PROBLEMS AND SOLUTIONS OF SCIENTIFIC AND INNOVATIVE RESEARCH
Volume 02, Issue 08, 2025

UDC: 546.732;547-326;547-327;

IR SPECTROSCOPY OF MIXED-LIGAND COORDINATION COMPOUNDS OF COBALT(II) ION WITH KETOROLAC

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Abstract. *This article presents the results of research on the synthesis and analysis of mixed-ligand coordination compounds of cobalt (II) ion with ketorolac and amides. Solvent-based methods were selected for the synthesis process, in which cobalt (II) salts (such as chloride or acetate), ketorolac, and various amides (formamide, acetamide, nicotinamide) reacted in specific molar ratios to form new coordination compounds. To determine the structure and composition of the complexes, IR, UV-Vis, and NMR spectral analyses, as well as elemental analysis and X-ray diffraction (XRD), were employed. Thermal analysis was used to establish the thermal stability of the complexes. During the study, the coordination interactions of ligands with cobalt (II) ions, their electronic configuration, and biological activity were examined, and corresponding conclusions were drawn.*
Keywords: *Ketorolac, formamide, acetamide, nicotinamide, coordination compound, synthesis, analysis, coordination capacity, thermal stability, solubility, reaction yield.*

Introduction. One of the most relevant areas of modern coordination chemistry and bioinorganic chemistry is the synthesis of new coordination compounds based on biologically active ligands and the study of their properties. In particular, complexes of transition metals such as cobalt attract special interest due to their wide range of biological activities, including antibacterial, antifungal, and antitumor properties [1,2]. The cobalt (II) ion, owing to its electronic configuration and wide coordination numbers, can form stable coordination compounds with a variety of ligands; their structural features and bioactivity largely depend on the nature of the ligands [3]. Ketorolac is a systemically active non-steroidal anti-inflammatory drug (NSAID), whose pharmacological effect is mainly achieved through the inhibition of prostaglandin synthesis. However, at high doses, it carries the risk of damaging the gastrointestinal mucosa [4]. In modern pharmaceutical chemistry, the synthesis of metal complexes of drugs is considered a promising approach to enhance drug efficacy

and reduce side effects. It is well established that when organic ligands form complexes with metal ions, their biological activity can significantly increase, often associated with improved metabolic stability and enhanced solubility in water [5].

Since the differences between the spectra of the initial components and those of the complexes provide information about new interactions and bond formations, IR spectroscopy data were used to analyze the structures of the obtained complexes. The IR absorption spectra were recorded in the range of 400–4000 cm^{-1} on a "SHIMADZU" IRAffinity-1S spectrometer [29]. The IR spectra of ketorolac, cobalt(II) chloride hexahydrate, and the complex compound synthesized from these two components were analyzed. In the spectrum of ketorolac, characteristic absorption bands of C=O stretching vibrations were observed at 1720 and 1705 cm^{-1} [30], corresponding to the carbonyl group of the carboxylic moiety. Additionally, O–H stretching vibrations of the carboxyl group appeared in the range of 2729–2749 cm^{-1}. In the spectrum of cobalt(II) chloride hexahydrate, vibrational modes of water molecules and the amino group were recorded: O–H stretching at 3369 and 3560 cm^{-1}, and asymmetric and symmetric N–H_2 stretching at 3311 and 3225 cm^{-1}, respectively. Low-frequency vibrations attributed to Co–O bonds were also observed in the range of 535–565 cm^{-1}. In the spectrum of the complex synthesized from ketorolac and cobalt(II) nitrate, the C=O stretching bands of ketorolac were shifted from 1732 to 1739 cm^{-1} and from 1693 to 1683 cm^{-1}, indicating coordination of the C=O group with the cobalt ion. Furthermore, the disappearance of the broad O–H stretching bands suggests deprotonation of the carboxyl group upon complex formation with Co(II). New absorption bands in the 530–570 cm^{-1} region confirm the formation of Co–O bonds.

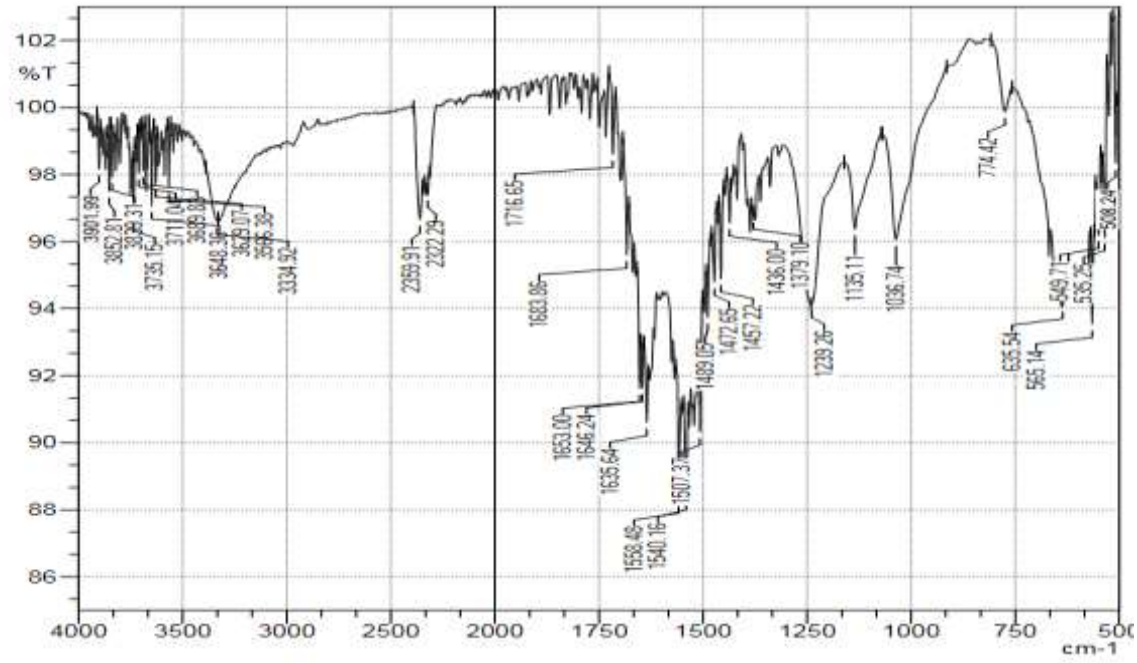

Figure 1. IR spectrum of the $[Co(Ket)_2(fm)_2(H_2O)_2]$ complex compound

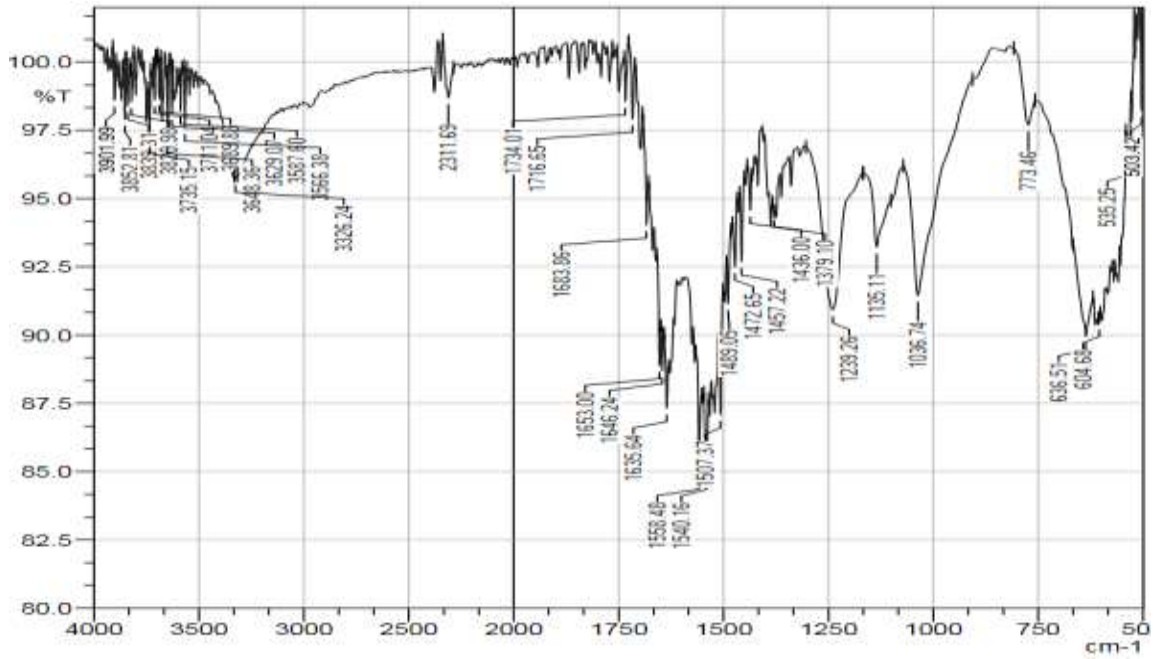

Figure 2. IR spectrum of the $[Co(Ket)_2(acm)_2(H_2O)_2]$ complex compound

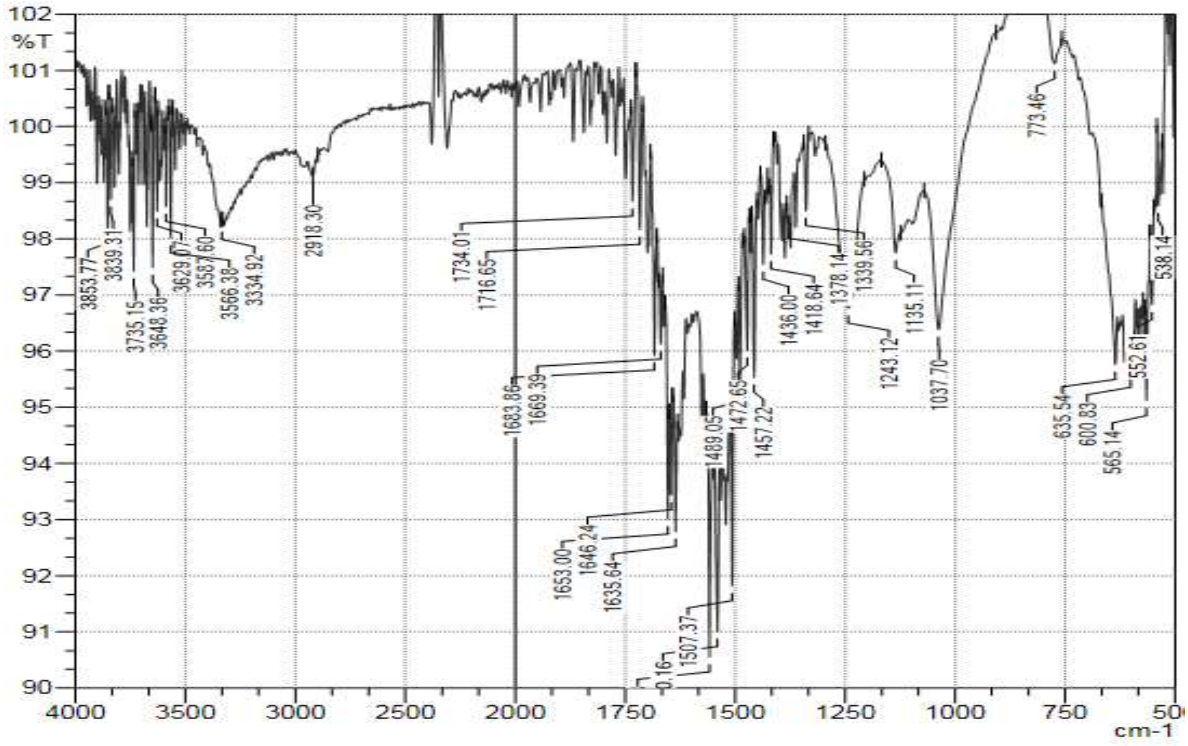

Figure 3. IR spectrum of the $[Co(Ket)_2(nia)_2(H_2O)_2]$ complex compound

Based on these IR spectral analyses, it is evident that a coordination complex is formed between ketorolac and cobalt(II) nitrate hexahydrate. The ketorolac molecule coordinates to the Co(II) ion via its carboxyl group. The shift of the C=O stretching vibrations, disappearance of O–H bands, and the appearance of new Co–O vibrations serve as direct evidence of complex formation (Figures 1–3).

The antibacterial properties of ketorolac and the metal–complex compounds synthesized on its basis were studied in vitro under laboratory conditions against strains from the microorganism collection of the Institute of Microbiology, Academy of Sciences of Uzbekistan: Bacillus subtilis-5, Escherichia coli-221, Pseudomonas aeruginosa-225, Staphylococcus aureus-91, and Candida albicans-247 [31]. The effects of the ligand (HL) and the complex compounds on non-spore-forming test strains were determined during the exponential growth phase (after 36–42 hours), while their effects on spore-forming test strains were assessed during the sporulation stage (after 48–72 hours). Antibacterial activity was evaluated on the 3rd–5th day of incubation, based on the diameter of the sterile zones formed in Petri dishes where the test strains were inoculated and the samples were applied (Egorov, 1995; Egorov, 2003). To minimize experimental error, all experiments were repeated three times.

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