addressed by collecting high quality data at low temperature using a microfocus Cu X-ray source and employing dual-space recycling (SHELXD) for structure solution. The very large numbers of independent molecules present good exercises for the RESI and BLOC commands during refinement. For example, one structure in space group I2 has a unit cell volume of nearly $43 \times 10^3$ Å$^3$ and contains fourteen independent molecules. Despite a fascinating topological interweaving, more than one-third of the unit cell volume is occupied by solvent molecules that are disordered to the point of being impractical to model. Following application of the SQUEEZE routine in PLATON, the residual $R_1$ decreased from 8.4% to 4.5%.

**Keywords:** Z-prime, pseudosymmetry, porous

**MS61.P05**


**X-ray structure-cytotoxicity relationship of the 6-deoxyclitoriacetal derivatives**

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6-Deoxyclitoriacetal (1) has been identified to have a good cytotoxic activity against various types of human carcinoma, possibly due to its ability to intercalate with DNA as evidenced in vitro assay [1]. The sulfonate derivatives of 6-deoxyclitoriacetal were synthesized to enhance its cytotoxic activities as novel anticancers [2,3]. Screening of these compounds for cytotoxic activity has shown that tosylate derivative (4) was more potent and selective than commercial doxorubicin hydrochloride. X-ray structures and their spectroscopic techniques [4].

1. The product of decomposition is a black-colored mixture of BeO and uranyl acetate. I crystallizes in tetragonal crystal system, unit cell parameters: $a = 10.3647$, $c = 23.4127\text{Å}$, $V = 2515.2\text{Å}^3$, $Z = 4$, space group $I4_1/a$, $R_e = 0.0194$ (for 1436 reflections). Each beryllium atom in structure of 1 is tetrahedrally surrounded by four oxygen atoms of water molecules and forms $[\text{Be}(\text{H}_2\text{O})_4]^{2-}$ complex. The crystal-chemical formula (CCF) of this complex is $\text{AM}_2\text{O}_4\text{CO}_3\text{H}_2\text{O}$.

A novel complex compound $[\text{Be}(\text{H}_2\text{O})_3\text{UO}_2\text{CH}_3\text{COO}]_3\text{I}_2$ (I) was synthesized and studied by X-Ray diffraction, IR spectroscopy and thermal analyses. Yellow prismatic crystals of I were obtained by slow evaporation of aqueous solution containing equimolar amounts of beryllium and uranyl acetates. I crystallizes in tetragonal crystal system, unit cell parameters: $a = 10.3647$, $c = 23.4127\text{Å}$, $V = 2515.2\text{Å}^3$, $Z = 4$, space group $I4_1/a$, $R_e = 0.0194$ (for 1436 reflections). Each beryllium atom in structure of I is tetrahedrally surrounded by four oxygen atoms of water molecules and forms $[\text{Be}(\text{H}_2\text{O})_4]^{2-}$ complex. The crystal-chemical formula (CCF) of this complex is $\text{AM}_2\text{O}_4\text{CO}_3\text{H}_2\text{O}$.

Thermal decomposition of I includes three stages. At the first stage (120-140°C) a removal of water molecules takes place. Further heating up to 220°C leads to sequential acetate anions decomposition. The product of decomposition is a black-colored mixture of BeO and UO$_2$.

IR spectrum of I contains uranyl, acetate and water absorption bands. It is in agreement with structure data obtained using single-crystal X-Ray diffraction, IR spectroscopy and thermal analyses. Yellow prismatic crystals of I were obtained by slow evaporation of aqueous solution containing equimolar amounts of beryllium and uranyl acetates. I crystallizes in tetragonal crystal system, unit cell parameters: $a = 10.3647$, $c = 23.4127\text{Å}$, $V = 2515.2\text{Å}^3$, $Z = 4$, space group $I4_1/a$, $R_e = 0.0194$ (for 1436 reflections). Each beryllium atom in structure of I is tetrahedrally surrounded by four oxygen atoms of water molecules and forms $[\text{Be}(\text{H}_2\text{O})_4]^{2-}$ complex. The crystal-chemical formula (CCF) of this complex is $\text{AM}_2\text{O}_4\text{CO}_3\text{H}_2\text{O}$.

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**Keywords:** uranyl, beryllium, acetate

**MS61.P07**


**Synthesis and structure of uranyl complexes with n-butyrate and n-valerate ions**

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A novel complex compound $[\text{Be}(\text{H}_2\text{O})_3\text{UO}_2\text{CH}_3\text{COO}]_3\text{I}_2$ (I) was synthesized and studied by X-Ray diffraction, IR spectroscopy and thermal analyses. Yellow prismatic crystals of I were obtained by slow evaporation of aqueous solution containing equimolar amounts of beryllium and uranyl acetates. I crystallizes in tetragonal crystal system, unit cell parameters: $a = 10.3647$, $c = 23.4127\text{Å}$, $V = 2515.2\text{Å}^3$, $Z = 4$, space group $I4_1/a$, $R_e = 0.0194$ (for 1436 reflections). Each beryllium atom in structure of I is tetrahedrally surrounded by four oxygen atoms of water molecules and forms $[\text{Be}(\text{H}_2\text{O})_4]^{2-}$ complex. The crystal-chemical formula (CCF) of this complex is $\text{AM}_2\text{O}_4\text{CO}_3\text{H}_2\text{O}$.

Thermal decomposition of I includes three stages. At the first stage (120-140°C) a removal of water molecules takes place. Further heating up to 220°C leads to sequential acetate anions decomposition. The product of decomposition is a black-colored mixture of BeO and UO$_2$.

IR spectrum of I contains uranyl, acetate and water absorption bands. It is in agreement with structure data obtained using single-crystal X-Ray diffraction experiment.

**Keywords:** uranyl, beryllium, acetate

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**Keywords:** 6-deoxyclitoriacetal, X-ray structure-cytotoxicity, topoisomerase II

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Poster Sessions

Todate, more than 70 acetate uranyl complexes have been researched, while uranyl complexes with anions of other monocarboxylic acids are considerably less studied. Thus, structure of only one uranyl complex with β-butyrate ligands is determined [1], and there exists no data about U(VI) compounds containing n-butyrate and n-valerate ions. In present research we defined crystal structures of Na₂UO₂(C₆H₅COO)₂·0.25H₂O (I), K₂UO₂(C₂H₅COO)₂ (II) and UO₂(C₆H₅COO)₂·2H₂O (III).

I and II were derived as prismatic yellow crystals while studying the interaction between uranyl nitrate and butyric acid in presence of sodium hydroxide (or potassium hydroxide). Prismatic yellow crystals III were derived as a result of interaction between uranium trioxide and aqueous solution of valeric acid. Fundamental absorption bands of Na₂UO₂·C₆06 (2011) A 222. E-mail: a222@icr.ru

Keywords: uranyl, butyrate, valerate


Keywords: uranyl, butyrate, valerate

MS61.P09

Complexes containing coordination centre OSIC₆X (X = Cl, Br) based on N-organosulfonyl-2-aminoacids

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Complexes with a coordination centre OSICl obtained from N-organosulfonyl-2-aminoacid containing three biologically active moieties (sulphonamide group, the residue of amino acid, and the five-membered O-Si-chelate ring) were studied by x-ray diffraction. Structure of the coordination polyhedron of the silicon atom in these complexes and the influence of crystal packing on their molecular structure were analyzed.

In the case of X=Cl the coordination polyhedron of the silicon atom correspond to a distorted trigonal bipyramid. The deviation of the silicon atom from the plane of equatorial substituents varies in the range from ~0.0408(5) to 0.0809(3) Å (sign “=” means that the Si atom deviates towards the Cl atom). The Si-O bond length depends on the electron-acceptor properties of N-organosulfonylprolin substituent; the smallest value corresponds to the compound I (R = Me), and the largest to the compound 2 (R = Ph). The changes in the interatomic Si...O distances are those for Si-O...Cl bond.

Keywords: uranyl, structure

MS61.P08

Crystal structure of complexes of uranyl chromate with isomers of pyridinecarboxylic acid

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The structures of uranyl sulfate with some isomers of pyridinecarboxylic acid are described in [1, 2]. To investigate the influence of nature of oxoanions on the structure of the complexes, complexation of uranyl chromate with nicotinic and isonicotinic acid in aqueous solutions was studied and new compound with compositions [UO₂CrO₂(C₆H₅NHCOO)H₂O (I) (C₆H₅NHCOO) – piperid-4-carboxylic acid] and [UO₂CrO₂(C₆H₅NHCOO)₂·0.5H₂O (II) (C₆H₅NHCOO) – piperid-3-carboxylic acid] were obtained. The structures of I and II were studied by X-ray diffraction. Both compounds crystallize in the monoclinic crystal system. The unit cell parameters for I: a = 7.5025, b = 11.5188, c = 13.0518 Å, β = 97.877°, V = 1117.3 Å³, space group P2₁/n; Z = 4, R = 0.0263 (3840 reflections); and for II: a = 7.2362, b = 13.8847, c = 10.7204 Å, β = 90.037°, V = 1077.1 Å³, space group P2₁/n, Z = 4, R = 0.0236 (5224 reflections).

The coordination polyhedron of the uranium atom in both structures I and II has the shape of a UO₆ pentagonal bipyramid. In structure I three equatorial oxygen atoms belong to three tridentate chromate ions (T³⁺ type) and another two oxygen atoms belong to two bidentate bridging molecules of isonicotinic acid (B²⁺ type), which occupy trans positions in relation to each other in equatorial plane of uranyl ion. The main structural unit of I is a layer [UO₂CrO₂(C₆H₅NHCOO)] belonging to the AT²B³ crystal chemical group, (A = UO₂, T = CrO₂⁻, B³⁺ = C₆H₅NHCOO molecules). The designations of coordination types and crystal chemical formulas are given in accordance with [3]. Layers are linked in framework by system of hydrogen bonds, which include outer sphere water molecules. In structure II chromate ions also have tridentate coordination and nicotinic acid molecules are bidentate chelate (B²⁺ type). The main structural unit of II is a chain [UO₂CrO₂(C₆H₅NHCOO)], belonging to the AT²B⁰ crystal chemical group, (A = UO₂, T = CrO₂⁻, B⁰ = C₆H₅NHCOO molecules).

Influence of nature of oxoanion and type of isomer on the structure of complexes of uranyl sulfate and chromate with some isomers of pyridinecarboxylic acid was discussed.

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Keywords: uranyl, butyrate, valerate

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