

IR SPECTROSCOPIC ANALYSIS OF THE COMPLEX OF COBALT(II) ION
WITH 2-(4-ISOBUTYLPHENYL)PROPIONIC ACID

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Annotatsiya: Ushbu ishda, kobalt(II)sulfatning, 2-(4-izobutilfenil) propion kislota (ibuprofen) bilan yangi kompleks birikmasi sintez qilingan va uning tarkibi, tuzilishi va ayrim kimyoviy xossalari fizik-kimyoviy metodlar: skanerlovchi elektron mikroskop-energiya dispersion tahlil (SEM-EDT), element analiz va I \mathcal{Q} -spektroskopiya tahlili yordamida o'rganilgan. Kompleks birikma hosil bo'lishida, markaziy atom kobalt, ikkita molekula 2-(4-izobutilfenil) propion kislota qoldig'i tarkibidagi karboksil guruhining kislorod atomi va ikkita suv molekulasi bilan o'zaro bog'lanib, koordinatsion soni 4 ga teng bo'lgan kompleks birikmani hosil qilgan. Kompleks birikma hosil bo'lishida, dastlabgi tuz tarkibidagi sulfat qoldig'i ishtirok qilmasligini alohida takidlab o'tish zarur. Kompleks birikma molekulasi $[\text{Co}(\text{Ibup})_2]\text{SO}_4 \cdot 2\text{H}_2\text{O}$ tuzilishga ega ekanligi, qayd qilingan analiz tahlillari yordamida isbotlab berildi.

Kalit so'zlar: Kobalt(II)sulfat heptagidrati, 2-(4-izobutilfenil) propion kislota (ibuprofen), ligand, element analiz SEM-EDX, kompleks birikma, koordinatsion son, I \mathcal{Q} -spektroskopiya tahlili.

Аннотация: В статье синтезирован новый комплекс сульфата кобальта(II) с 2-(4-изобутилфенил)пропионовой кислотой (ибупрофеном) и изучены его состав, структура и некоторые химические свойства с использованием физико-химических методов: сканирующей электронной микроскопии-энергодисперсионного анализа (СЭМ-ЭДТ), элементного анализа и ИК-спектроскопии. При образовании комплекса центральный атом кобальта, две молекулы остатка 2-(4-изобутилфенил)пропионовой кислоты взаимодействовали с атомом кислорода карбоксильной группы и двумя молекулами воды, образуя комплекс с координационным числом 4. Следует подчеркнуть, что сульфатный остаток в исходной соли не участвует в образовании комплекса. Структура комплексной молекулы $[\text{Co}(\text{Ibup})_2]\text{SO}_4 \cdot 2\text{H}_2\text{O}$ доказана указанными аналитическими анализами.

Ключевые слова: Гептагидрат сульфата кобальта(II), 2-(4-изобутилфенил)пропионосовая кислота (ибупрофен), лиганд, элементный анализ, SEM-EDX, комплексное соединение, координационное число, анализ ИК-спектроскопии.

Abstract: In the article, a new complex of cobalt(II) sulfate with 2-(4-isobutylphenyl) propionic acid (ibuprofen) was synthesized and its composition, structure and some chemical properties were studied using

physicochemical methods: scanning electron microscopy-energy dispersive analysis (SEM-EDT), elemental analysis and IR spectroscopy. In the formation of the complex, the central atom cobalt, two molecules of 2-(4-isobutylphenyl) propionic acid residue, interacted with the oxygen atom of the carboxyl group and two water molecules, forming a complex with a coordination number of 4. It should be emphasized that the sulfate residue in the original salt does not participate in the formation of the complex. The structure of the complex molecule $[\text{Co}(\text{Ibup})_2]\text{SO}_4 \cdot 2\text{H}_2\text{O}$ was proven by the mentioned analytical analyses.

Key words: Cobalt(II) sulfate heptahydrate, 2-(4-isobutylphenyl) propionic acid (ibuprofen), ligand, elemental analysis, SEM-EDX, complex compound, coordination number, IR spectroscopy analysis.

This research provides information on the synthesis of coordination compounds of biologically active ligands (Ibuprofen) with 3d transition metals — a new direction in the chemistry of coordination complexes — and their analysis using physicochemical methods.

At present, due to various changes occurring in the environment and the impact of different types of weapons used by humans, the number and diversity of diseases caused by microorganisms (such as parasitic fungi, bacteria, and viruses) are steadily increasing. For example, virologists have determined that the number of virus-induced inflammatory diseases has exceeded 300. Such diseases include rubella, measles, hepatitis, herpes, monkeypox, yellow fever, dengue fever, kuru, Japanese encephalitis, and others.

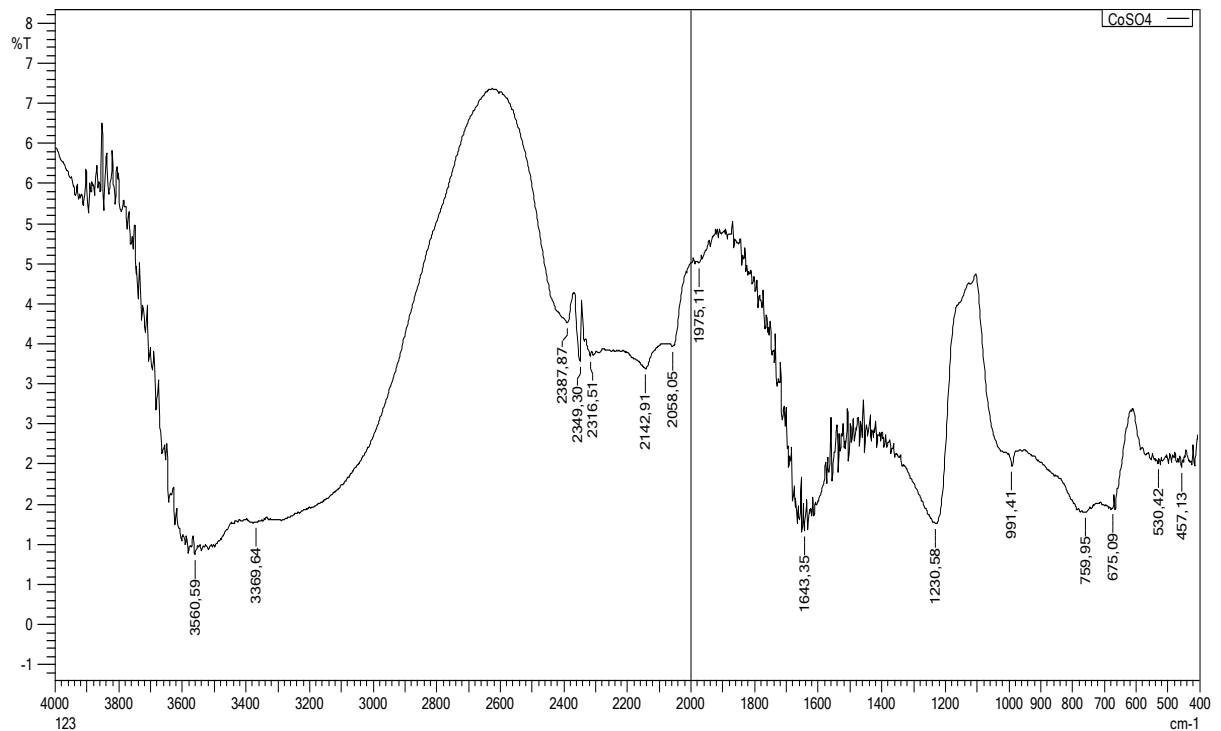
Various pharmaceutical drugs are currently being used to prevent and treat these diseases. Among them are ketorolac, diclofenac, indomethacin, ketoprofen, ibuprofen, paracetamol, mefenamic acid, and others. However, today, in order to combat diseases caused by the complex effects of harmful bacteria, microbes, and viruses on living organisms, it is necessary to use either more potent forms or higher concentrations of these drugs.

To enhance the therapeutic efficacy of ibuprofen, a coordination compound of this ligand with cobalt — a biogenic element — was synthesized. The molecular structure and configuration of the resulting complex were determined, and a methodology for its synthesis in solution under laboratory conditions was developed.

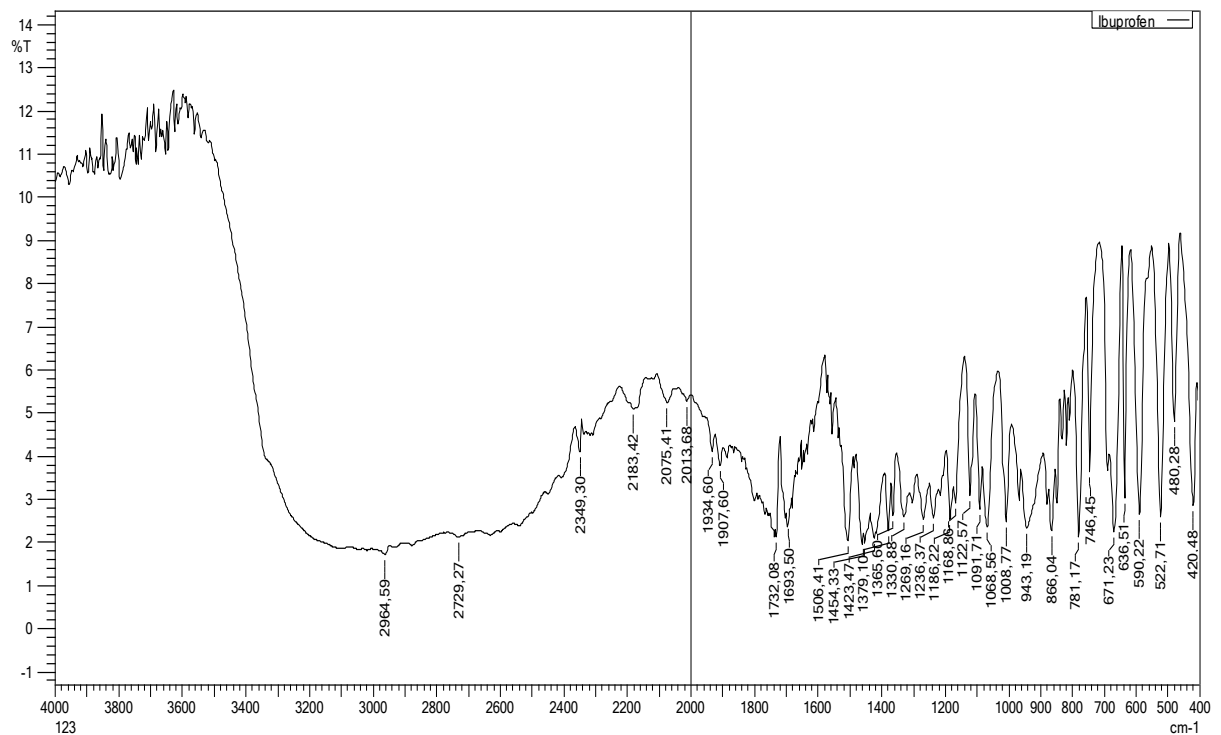
Research objective. The objective of this study is to synthesize and determine the composition, structure, and properties of a coordination compound formed from cobalt(II) sulfate hexahydrate and 2-(4-isobutylphenyl)propionic acid (ibuprofen). To achieve this goal, synthesis methods for the cobalt(II)-ibuprofen coordination compound were developed and the compound was successfully synthesized. The composition and structure of the synthesized complex were studied using elemental analysis and infrared (IR) spectroscopy methods.

Analysis and Results. To investigate the composition of the synthesized coordination compound, IR spectroscopy analysis was performed. First, the IR spectra of the individual components used in the synthesis were obtained. These spectra were then compared with the IR spectrum of the final product, and relevant conclusions were drawn based on the comparison [1]. The IR (infrared) spectra of ibuprofen, cobalt(II) sulfate heptahydrate, and

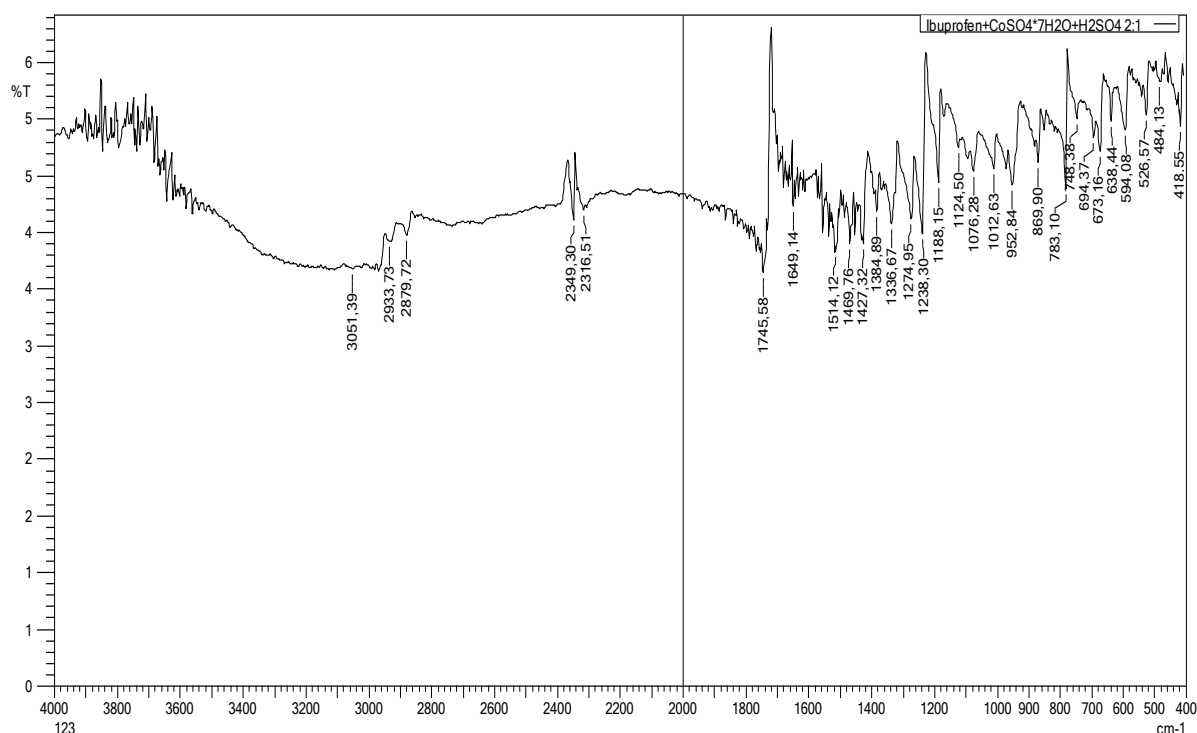
the coordination compound synthesized from these two substances were analyzed separately [2].



a)



b)



c)

Figure 1. a) IR spectrum of CoSO_4 b) IR spectrum of ibuprofen c) IR spectrum of the cobalt coordination compound

In the spectrum of ibuprofen, distinct absorption bands were observed at 1732 cm^{-1} and 1693 cm^{-1} , corresponding to the C=O stretching vibrations of the carboxyl group. Additionally, absorptions in the $2729\text{--}2749\text{ cm}^{-1}$ range were attributed to the O–H stretching vibrations of the same group.

In the spectrum of cobalt(II) sulfate heptahydrate, vibrational bands characteristic of water molecules and sulfate ions were observed: O–H stretching vibrations of water appeared at 3369 and 3560 cm^{-1} , while sulfate (SO_4^{2-}) absorption bands were recorded at 1230 and 1643 cm^{-1} . In the low-frequency region, between 457 and 759 cm^{-1} , Co–O bond vibrations were detected. In the IR spectrum of the synthesized coordination compound based on ibuprofen and cobalt(II) sulfate, the C=O stretching bands of ibuprofen shifted from 1732 to 1739 cm^{-1} and from 1693 to 1683 cm^{-1} . This shift indicates the coordination of the carbonyl group with the cobalt ion. Moreover, the O–H absorption bands disappeared from the spectrum, suggesting that the carboxyl group lost its proton and formed a complex with Co(II). Additionally, new bands were observed in the $418\text{--}592\text{ cm}^{-1}$ range, confirming the formation of Co–O bonds. The spectrum of the complex also showed absorption peaks at 1238 cm^{-1} (shifted from 1230 cm^{-1}) and in the range of $623\text{--}671\text{ cm}^{-1}$, which correlate with those of the SO_4^{2-} ion. These peaks are relatively well-resolved, not symmetrically arranged, and the shifts are not substantial (e.g., $1230 \rightarrow 1238\text{ cm}^{-1}$, a shift of only 8 cm^{-1}) [3]. These findings suggest that the sulfate ion does not participate in coordination but remains as a free anion outside the coordination sphere of the complex.

Conclusions. Based on the above IR spectral analyses, it was confirmed that a coordination compound was formed between ibuprofen and cobalt(II) sulfate

heptahydrate. The ibuprofen molecule coordinates to the Co(II) ion through its carboxyl group. The main evidence for this includes the shift in C=O stretching vibrations, the disappearance of O-H vibrations, and the emergence of new bands corresponding to Co-O bonds. These results indicate that pharmaceutical compounds such as ibuprofen are capable of forming stable complexes with metal ions, suggesting potential applications of such compounds in pharmaceutical and biological systems.

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