



## INFRARED SPECTRAL ANALYSIS OF THE IONITE BASED ON DIMETHYLOLCARBAMIDE AND ORTHOPHOSPHORIC ACID AND ITS COMPLEX WITH MERCURY (II) ION

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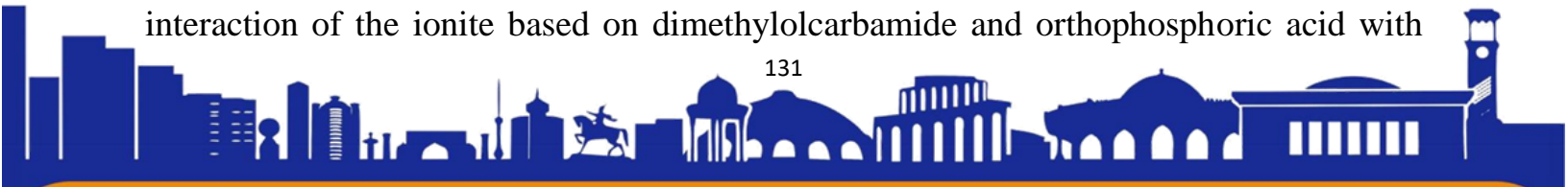
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### **Abstract:**

This study investigates the infrared (IR) spectra of an ionite synthesized from dimethylolcarbamide and orthophosphoric acid and its complex formed with mercury (II) ion. The presence of functional groups in the ionite and spectral changes after the formation of the complex were analyzed. Based on the results obtained, conclusions were drawn about the ionite's selectivity toward metal ions and the complexation mechanism.

### **Introduction:**

Ion exchange materials are of great importance in modern analytical chemistry, industrial technologies, and environmental protection. They are widely used in processes such as ion separation, purification, and selective sorption from solutions. The ion exchange capacity of ionites depends on their internal structure and active functional groups, which makes them sensitive and selectively interactive with heavy metals, radioactive elements, and other harmful pollutants. Ionites synthesized from dimethylolcarbamide and orthophosphoric acid possess a combination of multiple functional groups (amine, carbonyl, phosphate groups), which enable them to form strong coordination bonds with metal ions. The donor atoms (O, N) present in these ionites can combine with metal ions to form stable complexes, enhancing their selective sorption properties. In this study, the interaction of the ionite based on dimethylolcarbamide and orthophosphoric acid with





mercury (II) ion ( $\text{Hg}^{2+}$ ) was investigated. Due to the high toxicity and ecological risks of mercury ions, their selective removal and purification are of significant scientific and practical importance. Therefore, the complex formation characteristics of the ionite with mercury (II) ions were thoroughly analyzed.

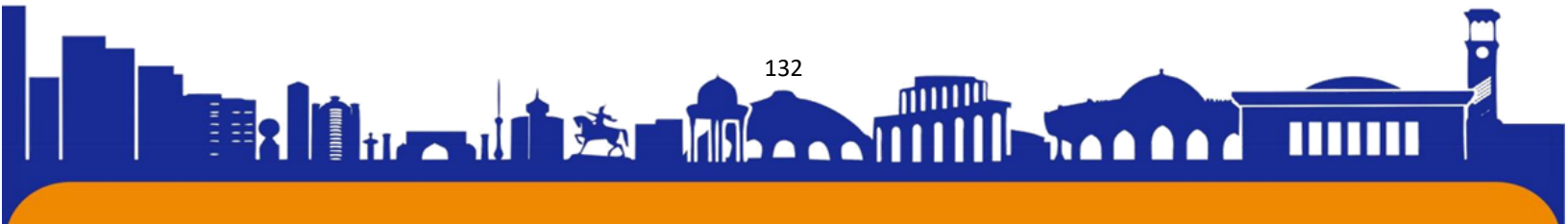
Infrared spectroscopy (IR spectral analysis) was used to determine the changes occurring between the ionite and mercury (II) ions, including the participation of functional groups and the formation of new coordination bonds. IR spectroscopy is an effective and non-invasive method for studying the molecular structure of ionites and their interactions with ions, providing important information on complexation processes through shifts in peaks and changes in intensities. Thus, this study aims to identify the potential of the ionite based on dimethylolcarbamide and orthophosphoric acid for selective separation of mercury (II) ions and to explore its prospects for use in environmental cleanup technologies.

### **Experimental Part:**

**Ionite Synthesis:** The ionite based on dimethylolcarbamide and orthophosphoric acid was synthesized in the laboratory. For this, dimethylolcarbamide and orthophosphoric acid were first mixed in a certain ratio in an aqueous environment. The mixture was stabilized under controlled temperature and pH conditions and allowed to react. During the polycondensation process, a branched macromolecular structure was formed through carbonyl and phosphate groups. The resulting ionite was dried, ground into fine particles, and prepared for further analysis.

**Complexation:** The prepared ionite sample was reacted with a mercury (II) ion ( $\text{Hg}^{2+}$ ) solution. For the complex formation process, the ionite was brought into contact with an aqueous  $\text{Hg}(\text{NO}_3)_2$  solution for a specified time (24 hours) under static conditions. During the reaction process, the functional groups (carbonyl, amine, and phosphate groups) of the ionite coordinated with the mercury ions, resulting in the formation of stable complex compounds on the surface of the ionite. After complexation, the samples were washed with water to remove free mercury ions, then dried.

1. **Spectral Measurement:** Infrared (IR) spectra of both the initial ionite and the ionite complexed with mercury (II) were obtained. The IR spectra were recorded in the  $4000\text{--}400\text{ cm}^{-1}$  range using modern Fourier Transform Infrared Spectroscopy (FTIR) equipment. The spectral measurements were performed using the KBr pellet





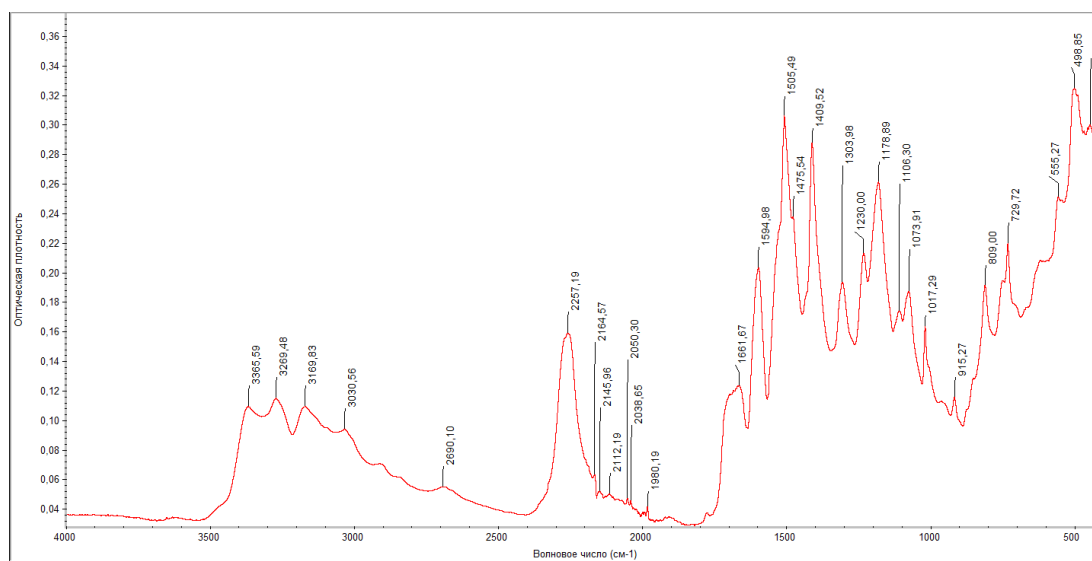
method, where ionite samples were mixed with KBr, pressed, and set in a transparent film form.

Analysis: Based on the obtained IR spectra, the state of the ionite before and after complexation with mercury (II) ions was compared. The spectra were analyzed for:

- The wave numbers ( $\text{cm}^{-1}$ ) corresponding to the main functional groups (O–H, N–H, C=O, P=O, P–O–C),
- Changes in the intensity of the peaks,
- Shifts in peaks and the appearance of new peaks.

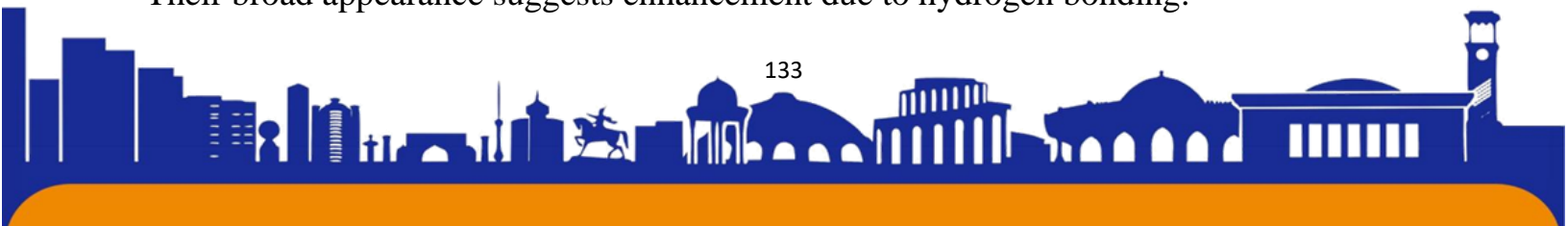
These changes helped to identify which functional groups were involved in the complexation process and to determine the nature of the interaction between the ionite and the mercury (II) ions.

### Results and Discussion:



**According to the results of infrared spectroscopy**, several characteristic vibrational bands were identified in the initial IR spectrum of the ionite based on dimethylolcarbamide and orthophosphoric acid:

**Broad peaks in the  $3660\text{--}3260\text{ cm}^{-1}$  range (3365, 3264, 3169  $\text{cm}^{-1}$ ):** These broad and intense peaks correspond to O–H and N–H stretching vibrations. These vibrations confirm the presence of amino and hydroxyl groups in the ionite structure. Their broad appearance suggests enhancement due to hydrogen bonding.





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**Peak at 3030  $\text{cm}^{-1}$ :** Associated with C–H stretching vibrations, indicating the presence of methyl ( $-\text{CH}_3$ ) and methylene ( $-\text{CH}_2-$ ) groups. These vibrations reflect C–H bonds in the organic part of the ionite.

**Peak at 2257  $\text{cm}^{-1}$ :** A sharp and distinct peak likely corresponding to  $\text{C}\equiv\text{N}$  stretching vibrations. This suggests the presence of nitrile groups or similar strong triple bond structures in the ionite. Such groups enhance the potential for strong coordination bonds with metal ions.

**Range 1650–1500  $\text{cm}^{-1}$  (peaks at 1616, 1595, 1505  $\text{cm}^{-1}$ ):** This region includes C=O stretching vibrations and deformation vibrations of N–H groups. Strong C=O stretching typical for urea fragments is evident, confirming the successful incorporation of dimethylolcarbamide into the ionite.

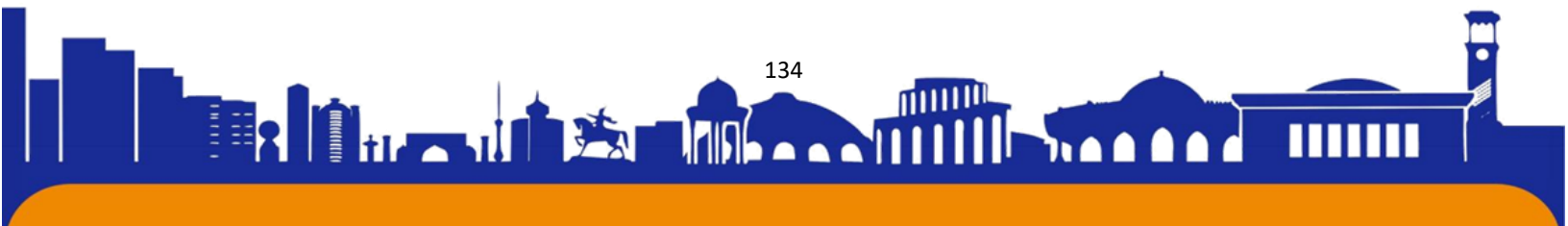
**Range 1200–1000  $\text{cm}^{-1}$  (peaks at 1230, 1178, 1108  $\text{cm}^{-1}$ ):** Strong peaks here correspond to P=O stretching and P–O–C bond vibrations. These indicate active involvement of orthophosphate groups in the ionite matrix, playing a key role in the formation of the branched structure during polycondensation.

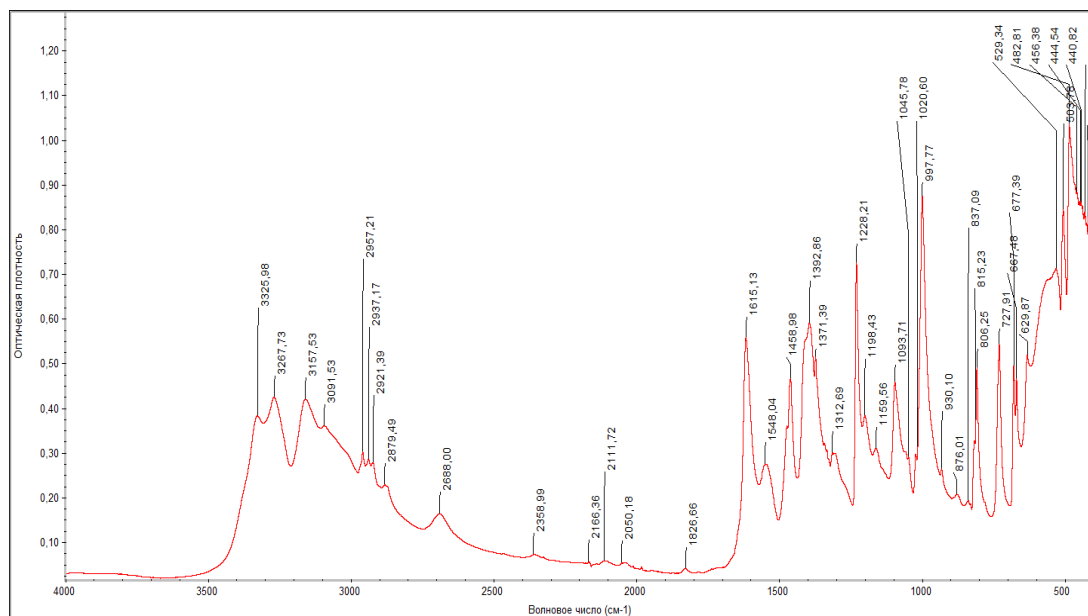
**Range 600–400  $\text{cm}^{-1}$  (peaks at 729, 555, 445  $\text{cm}^{-1}$ ):** Low-energy vibrations in this region are attributed to P–O–P and possibly C–N deformation vibrations. These vibrations point to the presence of a multi-branched and strongly bonded structural framework within the ionite.

**Overall spectral analysis:** The initial IR spectrum of the ionite clearly reveals the presence of rich functional groups:

- Urea fragments (C=O and N–H groups),
- Phosphate groups (P=O and P–O–C bonds),
- Nitrile or  $\text{C}\equiv\text{N}$  structures,
- Organic C–H bonds.

The presence of these groups allows the ionite to form strong coordination complexes with metal ions, especially heavy metals such as mercury (II). The combination of amino, carbonyl, and phosphate groups provides the ionite with multiple donor sites, significantly enhancing its selective sorption and complexation properties. Furthermore, the observed broad and intense hydrogen bonding networks suggest that the ionite may also possess improved mechanical and chemical stability.





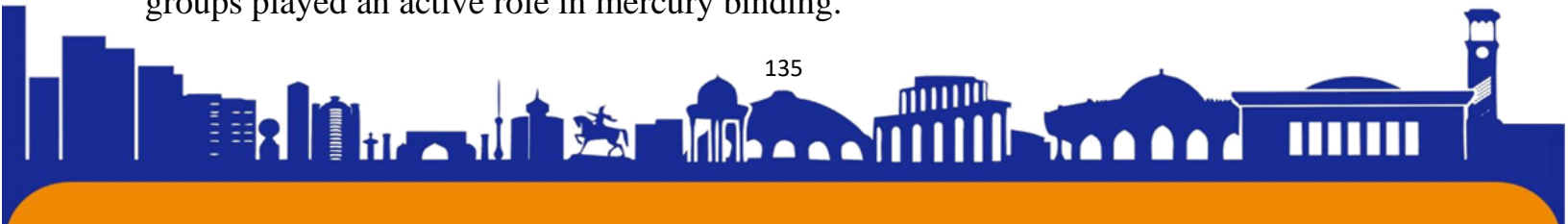
## 2. IR Spectrum of the Ionite After Complexation with Mercury (II) Ion:

Significant changes were observed in the IR spectrum of the ionite after it reacted with mercury (II) ions, indicating that complexation had occurred.

**Changes in the 3365–3160  $\text{cm}^{-1}$  region:** The shape and intensity of the O–H and N–H stretching vibrations changed considerably. The previously broad peaks became narrower and slightly sharper, suggesting the disruption or rearrangement of hydrogen bonding. The coordination of  $\text{Hg}^{2+}$  ions with N–H and O–H groups alters the hydrogen bonding network. This indicates a structural reorganization of the ionite molecule and direct interaction of mercury ions with amino and hydroxyl groups.

**2257  $\text{cm}^{-1}$  peak retained but intensified:** This peak corresponds to the  $\text{C}\equiv\text{N}$  (nitrile) stretching vibration. Its retention, but with increased intensity, suggests a weak but notable interaction between the  $\text{C}\equiv\text{N}$  group and mercury (II) ions. The approach of  $\text{Hg}^{2+}$  ions changes the electron density around the nitrile group, intensifying the vibration. This indicates that  $\text{C}\equiv\text{N}$  groups can also participate in metal ion binding.

**1616–1505  $\text{cm}^{-1}$  region:** Slight shifts and intensity changes in the  $\text{C}=\text{O}$  stretching vibration were observed. This suggests that the carbonyl group formed a coordination bond with  $\text{Hg}^{2+}$  ions. A decrease in stretching frequency indicates reduced electron density on the carbonyl oxygen, confirming a strong coordination interaction. Thus, carbonyl groups played an active role in mercury binding.





**1200–1000  $\text{cm}^{-1}$  region:** Peaks corresponding to P=O and P–O–C stretching vibrations intensified and slightly shifted. This is due to the interaction of phosphate group electron clouds with mercury (II) ions, altering their vibrational characteristics. This demonstrates that phosphate groups actively participated in the complexation process by coordinating with  $\text{Hg}^{2+}$  ions.

**600–400  $\text{cm}^{-1}$  region:** New deformation vibration peaks appeared in this low-frequency region, and existing peaks showed significant shifts. These confirm the formation of new coordination bonds of the Hg–O and Hg–N type. The distinctive vibrations of Hg–O and Hg–N appeared as new signals in the spectrum, clearly demonstrating the formation of a metal complex.

#### General Spectral Analysis:

After complexation with mercury (II) ions, the ionite spectrum showed:

- Changes in O–H and N–H stretching regions,
- Interaction of  $\text{C}\equiv\text{N}$  and  $\text{C}=\text{O}$  groups,
- Coordination of phosphate groups,
- Formation of new Hg–O and Hg–N bonds.

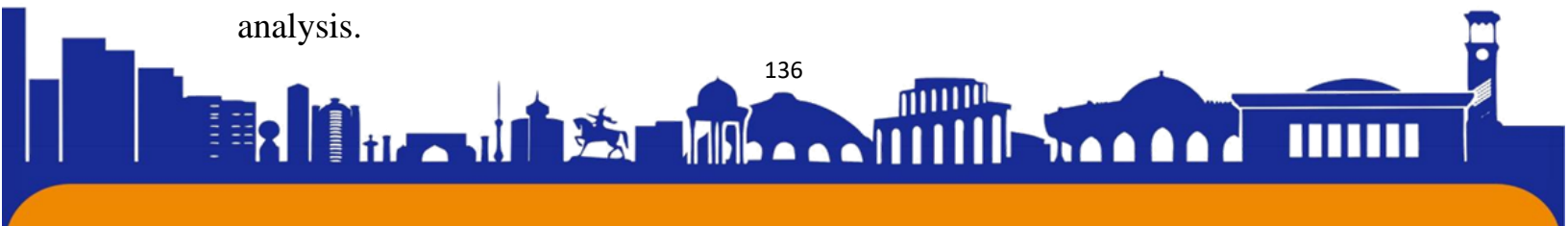
These changes confirm that complexation occurred and that several functional groups in the ionite (amino, carbonyl, phosphate, nitrile) actively participated in binding the metal ions. The ionite synthesized from dimethylolcarbamide and orthophosphoric acid forms effective complexes with mercury (II) ions, where amino, carbonyl, and phosphate groups serve as the primary coordination centers.

**General Conclusion:** As a result of complexation with mercury (II), the carbonyl and phosphate groups in the ionite formed coordination bonds, anchoring mercury ions firmly within the ionite matrix.

**Mechanism of complex formation:** The ionite synthesized from dimethylolcarbamide and orthophosphoric acid forms complexes with mercury (II) ions through coordination bonds. Primarily, carbonyl ( $\text{C}=\text{O}$ ), amino (N–H), and phosphate (P=O, P–O–C) groups are actively involved in this complexation process.

#### Conclusion:

- The presence of carbonyl, amino, and phosphate groups in the ionite synthesized from dimethylolcarbamide and orthophosphoric acid was confirmed via IR spectral analysis.





- The formation of strong complexes with mercury (II) ions was evidenced by shifts in IR peaks and the appearance of new vibrational bands.
- The study demonstrated that this ionite has great potential for selective sorption of heavy metal ions, particularly  $\text{Hg}^{2+}$ .

### References:

1. Khayit Turaev, Gulnora Umirova, Sherzod Kasimov, Malika Kobilova. *Synthesis and studying of nitrogen and oxygen-containing complexing sorbents during the sorption of some d-metals*, *Science and Innovation*, Vol. 2 (2023), pp. 277–282.
2. Lisa Malachowski, J. L. Stair, J. A. Holcombe. *Immobilized peptides/amino acids on solid supports for metal remediation*, *Pure Appl. Chem.*, Vol. 76 (2004), pp. 777–787.
3. Marco Luechinger, Alexander Kienhöfer, Gerhard D. Pirngruber. *Immobilized Complexes of Metals with Amino Acid Ligands – A First Step toward the Development of New Biomimetic Catalysts*, *Chemistry of Materials*, 2006, 18(5), 1330–1336.
4. Muhammad Pervaiz et al. *Synthesis, spectral and antimicrobial studies of amino acid derivative Schiff base metal (Co, Mn, Cu, and Cd) complexes*, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, Vol. 206 (2019), pp. 642–649.
5. A.O. Raji et al. *Mn(II), Co(II), Ni(II), and Cu(II) complexes of amino acid derived Schiff base ligand: Synthesis, characterization and in-vitro antibacterial investigations*, *Ethiopian Journal of Chemistry*, Vol. 35, pp. 97–106.
6. Nurmetova D.K. et al. *Synthesis of cobalt (II) complex with para-nitrobenzoic acid and ethylenediamine*, *Proceedings of International Scientific-Practical Conference on Coordination Chemistry*, 2022, pp. 8–9.
7. Ermuratova N.A., Kasimov Sh.A., Turayev K.K. *Synthesis and study of a chelating sorbent based on urea, formaldehyde and 2-aminopentanedioic acid*, *Universum: Technical Sciences*, 2021, No. 4(85), pp. 71–73.
8. Umiriva G.A., Kasimov Sh.A., Turayev K.K., Sharipov B.Sh. *Study of physicochemical properties of a synthesized complex-forming anionite*, *ARES*, 2021, No. 12, pp. 1372–1379.

