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 43 000 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 *R1* decreased from 8.4% to 4.5%.

Keywords: Z-prime, pseudosymmetry, porous

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

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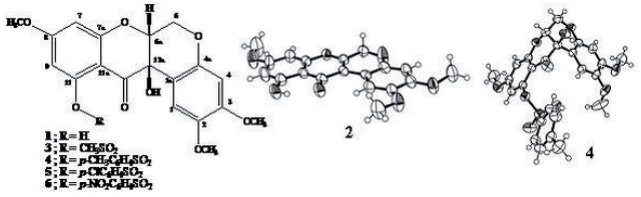
6-Deoxyclitoriacetal **(1)** has been identified to have a good cytotoxic activity against various types of human carcinoma, possibly due to its ability to intercalate with DNA as evidenced *in vitro* assay [1]. The sulfonate derivatives of 6-deoxyclitoriacetal were synthesized to enhance its cytotoxic 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 cytotoxic activities have considerably revealed that not only a bent-shaped structure but also the suitable functional groups at C11 play an important role in increasing their cytotoxicities. Preliminarily, molecular docking of **4** with d(CGATCG)$_2$ revealed that this derivative with a bent shape structure can intercalate between CG base pair, like doxorubicin behavior. Additionally, the sulfonate derivatives were evaluated their ability to inhibit topoisomerase II activity. They had potentially inhibited the topoisomerase II more 70% inhibition. Finally, we studied the DNA-binding affinity, thermal denaturation of 6-deoxyclitoriacetal and its sulfonate derivatives based on UV-Visible spectroscopic techniques [4].



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

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Synthesis, crystal structure and properties of $[Be(H_2O)_4][UO_2(CH_3COO)_3]_2$

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A novel complex compound $[Be(H_2O)][UO_2(CH_3COO)_3]_2$ (I) was synthesized and studied by X-Ray diffraction, IR spectroscopy and thermal analisys. 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 = 23.4127Å, V = 2515.2Å^3, Z = 4, space group $I4_1/a$, R_f = 0.0194 (for 1436 reflections). Each beryllium atom in structure of I is tetrahedrally surrounded by four oxygen atoms of water molecules and forms $[Be(H_2O)_4]^{2+}$ complex. The crystal-chemical formula (CCF) of this complex is AM^1_4 (A = Be^{2+}, $M^1 = H_2O$). CCF is given in accordance with [1]. Uranyl cation forms mononuclear $[UO_2(CH_3COO)_3]^-$ complex with AB^{01}_3 (A = UO_2^{2+}, B^{01} = CH_3COO^-) CCF. Coordination polyhedron of uranium atom is in shape of hexagonal bypiramid. Six oxygen atoms that are located in equatorial plane belong to three acetate groups, which act as bidentate chelate ligands (the B^{01} coordination type).

The $[Be(H_2O)_4]^{2+}$ and $[UO_2(CH_3COO)_3]^-$ in I are bound with each other by electrostatic interactions and hydrogen bonds. The hydrogen bonds are formed by atoms of water molecules and oxygen atoms of acetate groups. There are two crystallographically different H-bonds in I. According to Steiner classification [2], both of them are of moderate strength (the OH···O angles are equal to 175 and 170°, and the O···O distances are equal to 2.60 и 2.67 Å). Meanwhile Voronoi-Dirichlet polyhedron solid angles of the O···O face (expressed as a percentage of 4π steradian) calculated without hydrogen atoms equal 16.6 and 14.9% respectively. This result agrees with previously reported method [3] of H-bonds finding in structures which contain hydrogen atoms, but its coordinates have not been determined.

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 U_3O_8.

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.

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Keywords: uranyl, beryllium, acetate

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

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