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SYNTHESIS OF THE COORDINATION COMPOUND OF Zn(II) ION WITH KETOROLAC

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Annotatsiya. Ushbu maqolada rux nitrat va ketorolak asosida hosil qilingan yangi koordinatsion birikmaning sintezi va fizik-kimyoviy xossalari o'rganildi. Kompleks birikma $[Zn(ket)_2](NO_3)_2 \cdot 2H_2O$ suv va etanol aralashmasida pH = 5.5–6 sharoitida sintez qilindi. Oq kristall holida cho'kma sifatida ajralib chiqdi. Sintez qilingan modda IR-spektroskopiya, UV-Vis va elementar analiz metodlari yordamida tahlil qilindi. Natijalar birikmada Zn–O koordinatsion bog'lar hosil bo'lganini, ketorolak esa karboksil guruhi orqali rux ioniga bog'langanini ko'rsatdi. Tadqiqot natijalari yangi koordinatsion birikmalar sintezining farmatsevtika va noorganik kimyo sohalaridagi ahamiyatini tasdiqlaydi.

Kalit so'zlar: Ketorolak, formamid, atsetamid, karbamid, nikotinamid, kompleks birikma, aralash-ligandli kompleks birikma, metall kompleks, IR-spektroskopiya, UV-Vis, element analiz.

Аннотация. В данной статье представлен синтез и физико-химическая характеристика нового координационного соединения, полученного из нитрата цинка и кеторолака. Соединение $[Zn(ket)_2](NO_3)_2 \cdot 2H_2O$ было синтезировано в смеси вода–этанол при pH 5,5–6 и выделено в виде белых кристаллов. Синтезированное соединение было проанализировано с использованием ИК-спектроскопии, УФ-видимой спектроскопии и элементного анализа. Результаты подтвердили образование координационных связей Zn–O, при этом кеторолак выступает в качестве лиганда через свою карбоксильную группу. В исследовании подчеркивается значимость синтеза новых координационных соединений для применения в фармацевтической и неорганической химии.

Ключевые слова: Кеторолак, формамид, ацетамид, карбамид, никотинамид, комплексное соединение, смешанно-лигандное комплексное соединение, металлический комплекс, ИК-спектроскопия, УФ-видимая спектроскопия, элементный анализ.

Abstract: This article presents the synthesis and physicochemical characterization of a novel coordination compound formed from zinc nitrate and ketorolac. The compound $[Zn(ket)_2](NO_3)_2 \cdot 2H_2O$ was synthesized in a water–ethanol mixture under pH conditions of 5.5–6 and precipitated as white crystals. The synthesized compound was analyzed using IR spectroscopy, UV-Vis spectroscopy, and elemental analysis. The results confirmed the formation of Zn–O coordination bonds, with ketorolac acting as a ligand through its carboxyl group. The study emphasizes the significance of synthesizing new coordination compounds for applications in pharmaceutical and inorganic chemistry.

Keywords: Ketorolac, formamide, coordination compound, mixed-ligand coordination compound, metal complex, IR spectroscopy (Infrared spectroscopy), UV-Vis spectroscopy (Ultraviolet–Visible spectroscopy), elemental analysis.

Coordination chemistry is a rapidly expanding field of research with significant applications in pharmaceuticals, biomedicine, and inorganic chemistry. In recent years, complex compounds

formed between bioactive substances and metal ions have garnered considerable attention due to their pronounced antibacterial and antiviral activities. Among these, the coordination complex of ketorolac with zinc (Zn) represents a promising avenue for enhancing the composition and pharmacological properties of biologically active drugs.

Ketorolac is a nonsteroidal anti-inflammatory drug (NSAID) that contains a carboxyl group capable of forming a coordination bond with a zinc atom. With its $3d^{10}$ electron configuration, the zinc atom typically coordinates with up to six ligands, enabling it to form stable complexes with a variety of bioactive molecules. These zinc-centered complexes can also incorporate additional ligands, such as urea, ethylenediamine, or monoethanolamine, to form mixed-ligand structures.

Scientific literature confirms that newly synthesized coordination compounds of the type [Zn(ketorolac)(ligand)n] exhibit greater antibacterial activity compared to ketorolac alone. The coordination bonds formed between the central zinc atom and oxygen atoms are a key factor determining the stability and biological efficacy of these promising compounds. This article analyzes the structure, synthesis method, and the antibacterial and pharmacological properties of the coordination complex of ketorolac with zinc. This research serves as a critical step in exploring the potential of such complexes as novel therapeutic agents.

Research Methodology: Initially, all necessary reagents and glassware required for the synthesis were collected, including $Zn(NO_3)_2 \cdot xH_2O$, $C_{15}H_{13}NO_3$ (ketorolac), ethanol or dimethylformamide (DMF), NaOH, distilled water, and appropriate laboratory vessels. The synthesis of the coordination compound with the composition $[Zn(ket)_2](NO_3)_2 \cdot 2H_2O$ was carried out according to the procedure described in [1,2]. For complex formation, 0.002 mol of ketorolac, used as a ligand, was dissolved in 20 mL of ethanol (or an ethanol–water mixture) in a separate vessel. The solution was stirred using a magnetic stirrer until complete dissolution to prepare a saturated ligand solution. In the next step, 0.001 mol of $Zn(NO_3)_2 \cdot 6H_2O$ was accurately weighed and dissolved in 20 mL of distilled water. Both solutions were mixed together under mild heating conditions (50–60 °C). The pH of the mixture was maintained at approximately 6.0–6.5 throughout the reaction. The reaction mixture was continuously stirred for 2–3 hours. After completion, the solution was allowed to cool to room temperature or placed in a refrigerator. Within 24–48 hours, a white crystalline precipitate formed. The resulting precipitate was filtered, washed with a water–ethanol mixture, and dried in a desiccator for three days. The final product was stored for further analysis [3].

The reaction can be represented by the following equation:

$$Zn(NO_3)_2 \cdot 6H_2O + 2HL \longrightarrow [Zn(L)_2](NO_3)_2 \cdot 2H_2O + 4H_2O$$

HL – the ketorolac molecule in its protonated carboxylic acid form.

L^- – denotes the deprotonated form of ketorolac.

$[Zn(L)_2](NO_3)_2 \cdot 2H_2O$ – the coordination compound, which consists of two ketorolac ligands and two nitrate ions in the form of a salt.

The elemental composition of the synthesized coordination compound $[Zn(L)_2](NO_3)_2 \cdot 2H_2O$ was determined by elemental analysis [4].

Table 1

Elemental Analysis of the $[Zn(L)_2](NO_3)_2 \cdot 2H_2O$ Coordination Compound

Molecular Formula of the Coordination Compound	Element	Theoretical (%)	Experimental (%)
	C	52,94	52,44

$[Zn(L)_2](NO_3)_2 \cdot 2H_2O$ Molecular formula: $C_{32}H_{28}N_4O_{12}Zn$ M=726 g/mol	H	3,89	3,44
	N	7,72	7,37
	O	26,45	26,05
	Zn	9,01	8,54

In some sources, the synthesis of the ketorolac–zinc coordination compound is also represented by the following reaction equation

$$Zn(NO_3)_2 \cdot xH_2O + 2HL \longrightarrow [Zn(L)_2] + 2HNO_3 + xH_2O$$

HL – ketorolac in its non-ionized (protonated) carboxylic acid form.

L^- – the deprotonated ketorolac (carboxylate anion).

$[Zn(L)_2]$ – the synthesized complex containing two ligands coordinated to a Zn(II) center.

Conclusion: In this study, a novel coordination compound, $[Zn(ket)_2](NO_3)_2 \cdot 2H_2O$, was successfully synthesized from zinc(II) nitrate and ketorolac. The synthesis was carried out in a water–ethanol medium at pH 5.5–6, resulting in the formation of a white crystalline precipitate. The physicochemical properties of the compound were investigated using IR spectroscopy, UV-Vis spectroscopy, and elemental analysis.

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