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Д.В.Сокольский атындағы «Жанармай,
катализ және электрохимия институты» АҚ

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ИЗВЕСТИЯ

НАЦИОНАЛЬНОЙ АКАДЕМИИ НАУК
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АО «Институт топлива, катализа и
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NAS RK is pleased to announce that News of NAS RK. Series of chemistry and technologies scientific journal has been accepted for indexing in the Emerging Sources Citation Index, a new edition of Web of Science. Content in this index is under consideration by Clarivate Analytics to be accepted in the Science Citation Index Expanded, the Social Sciences Citation Index, and the Arts & Humanities Citation Index. The quality and depth of content Web of Science offers to researchers, authors, publishers, and institutions sets it apart from other research databases. The inclusion of News of NAS RK. Series of chemistry and technologies in the Emerging Sources Citation Index demonstrates our dedication to providing the most relevant and influential content of chemical sciences to our community.

Қазақстан Республикасы Ұлттық ғылым академиясы "ҚР ҰҒА Хабарлары. Химия және технология сериясы" ғылыми журналының Web of Science-тің жаңаланған нұсқасы Emerging Sources Citation Index-те индекстелуге қабылданғанын хабарлайды. Бұл индекстелу барысында Clarivate Analytics компаниясы журналды одан әрі the Science Citation Index Expanded, the Social Sciences Citation Index және the Arts & Humanities Citation Index-ке қабылдау мәселесін қарастыруда. Webof Science зерттеушілер, авторлар, баспашылар мен мекемелерге контент тереңдігі мен сапасын ұсынады. ҚР ҰҒА Хабарлары. Химия және технология сериясы Emerging Sources Citation Index-ке енуі біздің қоғамдастық үшін ең өзекті және беделді химиялық ғылымдар бойынша контентке адалдығымызды білдіреді.

НАН РК сообщает, что научный журнал «Известия НАН РК. Серия химии и технологий» был принят для индексирования в Emerging Sources Citation Index, обновленной версии Web of Science. Содержание в этом индексировании находится в стадии рассмотрения компанией Clarivate Analytics для дальнейшего принятия журнала в the Science Citation Index Expanded, the Social Sciences Citation Index и the Arts & Humanities Citation Index. Web of Science предлагает качество и глубину контента для исследователей, авторов, издателей и учреждений. Включение Известия НАН РК в Emerging Sources Citation Index демонстрирует нашу приверженность к наиболее актуальному и влиятельному контенту по химическим наукам для нашего сообщества.

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NEW SEMIORGANIC IODINE COMPLEX, ITS STRUCTURE AND BIOLOGICAL ACTIVITY

Abstract. The crystal structure of a new coordination compound formed in the tryptophan:NaI:iodine system was examined, and unit cell parameters were determined. A chemical structure of the compound was determined by X-ray diffraction analysis as $C_{11}H_{12}N_2O_2 \bullet (C_{11}H_{13}N_2O_2)^+ \bullet Na^+ \bullet 2H_2O \bullet (I_4)^{2-}$. The coordination compound showed low toxicity and exhibited bactericidal activity against both susceptible and multiresistant strains of bacteria *S. aureus*, *P. aeruginosa*, and *E. coli*.

Keywords: crystal structure, tryptophan, iodine, X-ray diffraction analysis, cytotoxicity, bactericidal activity.

Introduction. In connection with the problem of antibiotic resistance in pathogenic microorganisms, the World Health Organization (WHO) urges the government of WHO member countries and scientists all over the world to intensify the search for new effective drugs that can withstand the spread of drug resistant microorganisms and the diseases caused by them [1].

In a number of promising compounds for the control of drug-resistant pathogens, the semiorganic iodine coordination compounds with biologically active organic ligands and alkali metal halides are among the most perspective [2–5].

For a purposeful search for new iodine coordination compounds with biologically active ligands, it is necessary to study the influence of the ligand nature and structure of coordination compounds on pathogenic microorganisms at the molecular level, and to associate the structure with antimicrobial effectiveness.

It is necessary to find out the mechanism of action of biologically active compounds on pathogenic microorganisms at the molecular level. This formulation of the problem emphasizes the importance of knowledge of atomic structures of compounds. Of all the modern physicochemical methods for studying the atomic structure of molecules, X-ray diffraction analysis (XRD) is the most reliable technique. Starting from the second half of the last century, these XRD data for new compounds are collected in the Cambridge Structural Database [6].

Materials and Methods

Synthesis. 2.000 g of tryptophan, 11 mL of purified water, and 3 ml of hydrochloric acid (18%) were added to a 50 mL beaker. The mixture was stirred with a glass rod until complete dissolution of the amino acid, while heating the beaker on a water bath. The molar ratio of tryptophan: NaI : I_2 was 1:0.5:1. 0.7340 g of sodium iodide, 1.0132 g of iodine, previously crushed in an agate mortar to a fine powder, and 20 mL of ethanol (96%) were added to a 100 mL flask with ground-in stopper. The mixture was stirred until complete dissolution, while heating on a water bath. The sodium triiodide solution was added to the tryptophan solution. The resulting reaction mixture was capped and stirred at room temperature for 5 minutes. The prepared product was kept in a dark place at room temperature. A day later the complex solution was poured into a

crystallizer, a crystallizer with the complex solution was further placed into a desiccator with anhydrous calcium chloride to evaporate the solvent at room temperature. The yield of monocrystals of the complex was 1.95 g (65% of the theoretical).

X-ray diffraction analysis. The purpose of these studies was to determine and refine the crystal structure of the new coordination compound formed in the tryptophan:NaI:iodine system. As a result of crystallization of the synthesized compound, small crystals were formed. To carry out the diffraction experiment, we have managed to find a small crystal sample a in the form of a plate with a size of 0.22x0.10x0.005mm, not very suitable for ensuring high quality diffraction measurements. All diffraction measurements were carried out using Enraf-Nonius CAD4 autodiffractometer (Nederland) (graphite monochromator, Mo-K_α radiation, $\theta/2\theta$ scan, CAD4 software) [7]. The parameters of triclinic unit cell were determined (Table 1) and refined based on 25 reflexes with $10.2 < \theta < 12.9$.

The main fragment of the structure was decoded by a direct method. The coordinates of missing atoms were determined by difference Fourier syntheses of electron density. Due to the presence of heavy atoms in the structure, it was not possible to detect hydrogen atoms by difference Fourier syntheses of electron density. Therefore, the coordinates of hydrogen atoms were determined by geometric calculations and refined using the "rider" model with the following conditions: C-H bond length = 0.96Å, $U_{iso}(H) = 1.5U_{eq}$ (C) for CH_2 groups, CH = 0.93Å, Uiso (H) =1.5Ueq (C) for CH groups, NH = 0.86Å, Uiso (H) = 1.2Ueq (N) for NH groups, NH = 0.89Å, Uiso (H) = 1.2Ueq (N) for NH_3 groups and O- H = 0.86Å, Uiso (H) = 1.2Ueq (O) for water molecules. The structure was refined using full matrix OLS in the anisotropic approximation for non-hydrogen atoms and in the isotropic approximation for hydrogen atoms. All structural calculations were carried out using the SHELXTL [7] and JANA2006 [9] software packages; the purity of structural data was checked using the PLATON software package [10]. According to the obtained structural data, a search was conducted in the Cambridge Structural Database in order to establish the originality of the results or find analogues in the case of their availability. The search indicated that these crystals are original, were not previously obtained and studied, and new crystallographic data in the CIF format were deposited in the Cambridge Crystallographic Data Centre, the deposit number is CCDC 1877292.

The experimental conditions and main crystallographic data are listed in Table 1. According to the results of the calculations performed, the chemical structure of the compound can be represented as $C_{11}H_{12}N_2O_2 \bullet (C_{11}H_{13}N_2O_2)^+ \bullet Na^+ \bullet 2H_2O \bullet (I_4)^{2-}$. Interatomic distances and valent angles in the crystal structure are given in Tables 2 and 3.

Determination of cytotoxicity. *In vitro* cytotoxicity was evaluated using the MTT assay [11].

Determination of *in vitro* antiviral effect of the substances under study. Six concentrations of compound 127 were used to determine the therapeutic activity, starting with 1/2 of the cytotoxic concentration CTC_{50}. To determine the virus-inhibiting activity, three concentrations of the examined substance were used with a dilution factor of 2, starting with the CTC_{50} value. The results of determining virus-inhibiting activity were recorded after 72 hours. The presence or absence of influenza virus in the cell culture was confirmed by the results of the hemagglutination assay [12]. The infectivity titer of residual virus was calculated by the Reed and Mench method [13]. The drug effectiveness was evaluated by the inhibition quotient (*IQ*) [14]. The therapeutic activity of substances against influenza virus was recognized as a result of a decrease in the infectivity titer of residual virus in the hemagglutination assay [12]. All studies were conducted with five replicates.

Studies on antimicrobial activity of iodine coordination compound. The antimicrobial activity of the coordination compound was studied using the twofold serial dilution method in a liquid nutrient medium [15-17].

Test strains. Test strains used in the study were obtained from the American Type Culture Collection (ATCC). The museum susceptible, museum multiresistant, and one clinical test strains were used in the experiment: *S. aureus* ATCC 6538-P (museum susceptible strain); *S. aureus* ATCC-BAA-39 (museum multiresistant strain); *E. coli* ATCC 8739 (museum susceptible strain); *E. coli* ATCC-BAA-196 (museum multiresistant strain); *P. aeruginosa* ATCC 9027 (museum susceptible strain); *P. aeruginosa* TA2 (clinical multiresistant strain).

Results

The independent part of the unit cell contains two molecules of tryptophan $C_{11}H_{12}N_2O_2$, two molecules of water H_2O, sodium cation Na^+, and iodine polyanion $(I_4)^{-2}$. At the same time, one of the

tryptophan molecules is positively charged $(C_{11}H_{13}N_2O_2)^+$ due to the addition of a proton. The negative charge of the polyanion $(I_4)^{-2}$ is compensated by the positive charge of tryptophanium $(C_{11}H_{13}N_2O_2)^+$ and Na^+ cation (Fig. 1). In three-dimensional packing of the crystal structure of the compound $C_{11}H_{12}N_2O_2•(C_{11}H_{13}N_2O_2)^+ •Na^+ •2H_2O •(I_4)^{2-}$, Na^+ cations are octahedrally coordinated by six oxygen atoms, forming infinite tapes in the plane direction [100] (Fig. 2).

At that four oxygen atoms belong to two neighboring tryptophan molecules and the other two to water molecules. In three-dimensional packing, the tapes are connected by hydrogen bonds with with tetraiodide polyanions (Table 4 and Fig. 3).

Table 1 - Crystallographic data for $C_{11}H_{12}N_2O_2•(C_{11}H_{13}N_2O_2)^+•(I_4)^{2-}•Na^+•2H_2O$, determination accuracy is given in parentheses

Crystallographic data for 127	
Formula	$C_{11}H_{12}N_2O_2·(C_{11}H_{13}N_2O_2)^+ · Na^+ ·2H_2O· (I_4)^{-2}$
Molecular weight	976.08
Syngony; Space group	Triclinic, P1
Lattice parameters a, b, c [Å]	5.4298(11), 11.427(2), 13.388(3)
alpha, beta, gamma [deg]	101.58(3), 100.96(3), 93.43(3)
V [Å]^3 ; Z	794.8(3); 1
D(calc)[g/cm^3]; F(000)	2.039; 460
Mu(MoKα) [mm^{-1}]	3.973
Crystal sizes [mm]	0.22x0.10x0.005
Measurements	
Temperature (K); Radiation+ [Å]	293; MoKα; λ=0.71073
$\theta_{min};\theta_{max}$[Deg]	1.6, 30.0
Measuring area	-7≤h≤7; -16≤k≤16; -18≤l≤18
Number of reflexes	7080
Observed data [I > 2.0 sigma(I)]	2408
Refinement	
Number of reflexes, Number of parameters	7080, 363
R, wR^2, S	0.0784, 0.2176, 0.97
w = 1/[\s^2^(Fo^2^)+(0.0349P)^2^+8.8867P] where P=(Fo^2^+2Fc^2^)/3	
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Å^3]	-0.45, 0.41

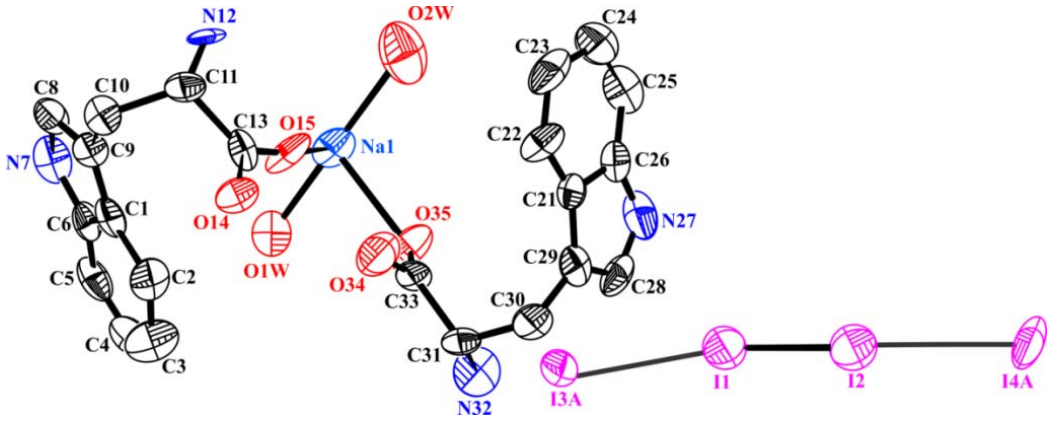


Figure 1 – Model of atomic structure $C_{11}H_{12}N_2O_2•(C_{11}H_{13}N_2O_2)^+ •Na^+ •2H_2O •(I_4)^{2-}$. Ellipsoids of anisotropic thermal oscillations are shown at the 50% probability level, hydrogen atoms and disordered polyanions $(I_4)^{-2}$ are not demonstrated

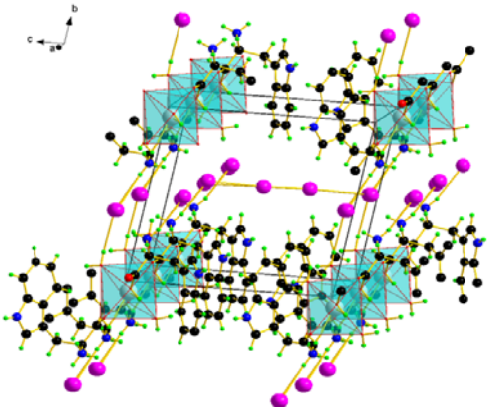


Figure 2- Perspective view of the crystal structure $C_{11}H_{12}N_2O_2 \bullet (C_{11}H_{13}N_2O_2)^+ \bullet Na^+ \bullet 2H_2O \bullet (I_4)^{2-}$

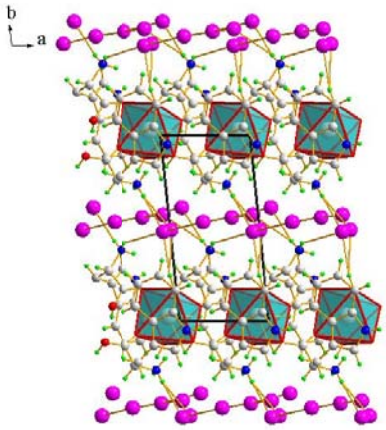


Figure 3 - Projection of the structure $C_{11}H_{12}N_2O_2 \bullet (C_{11}H_{13}N_2O_2)^+ \bullet Na^+ \bullet 2H_2O \bullet (I_4)^{2-}$ on the plane (100)

Table 2- Main interatomic distances in the structure $C_{11}H_{12}N_2O_2 \bullet (C_{11}H_{13}N_2O_2)^+ \bullet Na^+ \bullet 2H_2O \bullet (I_4)^{2-}$

Atoms	Distance (Å)	Atoms	Distance (Å)	Atoms	Distance (Å)
I1-I2	2.762(4)	C4-C5	1.38(5)	C1-C2	1.44(4)
I1-I3A	3.431(4)	I1-I3B	3.444(4)	C1-C6	1.41(3)
I2-I4B	3.628(4)	I2-I4A	3.629(4)	C1-C9	1.42(5)
Na1-O1W	2.30(2)	C5-C6	1.35(4)	C2-C3	1.41(5)
Na1-O2W	2.36(3)	N7-H7	0.8600	C3-C4	1.40(5)
Na1-O35	2.43(2)	C8-C9	1.41(4)	C5-H5	0.9300
Na1-O14_b	2.39(2)	C9-C10	1.45(4)	C8-H8	0.9300
Na1-O15	2.42(2)	C10-C11	1.55(3)	C10-H10A	0.9700
Na1-O34_b	2.34(3)	C11-C13	1.51(3)	C10-H10B	0.9800
O14-C13	1.29(3)	N12-H12B	0.8900	C11-H11	0.9800
O15-C13	1.21(3)	N12-H12C	0.8900	C22-H22	0.9300
O34-C33	1.35(4)	N12-H12A	0.8900	C23-H23	0.9300
O35-C33	1.17(4)	C21-C22	1.34(4)	N32-H32C	0.8900
O1W-H1W2	0.87(11)	C21-C26	1.49(4)	N32-H32B	0.8900
O1W-H1W1	0.86(7)	C21-C29	1.40(5)	C2-H2	0.9300
O2W-H2W1	0.86(17)	C22-C23	1.31(4)	C3-H3	0.9300
O2W-H2W2	0.86(6)	C23-C24	1.47(5)	C4-H4	0.9300
N7-C6	1.37(3)	C24-C25	1.30(5)	C24-H24	0.9300
N7-C8	1.39(4)	C25-C26	1.37(4)	C25-H25	0.9300
N12-C11	1.43(3)	N27-H27	0.8600	C28-H28	0.9200
O14-H14	0.8200	C28-C29	1.37(4)	C30-H30B	0.9700
N27-C28	1.34(4)	C29-C30	1.50(4)	C30-H30A	0.9700
N27-C26	1.36(4)	C30-C31	1.52(3)	C31-H31	0.9800
N32-C31	1.49(4)	C31-C33	1.51(4)		
O34-H34	0.8200	N32-H32A	0.8900		

Table 3 – Main valence angles (degree) in the structure $C_{11}H_{12}N_2O_2$•$(C_{11}H_{13}N_2O_2)^+$ •Na^+ •$2H_2O$ •$(I_4)^{2-}$

Atoms	Angles(deg.)	Atoms	Angles(deg.)	Atoms	Angles(deg.)
O1W-Na1-O2W	174.6(10)	C26-N27-C28	108(2)	C28-C29-C30	129(3)
O1W-Na1-O15	101.5(9)	C33-O34-H34	109.00	C21-C29-C28	108(2)
O1W-Na1-O35	81.3(9)	Na1_a-O34-H34	92.00	C29-C30-C31	114(2)
O1W-Na1-O14_b	92.4(8)	C6-C1-C9	111(2)	N32-C31-C30	110(2)
O1W-Na1-O34_b	88.7(9)	C2-C1-C6	118(3)	N32-C31-C33	110(2)
O2W-Na1-O15	83.8(9)	C2-C1-C9	131(2)	C30-C31-C33	110(2)
O2W-Na1-O35	100.4(10)	C1-C2-C3	117(3)	C31-N32-H32A	109.00
O2W-Na1-O14_b	86.2(9)	C2-C3-C4	121(3)	C31-N32-H32B	109.00
O2W-Na1-O34_b	86.0(9)	C3-C4-C5	120(3)	C31-N32-H32C	109.00
O15-Na1-O35	86.6(8)	C4-C5-C6	120(3)	H32A-N32-H32B	110.00
O14_b-Na1-O15	92.3(8)	N7-C6-C1	106(2)	C25-C24-H24	121.00
O15-Na1-O34_b	168.3(9)	N7-C6-C5	132(2)	C24-C25-H25	119.00
O14_b-Na1-O35	173.2(8)	C1-C6-C5	123(2)	C26-C25-H25	119.00
O34_b-Na1-O35	100.8(9)	C6-N7-H7	125.00	N27-C28-H28	124.00
O14_b-Na1-O34_b	81.4(8)	C8-N7-H7	125.00	C29-C28-H28	124.00
Na1_a-O14-C13	126.2(14)	N7-C8-C9	110(3)	C29-C30-H30A	109.00
Na1-O15-C13	158.8(19)	C8-C9-C10	124(3)	C29-C30-H30B	109.00
Na1_a-O34-C33	145(2)	C1-C9-C8	104(2)	C11-C10-H10B	108.00
Na1-O35-C33	125(2)	C1-C9-C10	133(3)	H10A-C10-H10B	107.00
H1W1-O1W-H1W2	102(10)	C9-C10-C11	117(2)	N12-C11-H11	108.00
Na1-O1W-H1W2	125(8)	N12-C11-C10	111(2)	C10-C11-H11	108.00
Na1-O1W-H1W1	128(5)	N12-C11-C13	109(2)	C13-C11-H11	108.00
Na1-O2W-H2W2	124(6)	C10-C11-C13	112.5(19)	C21-C22-H22	118.00
Na1-O2W-H2W1	123(11)	C11-N12-H12A	110.00	C23-C22-H22	118.00
H2W1-O2W-H2W2	101(15)	C11-N12-H12B	109.00	C22-C23-H23	119.00
C6-N7-C8	110(2)	C11-N12-H12C	110.00	C24-C23-H23	120.00
C13-O14-H14	109.00	H12A-N12-H12B	109.00	C23-C24-H24	121.00
Na1_a-O14-H14	88.00	H12A-N12-H12C	109.00	C31-C30-H30A	109.00
H12B-N12-H12C	109.00	H32A-N32-H32C	110.00	C31-C30-H30B	109.00
O14-C13-O15	127(2)	H32B-N32-H32C	110.00	H30A-C30-H30B	107.00
O15-C13-C11	118(2)	O34-C33-C31	114(2)	N32-C31-H31	109.00
O14-C13-C11	115(2)	O35-C33-C31	122(3)	C30-C31-H31	109.00
C22-C21-C29	140(3)	O34-C33-O35	124(3)	C33-C31-H31	108.00
C22-C21-C26	116(3)	C1-C2-H2	122.00	C28-N27-H27	126.00
C26-C21-C29	104(3)	C3-C2-H2	121.00	C26-N27-H27	126.00
C21-C22-C23	124(3)	C2-C3-H3	120.00	N27-C28-C29	112(2)
C22-C23-C24	120(3)	C4-C3-H3	120.00	C21-C29-C30	123(3)
C23-C24-C25	118(3)	C3-C4-H4	120.00	C9-C8-H8	125.00
C24-C25-C26	122(3)	C5-C4-H4	120.00	C9-C10-H10A	108.00
C21-C26-C25	119(3)	C4-C5-H5	120.00	C9-C10-H10B	108.00
N27-C26-C21	108(3)	C6-C5-H5	120.00	C11-C10-H10A	108.00
N27-C26-C25	133(3)	N7-C8-H8	125.00		

To determine the maximum concentrations that do not have toxic properties, the cytotoxic effect of the coordination compound was studied. Monolayer transplantable cell culture MDCK was used to evaluate the toxicity. The results of the study assessing the cytotoxic effect of the coordination compound on MDCK cell culture are presented in Figure 4.

Table 4- Hydrogen bonds in the structure $C_{11}H_{12}N_2O_2$•$(C_{11}H_{13}N_2O_2)^+$ •Na^+ •$2H_2O$ •$(I_4)^{2-}$

D--H…A	D--H(Å)	H…A(Å)	D…A(Å)	D--H…A(deg.)
O1W--H1W2...I4A	0.87(11)	2.74(11)	3.58(3)	164.00
O1W--H1W2...I4B	0.87(11)	2.90(10)	3.70(3)	153(16)
O2W--H2W1...I3A	0.87(11)	3.085(3)	3.623(3)	122.71(3)
N12--H12B...I4A	0.8900	2.6700	3.56(2)	176.00
N12--H12C...O14	0.8900	2.1000	2.87(2)	145.00
N12--H12A...I3A	0.8900	3.087	3.73(2)	130.95
O14--H14...N12	0.8200	2.2800	2.87(2)	129.00
N32--H32A...O35	0.8900	2.3600	2.70(3)	103.00
N32--H32B...I4A	0.8900	2.9600	3.66(3)	137.00
N32--H32C...I3B	0.8900	2.6076	3.4799(3)	166.75

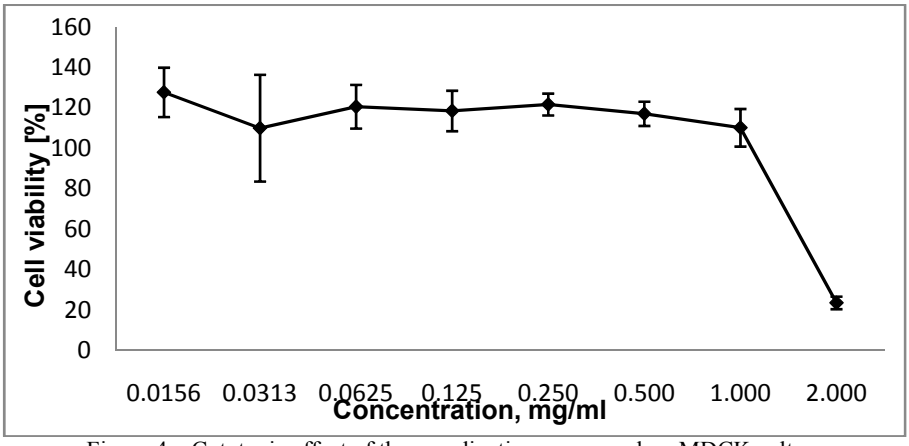


Figure 4 – Cytotoxic effect of the coordination compound on MDCK culture

The toxicity value for the coordination compound was 1.70 mg/mL, which characterizes the examined substance as a low toxic compound.

Antimicrobial activity of iodine coordination compound with tryptophan. The results of testing for antimicrobial activity are presented in Table 5.

Table 5 - Minimum bactericidal concentrations values of the coordination compound, μg/mL

Sample	Test strain	Minimum bactericidal concentrations of the complex, μg/mL
$C_{11}H_{12}N_2O_2$• $(C_{11}H_{13}N_2O_2)^+$ • Na^+•$2H_2O$ •$(I_4)^{2-}$	*S. aureus* ATCC 6538-P	125
	S. aureus ATCC-BAA-33591	125
	E. coli ATCC 8739	250
	E. coli ATCC-BAA 2523	125
	P. aeruginosa ATCC 9027	250
	P. aeruginosa TA 2	250

Discussion of the results. The composition of the semiorganic complex compound formed in the tryptophan-sodium iodide-iodine-water-ethanol system indicates that the system is non-equilibrium. The iodine hydrolysis reaction takes place in it.

$$H_2O + I_2 \rightarrow HI + HOI \quad (1)$$

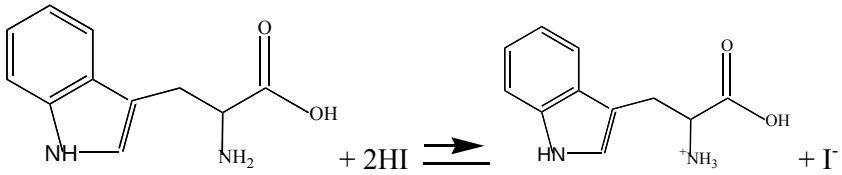
$$2HOI \rightarrow 2HI + O_2\uparrow \quad (2)$$

The resulting hydroiodic acid protonates part of the tryptophan molecules at the nitrogen atom of -NH_2-group.

Therefore, in the equilibria in the tryptophan-NaI-I_2-H_2O-ethanol system, along with the initial components there are protonated tryptophan and triiodide ions, which are formed by the reaction $I_2 + I^- \rightarrow I_3^-$.

As it is shown in Figure 1, Na^+ cation coordinates one tryptophan molecule and one protonated tryptophan molecule (tryptophanium) on the oxygen atoms of the carboxyl groups, as well as two water molecules.

Iodide ions formed during dissociation of sodium iodide and iodide ions of hydroiodic acid form with molecular iodine tetraiodide I_4^{2-}.



(3)

The bond length in the iodine molecule (I1-I2, Table 2) is 2.762 Å, while the bond length of ions I_3^- and I_4^- attached to the molecule is as follows: I1-I3 - 3.431 Å I2-I4 - 3.628 Å. In the polyanion I_4^- a rare case is realized when two iodide anions polarize the electrons of the iodine molecule with the formation of a partially positive charge on each atom

$$I^- \overset{3.431Å}{} I^{\delta+} \overset{2.762Å}{} I^{\delta+} \overset{3.628\ Å}{} I^- \quad (4)$$

As may be seen from the above, the semiorganic complex contains molecular iodine in its structure, which has antimicrobial properties. Its content in the complex is 26 mass% , and the coordination compound is therefore of particular interest due to its potential antimicrobial activity. This compound is effective against both susceptible and resistant strains of *S. aureus* ATCC 6538-P and *S. aureus* ATCC-BAA-33591, value of the minimum bactericidal concentration is 125 μg/mL.

The coordination compound is effective against the susceptible *P. aeruginosa* strain ATCC 9027, as well as the clinical multiresistant of *P. aeruginosa* strain TA2, at a concentration of 250 μg/mL.

The minimum bactericidal concentrations of the compound under testing against the susceptible *E. coli* strain ATCC 8739 and multiresistant *E. coli* strain ATCC-BAA 2523 are 250 μg/mL and 125 μg/mL, respectively. The complex exhibits bactericidal activity against both susceptible and multiresistant bacterial strains.

Conclusion. As follows from the obtained data, a new semiorganic complex $C_{11}H_{12}N_2O_2 \bullet (C_{11}H_{13}N_2O_2)^+ \bullet Na^+ \bullet 2H_2O \bullet (I_4)^{2-}$ has low cytotoxicity, direct antiviral effect, broad-spectrum antimicrobial activity against antibiotic-resistant strains of microorganisms and is therefore promising for further use as an active antimicrobial substance.

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ИОДТЫҢ ЖАҢА ЖЕТІ ОРГАНИКАЛЫҚ КЕШЕНІ, ОНЫҢ ҚҰРЫЛЫМЫ МЕН БИОЛОГИЯЛЫҚ БЕЛСЕНДІЛІГІ

Аннотация. Триптофан:NaI:йод жүйесінде пайда болған жаңа координациялық қосылыстардың кристаллдық құрылымы зерттеліп, элементарлық ұяшық параметрі анықталды. Рентген құрылымдық талдаумен $C_{11}H_{12}N_2O_2 \bullet (C_{11}H_{13}N_2O_2)^+ \bullet (I_4)^{2-} \bullet Na^+ \bullet 2H_2O$ қосылыстарының химиялық құрылымы анықталды. Координациялық қосылыстар аз уыттылықты көрсетіп, *S. Aureus, P. Aeruginosa* и *E. coli* бактерияларының мультирезистенттік штаммдарына да, сезімталдарына да бактерицидтік белсенділігін көрсетті.

УДК 54.022

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НОВЫЙ СЕМИОРГАНИЧЕСКИЙ КОМПЛЕКС ИОДА, ЕГО СТРУКТУРА И БИОЛОГИЧЕСКАЯ АКТИВНОСТЬ

Аннотация. Изучена кристаллическая структура нового координационного соединения, образующиеся в системе триптофан:NaI:йод и определены параметры элементарной ячейки. Рентгеноструктурным анализом установлена химическая структура соединения $C_{11}H_{12}N_2O_2 \bullet (C_{11}H_{13}N_2O_2)^+ \bullet (I_4)^{2-} \bullet Na^+ \bullet 2H_2O$. Координационное соединение показало малую токсичность и проявило бактерицидную активность в отношении как чувствительных, так мультирезистентных штаммов бактерий *S. Aureus, P. Aeruginosa и E. coli*.

Ключевые слова: кристаллическая структура, триптофан, йод, рентгеноструктурный анализ, цитотоксичность, бактерицидная активность

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