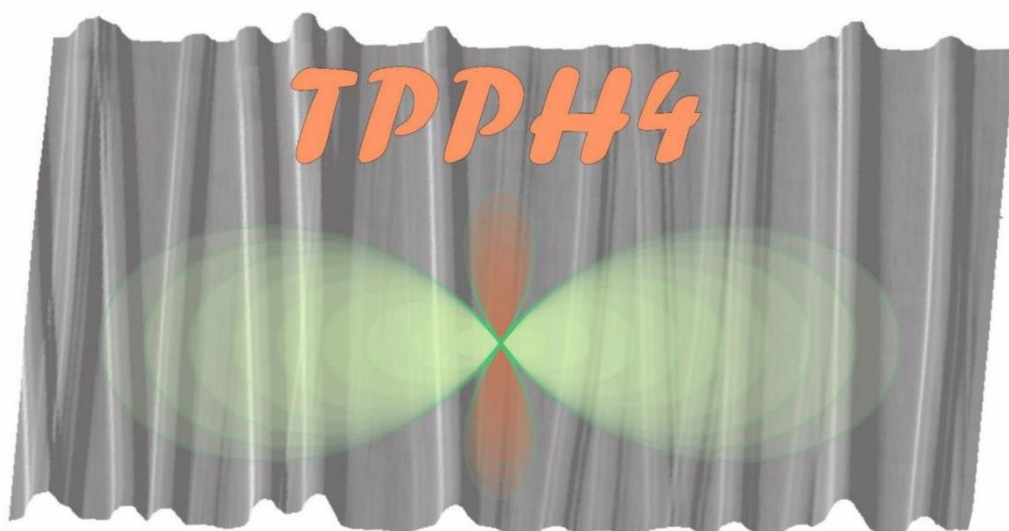


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спектроскопии минералов  
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**IV Конференция и Школа  
для молодых ученых  
Терморентгенография и рентгенография  
наноматериалов**



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## **Book of Abstracts**

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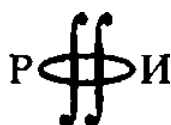
В сборнике представлены новые экспериментальные данные и методики по дифракционным исследованиям порошков, монокристаллов и наноматериалов. Особое внимание уделено исследованиям изменений кристаллической структуры при воздействии температур, давлений и структурных замещений.

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The book of abstracts presents new experimental data and methods for diffraction studies of powders, single crystals and nanomaterials. Particular attention is paid to studies of changes in the crystal structure under the conditions of temperature, pressure and structural substitutions.

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**Synthesis, characterization and morphotropic transitions in a family of  $M[(\text{UO}_2)(\text{CH}_3\text{COO})_3](\text{H}_2\text{O})_n$  ( $M = \text{Na, K, Rb, Cs}$ ;  $n = 0-1.0$ ) compounds.**

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Single crystals of  $\text{Na}[\text{UO}_2(\text{CH}_3\text{COO})_3]$  (**I**),  $\text{K}[\text{UO}_2(\text{CH}_3\text{COO})_3](\text{H}_2\text{O})_{0.5}$  (**2**),  $\text{Rb}[\text{UO}_2(\text{CH}_3\text{COO})_3]$  (**3**) and  $\text{Cs}[\text{UO}_2(\text{CH}_3\text{COO})_3](\text{H}_2\text{O})_{0.5}$  (**4**) have been prepared by evaporation from 3 ml aqueous solution of uranyl acetate dihydrate, ammonium carbonate, and sodium chloride, potassium chloride, rubidium chloride or cesium chloride for **I**, **II**, **III** and **IV**, respectively. Single crystal X-Ray Diffraction data had been collected at 100 K for **II**, **III**, **IV** and 296 K for **I** using Bruker Kappa Apex II Duo diffractometer.

The unit cell parameters were determined and refined by least squares method [0]. The crystal structures were solved by direct methods and refined using the Shelx programs incorporated in Olex2 program package. **I**:  $P2_13$ ,  $a = 10.721(6)$  Å,  $V = 1232.4(19)$  Å<sup>3</sup>,  $Z = 4$ ,  $R_1 = 0.041$ . **II**:  $I4_1/a$ ,  $a = 14.222(5)$ ,  $c = 25.715(8)$  Å,  $V = 5201(4)$  Å<sup>3</sup>,  $Z = 16$ ,  $R_1 = 0.037$ . **III**:  $I4_1/a$ ,  $a = 13.787(3)$ ,  $c = 27.511(7)$  Å,  $V = 5230(3)$  Å<sup>3</sup>,  $Z = 16$ ,  $R_1 = 0.037$ . **IV**:  $P\bar{1}$ ,  $a = 8.353(4)$ ,  $b = 11.008(5)$ ,  $c = 15.354(7)$  Å,  $\alpha = 108.409(11)$ ,  $\beta = 100.140(9)$ ,  $\gamma = 96.370(9)^\circ$ ,  $V = 1297.5(10)$  Å<sup>3</sup>,  $Z = 4$ ,  $R_1 = 0.036$ .

Structures **I**, **II** and **III** contain one symmetrically nonequivalent uranium atom each. The structure of **IV** contains two independent uranium atoms. Each uranyl ion is coordinated by six oxygen atoms in the equatorial plane, which belong to three acetate groups. Resulting hexagonal bipyramids (coordination polyhedrons of  $\text{U}^{6+}$  atoms) share three common edges with  $(\text{CH}_3\text{COO})$  groups, forming uranyl-three-carbonate clusters, which are a core unit of structures **I-IV**.

The amount of symmetrically nonequivalent acetate groups increases from one in the structure of **I** to three in the structures of **II** и **III** and six in the structure of **IV**. The number of nonequivalent uranium atoms also increases with the decreasing of symmetry (from cubic in **I** to triclinic in **IV**).

The main structural differences within morphotropic transitions in family of  $M[(\text{UO}_2)(\text{CH}_3\text{COO})_3](\text{H}_2\text{O})_n$  ( $M = \text{Na, K, Rb, Cs}$ ;  $n = 0-1.0$ ) compounds are associated with changes in the ionic radii of alkali metal cations. The first structural transformation is induced by the Na-to-K substitution and results in the symmetry decrease from cubic  $P2_13$  to tetragonal  $I4_1/a$ . It happens due to the significant difference in the ionic radii of Na и K (~0.44 Å). The K-to-Rb substitution does not lead to any significant structural changes, because of the less significant difference in the ionic radii (~0.06 Å). The Rb-to-Cs substitution again causes structural changes due to large difference in the ionic radii (~0.17 Å), resulting in the symmetry decrease to triclinic.

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1. Korniyakov I.V. Synthesis, characterization and morphotropic transitions in a family of  $M[(\text{UO}_2)(\text{CH}_3\text{COO})_3](\text{H}_2\text{O})_n$  ( $M = \text{Na, K, Rb, Cs}$ ;  $n = 0-1.0$ ) compounds. Zeitschrift für kristallographie. 2020. V. 235(3). P. 95-103.