



## SPECTROSCOPIC ANALYSIS OF 2-METHYLTHIOBENZOXAZOLE AND THEIR COMPLEX COMPOUNDS WITH 3D-METALS

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**Relevance of the research:** derivatives of benzoxazole, which is a heterocyclic compound containing nitrogen and oxygen, are used in research as a starting material for the synthesis of many bioactive structures, and many scientific studies have been conducted on their structure and properties.

Derivatives of oxazole and 2-aminothiobenzoxazole are recognized as substances of medical importance. It is known that oxazole derivatives are substances with various pharmacological effects. For example, it is used as a remedy against cancer, microbes, inflammation, herbicide, antibacterial, antiviral, antihistamine, antioxidant, estrogen receptor inhibitor, and hepatitis C virus. Compounds of 2-aminothiobenzoxazole also have luminescent properties.

**Purpose of the study:** Synthesis of new complex compounds based on the ligand of benzoxazole derivatives of Co (II) and Cu (II) salts and study of their composition, structure and properties, as well as determination of the regularities of complex formation.

**Methods and techniques of the topic:** Based on the results of IR spectroscopy of metal complexes obtained on the basis of 2-aminothiobenzoxazole derivatives of Co (II) and Cu (II) salts, the results of IR spectroscopy were studied.

**Result:** Comparing the IR spectra of L and its complexes with cobalt and copper nitrate salts, it can be said that the position of symmetrical valence vibrations of the C=N bond and asymmetrical valence vibrations of -C-N= in the spectra, during the transition from the ligand to the complexes, a heterocyclic bond is formed, shifted by 12-26 cm<sup>-1</sup> for the first to the low-frequency region, and by 3-10 cm<sup>-1</sup> for the second (Table 1). The regions of asymmetric valence vibrations of the C=N bond shift to low frequencies by 12-26 cm<sup>-1</sup>. This change can be explained by the shift in electron density during complex formation at one of the nitrogen atoms of the oxazole ring. The position of the valence vibration region of the S-CH<sub>3</sub> bond, located in the region of 1031 cm<sup>-1</sup>, remains unchanged. Due to the presence of a small amount of moisture in the ligand molecule, the valence vibrations also occurred in the region of 3080-3271 cm<sup>-1</sup>, which remained unchanged in the complex, but in the IR spectrum of the complexes, these lines are more resolved and it has maxima at 3095 and 3271 cm<sup>-1</sup>.

**Table 1**

**In the IR spectra of ligands (L) and complexes based on them, the main oscillation frequencies (cm<sup>-1</sup>)**

| Birikma                                             | (-CH <sub>3</sub> ) | (=C-H) | v(CH <sub>3</sub> -S-) | σ(-C-N-) | v(-C=N-) | σ(-C-O-) | M-N |
|-----------------------------------------------------|---------------------|--------|------------------------|----------|----------|----------|-----|
| L                                                   | 1628                | 1418   | 1031                   | 3271     | 684      | 1519     | -   |
| [CoL <sub>2</sub> (NO <sub>3</sub> ) <sub>2</sub> ] | 1621                | 1496   | 1094                   | 3362     | 680      | 1556     | 419 |
| [CuL <sub>2</sub> (NO <sub>3</sub> ) <sub>2</sub> ] | 1624                | 1476   | 1044                   | 3193     | 696      | 1551     | 419 |

**Summary:** In the IR spectra of the complexes, the lines appearing at 481-459 cm<sup>-1</sup> are associated with the valence vibrations of the N-M bond. Consequently, we can conclude that the coordination of heterocyclic ligands occurs at the expense of endocyclic nitrogen atoms. In the spectrum of the analyzed complex, an intense band of symmetrical valence vibrations of the NO<sub>3</sub>-



group appeared at 1375 cm<sup>-1</sup>. This indicates that the nitrate group is monodentately attached to the central atom via oxygen. Thus, according to the IR spectroscopy of Co (II) complexes, the nitrate ion is monodentately coordinated with the central atom as an acidoligand. The conclusions obtained from the IR spectrum data are consistent with the results of X-ray.