Introduction. The synthesis of metal-ligand complexes has been a topic of great interest due to their wide-ranging applications in catalysis, material science, and drug development. Metal complexes, particularly those involving transition metals, exhibit unique properties due to the coordination between the metal center and organic ligands, which can significantly influence their chemical reactivity, stability, and biological activity. Manganese-based complexes, in particular, have gained attention for their catalytic properties, biological activities, and potential applications in various fields, including environmental remediation and pharmaceuticals[1].

Piperidine derivatives, as nitrogen-containing heterocyclic compounds, are known for their diverse biological activities, including analgesic, anti-inflammatory, and antimicrobial effects. Their ability to form stable complexes with metal ions enhances their potential applications, particularly in the development of new drugs and materials. Piperidinobetaine, a derivative of piperidine, is of particular interest due to its ability to coordinate with metal ions, forming stable complexes with transition metals like manganese[2]. These complexes can exhibit improved chemical and biological properties compared to the parent ligand alone.

In this study, we aim to investigate the synthesis and characterization of a novel manganese (II) complex formed by the reaction of piperidinobetaine and manganese (II) chloride. The physical-chemical properties of the synthesized complex were studied using various analytical techniques, including infrared (IR) spectroscopy, ultraviolet-visible (UV-Vis) spectroscopy, electron microscopy, and quantum chemical calculations. The study focuses on understanding the structural features, bonding interactions, and electronic properties of the complex, with a particular emphasis on its stability, coordination environment, and potential applications in catalysis and drug development.

This work also aims to provide valuable insights into the role of piperidine derivatives in metal complexation and to explore the possibilities of designing new metal-ligand systems with enhanced properties for use in various practical applications[3]. By examining the interaction between piperidinobetaine and manganese (II) chloride, we seek to contribute to the development of more efficient and versatile metal complexes for industrial and pharmaceutical applications[4].

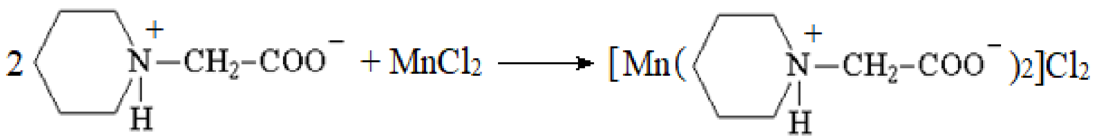
Methods. The synthesis of the metal complex was carried out by reacting piperidinobetaine with Manganese (II) chloride in an aqueous solution. Water was chosen as the solvent due to its effectiveness in dissolving the reactants and promoting the formation of the metal-ligand complex. The reaction conditions, including the concentration of the reactants, reaction time, and temperature, were carefully optimized to ensure the highest yield and purity of the complex. Various experimental parameters were tested to determine the optimal conditions for the synthesis. The interaction between Manganese (II) chloride and piperidinobetaine was monitored and confirmed using spectroscopic techniques[5].

For the structural and chemical characterization of the synthesized complex, Infrared (IR) spectroscopy was used to identify the characteristic vibrational frequencies of the functional groups present in the complex, including the metal-ligand bonds. The UV-Visible (UV) spectroscopy provided insights into the electronic transitions and ligand field splitting within the complex, allowing for the analysis of the coordination environment of the metal center[6].

The microstructure and morphology of the complex were examined using an electron microscope (Biobllue BB4253). The morphological features, including the particle size distribution and nanostructure, were analyzed[7]. Quantum chemical calculations were performed using Molview software to study the electronic structure, bond lengths, and spatial arrangement of atoms in the metal complex. These calculations provided detailed information about the dipole interactions between atoms, atomic energies, and the overall stability of the synthesized complex[8].

Results: Apart from piperidine, all alkaloids exhibit a high degree of bioactivity. This indicates that the combination of these three functions (the piperon nucleus, the piperidine nucleus, and the presence of the α,β-unsaturated ketonic group) is responsible for manifesting biological activity [9]. The actions of several piperidine derivatives are relevant and promising for research aimed at discovering new, highly effective drugs with broad pharmacological effects [10].

A metal complex compound was synthesized based on piperidine betaine and manganese (II) chloride. Water was chosen as the solvent for the initial substances. Experimental work was carried out with various parameters during the formation of the metal complex compound. The interaction of manganese (II) chloride with piperidine betaine proceeds according to the following reaction equation.



The structure of the synthesized metal-organic complex compound was determined using IR spectroscopy (Figures 1-2-3) [11].

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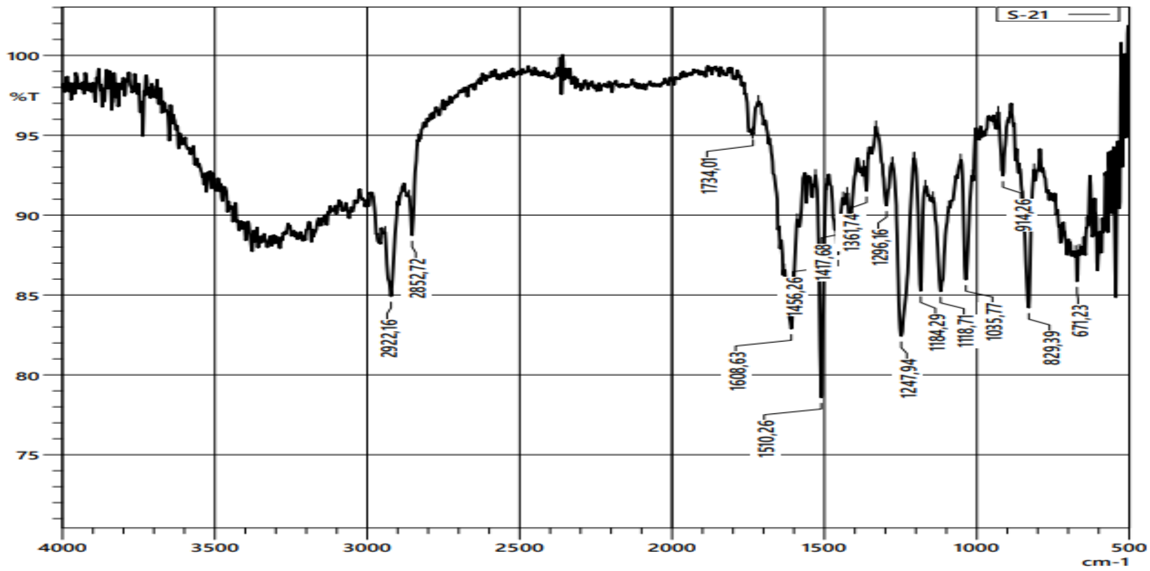

Figure 1. IR spectrum of manganese (II) chloride

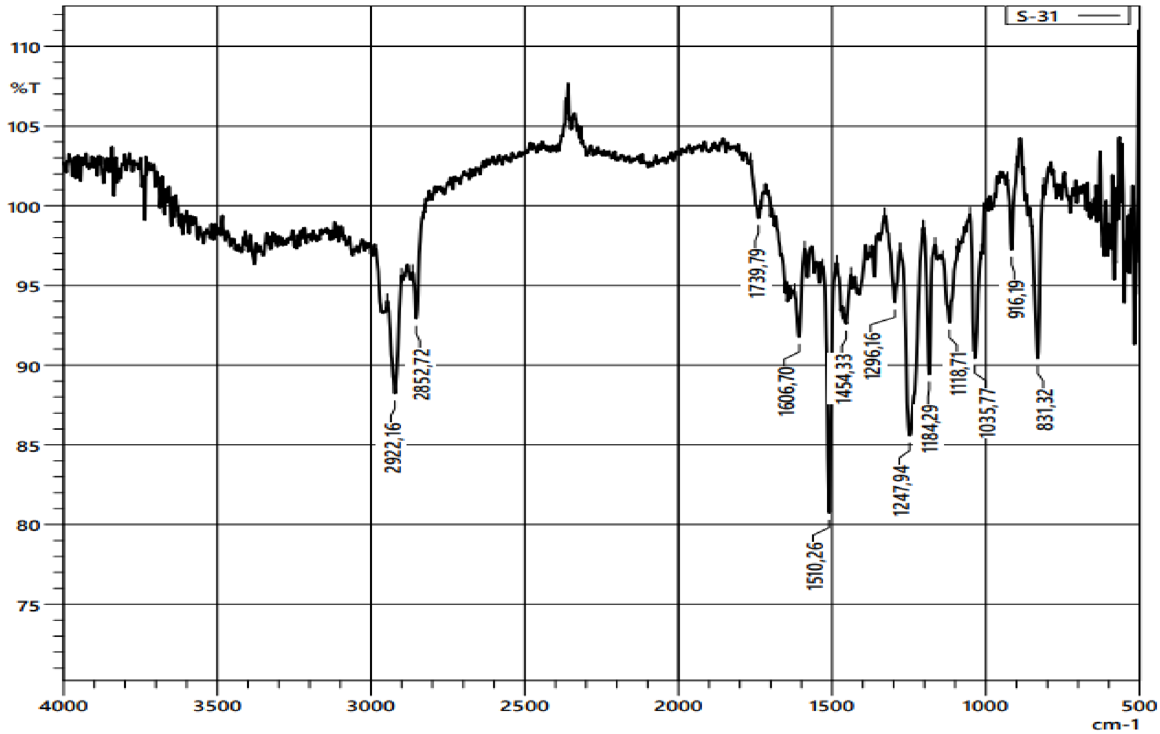

Figure 2. IR spectrum of piperidine betaine

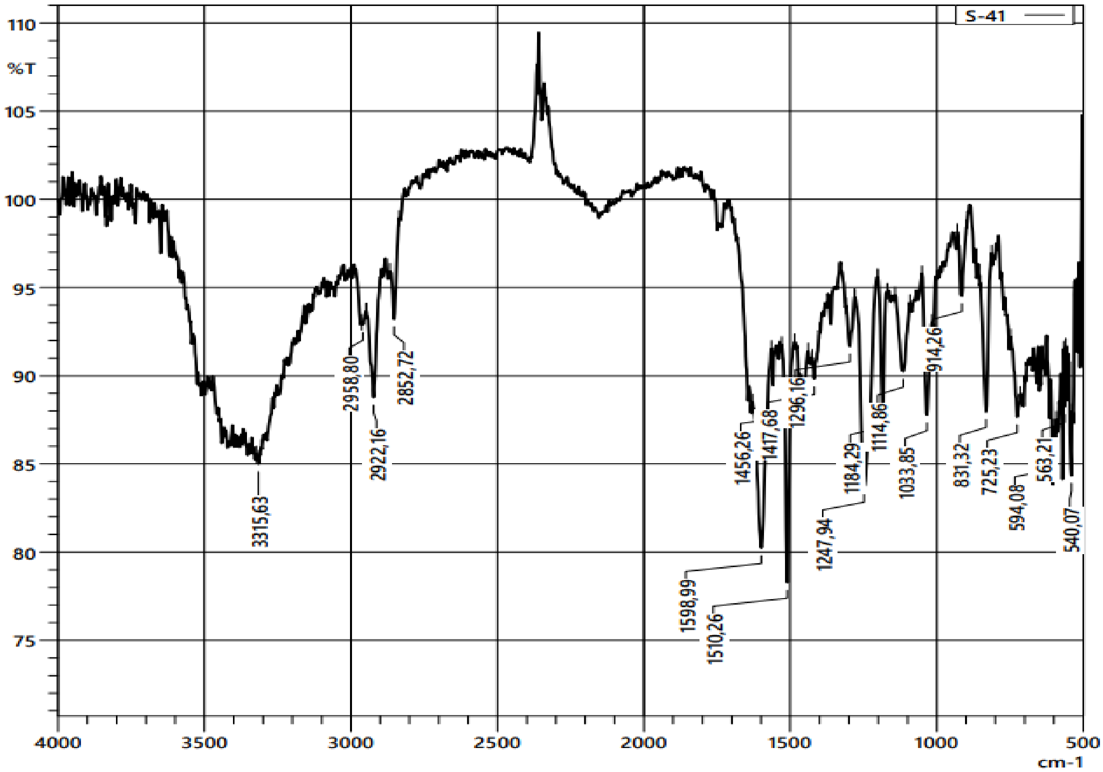

Figure 3. IR spectrum of the complex compound based on manganese (II) chloride and piperidine betaine

In the IR spectrum of the complex compound based on manganese (II) chloride and piperidine betaine, absorption zones corresponding to the stretching vibrations of quaternary nitrogen are observed in the 2922 cm^{-1} region, while the C-O-C bonds exhibit stretching vibrations in the 1035–1111 cm^{-1} range. The presence of C-H bonds is indicated by deformation vibrations in the 1456 cm^{-1} region. The presence of manganese compounds in the structure is characterized by stretching vibrations in the 657–671 cm^{-1} region. Additionally, the presence of a carboxylate anion is confirmed by stretching vibrations in the 1608 cm^{-1} region.

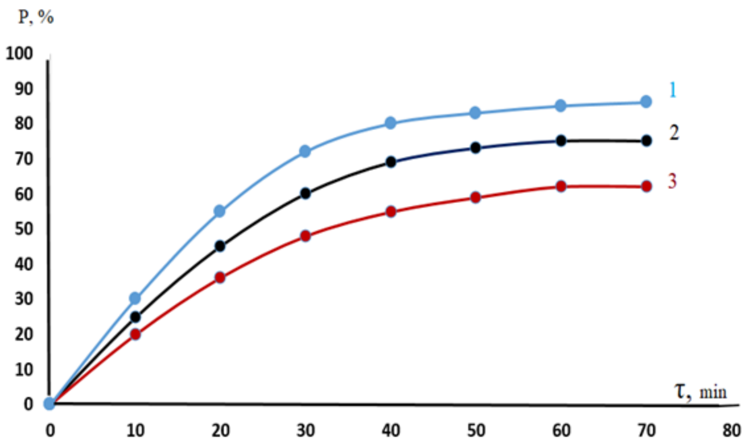

Figure 4. Graph showing the effect of reactant ratios on product yield

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The UV spectra of the synthesized complex compound and the starting materials were obtained, and the UV spectra of each substance were compared. Below are the UV spectra of the starting materials and the synthesized product.

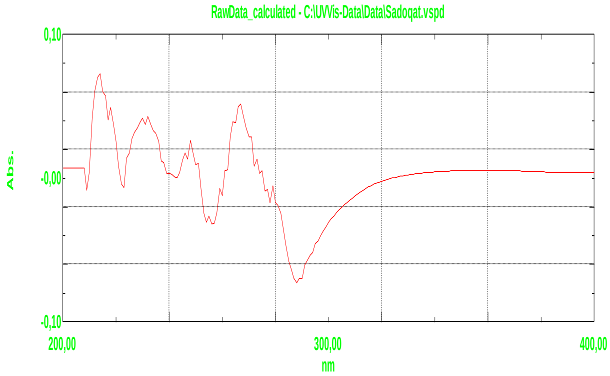


Figure 5. UV spectrum of piperidine betaine

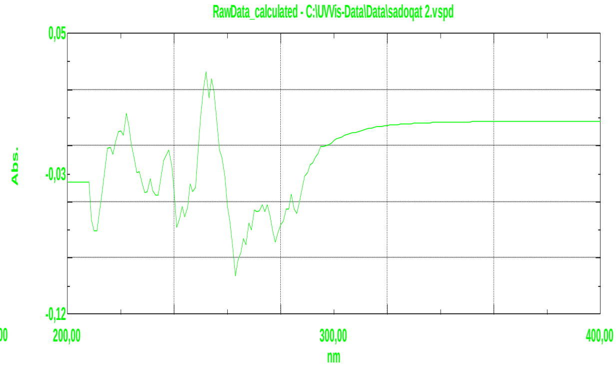


Figure 6. UV spectrum of manganese (II) chloride

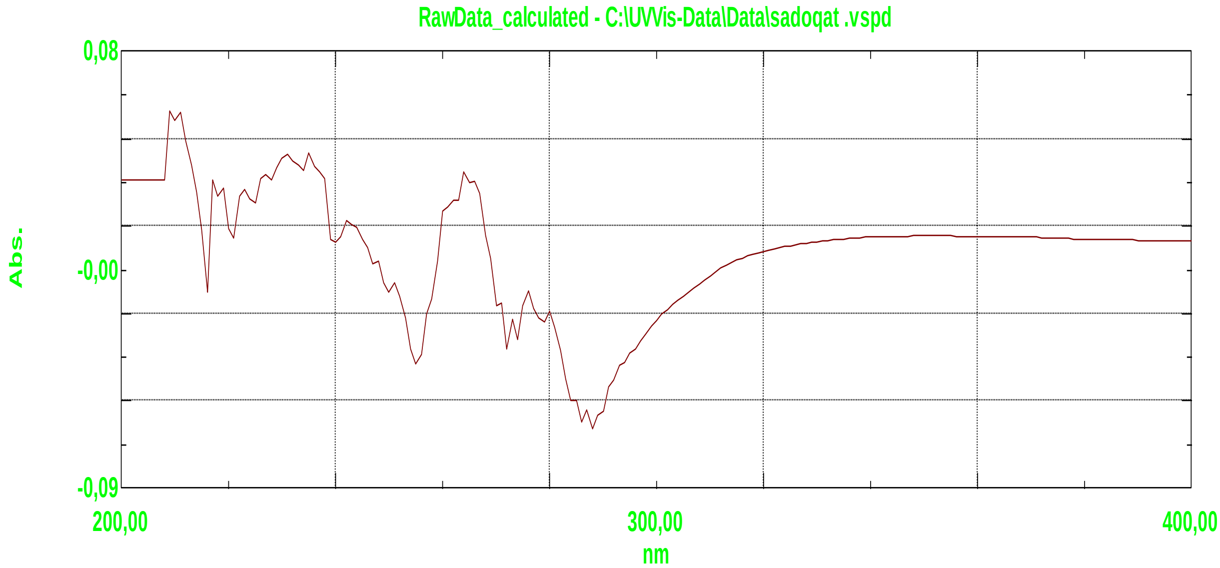


Figure 7. UV spectrum of the mixture of piperidine betaine and manganese (II) chloride

The process of combining 0.01 mol/L solutions of piperidine betaine and manganese (II) chloride was examined using a UV-1900 spectrophotometer. The UV spectrum of the mixture of piperidine betaine and manganese (II) chloride was compared with the individual UV spectra of the starting materials, piperidine betaine and manganese (II) chloride. A new absorption region at 320 nm can be observed for the formed complex compound. The maximum absorption regions of the starting materials and the new compound are presented in the table below.

Table 8. Absorption regions of the complex compound and starting materials

№	Substance Name	λmax 1 (nm)	λmax 2 (nm)	λmax 3 (nm)
1	Piperidine betaine	225	255	288
2	Manganese (II) chloride	210	242	262
3	Piperidine betaine and manganese (II) chloride metal complex	218	272	320

Quantum-chemical calculations were performed using the Molview software on the synthesized compounds. The program was used to study the structure, bond lengths, spatial arrangement of electron clouds, and atomic energies of the metal complex formed from Manganese (II) chloride and piperidinobetaine.

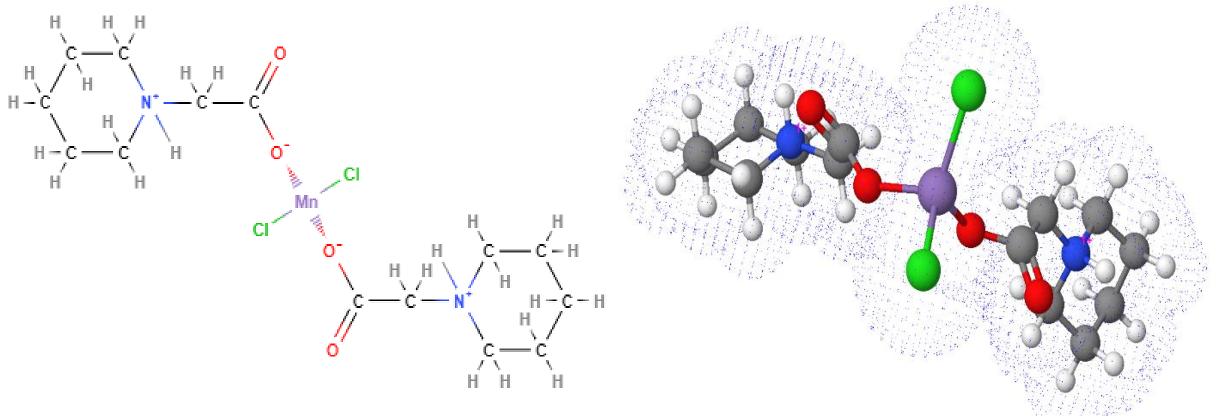


Figure 3.5.5. 2D and 3D structures of the complex compound formed from piperidinobetaine and Manganese (II) chloride.

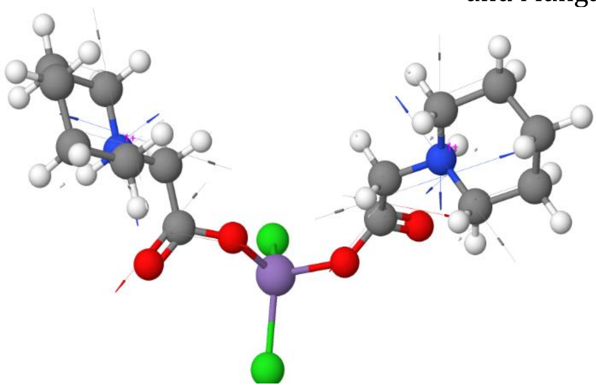


Figure 3.5.6. Dipole bonding of the complex compound formed from piperidinobetaine and Manganese (II) chloride.

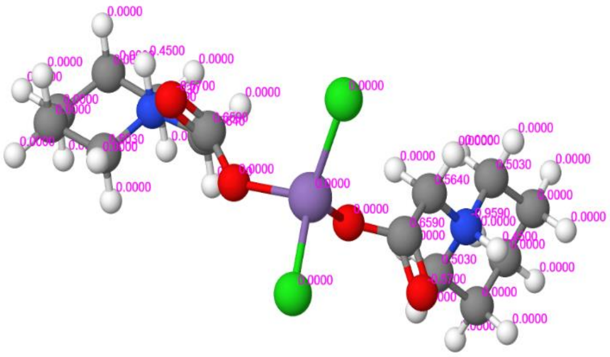


Figure 3.5.7. Atomic energies of the atoms in the complex compound formed from piperidinobetaine and Manganese (II) chloride.

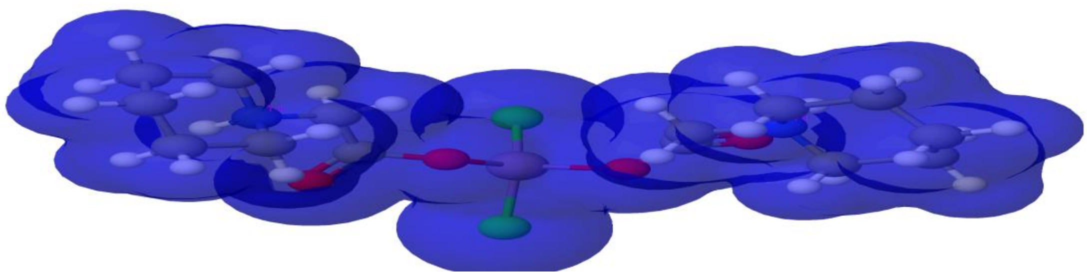
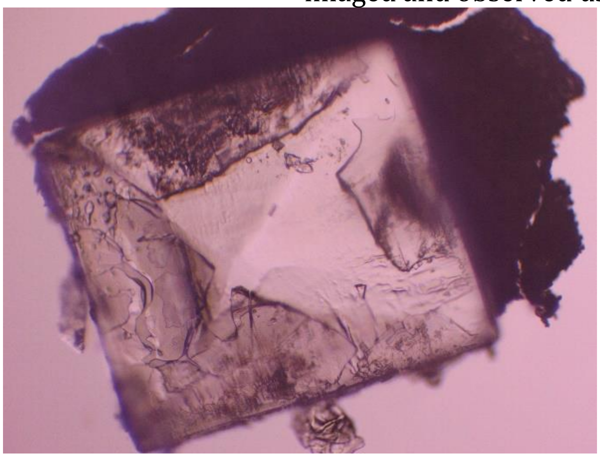


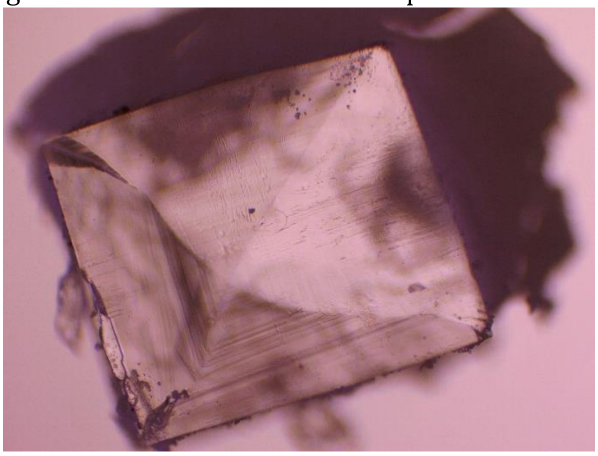
Figure 3.5.8. Electron cloud structure of the complex compound formed from piperidinobetaine and Manganese (II) chloride.

Ligand atoms:

№	Name	Total	№	Name	Total
0	C	0.774352	21	O	2.49931
3	C	0.756453	22	C	-1.27712
6	C	0.701633	25	N	3.00883
9	N	3.00859	27	C	4.04132
11	C	-1.23369	30	C	0.600903
14	C	-0.180323	33	C	0.774693
15	O	-1.09408	36	C	0.756252
16	MN	-0.951848	39	C	0.709006
17	CL	-0.829777	42	O	2.5147
18	CL	-0.842683	43	C	4.0636
19	O	-1.08578	46	C	0.593469
20	C	-0.141854			

The synthesized metal complex compound was imaged and observed using the Biobllue BB4253 microscope.





Crystal Shape and Geometric Structure: The crystal shape corresponds to cubic or tetragonal symmetry, indicating its highly ordered growth. Clear geometric shapes are visible on the crystal surface, but some deformations and flaws are present.Surface Deformations and Cracks: The surface in the first image is relatively smooth, whereas in the second image, there are large cracks and deformations. These cracks and lines are likely caused by stress or external factors during the crystal's growth process.Optical and Mechanical Properties: The light reflection and refraction on the crystal surface show its optical properties. Cracks and uneven surfaces may indicate mechanical weakness, which could reduce the material's strength. Crystallization Process: The crystal in the first image grew in a perfect shape, while the crystal in the second image shows signs of deformation due to altered growth conditions. This may be a result of the growth environment and external stresses. Chemical Composition and Structure: The crystal is composed of a metal-complex compound, with its structure based on the interactions between ligands and metal ions. The surface defects and cracks could influence how the crystal behaves in chemical reactions.

In this study, the physicochemical properties, structures, and electronic structures of the metal complex synthesized based on piperidinobetaine and manganese (II) chloride were thoroughly investigated. Functional groups and electronic transition processes of the complex were identified using infrared (IR) and ultraviolet (UV) spectroscopy, which helped in better understanding the chemical properties of the complex. Quantum-chemical calculations performed using the Molview software allowed for the study of the electronic structure, bond lengths, and atomic energies of the complex, providing insights into its stability and reactivity.

The microstructure and morphology of the complex were examined using electron microscopy, and these data described its nanostructures. Analysis of the complex's spatial structure and electron clouds enabled a deeper understanding of its chemical reactivity and potential. It can be concluded that the synthesized complex has the potential for use as new drugs, catalysts, or functional materials. Moreover, the structural characteristics and reactivity of the complex could serve as a basis for future research, especially in the development of new innovative solutions in the fields of pharmaceuticals and materials science. The research findings will help identify new applications for metal complexes based on piperidine derivatives and enhance their significance in both scientific and industrial fields.

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