

ISSN 2518-1483 (Online),
ISSN 2224-5227 (Print)

2017 • 3

ҚАЗАҚСТАН РЕСПУБЛИКАСЫ
ҰЛТТЫҚ ҒЫЛЫМ АКАДЕМИЯСЫНЫҢ

БАЯНДАМАЛАРЫ

ДОКЛАДЫ

НАЦИОНАЛЬНОЙ АКАДЕМИИ НАУК
РЕСПУБЛИКИ КАЗАХСТАН

REPORTS

OF THE NATIONAL ACADEMY OF SCIENCES
OF THE REPUBLIC OF KAZAKHSTAN

ЖУРНАЛ 1944 ЖЫЛДАН ШЫҒА БАСТАҒАН

ЖУРНАЛ ИЗДАЕТСЯ С 1944 г.

PUBLISHED SINCE 1944



Б а с р е д а к т о р ы
х.ғ.д., проф., ҚР ҰҒА академигі **М.Ж. Жұрынов**

Р е д а к ц и я а л қ а с ы:

Адекенов С.М. проф., академик (Қазақстан) (бас ред. орынбасары)
Боос Э.Г. проф., академик (Қазақстан)
Величкин В.И. проф., корр.-мүшесі (Ресей)
Вольдемар Вуйчик проф. (Польша)
Гончарук В.В. проф., академик (Украина)
Гордиенко А.И. проф., академик (Белорус)
Дука Г. проф., академик (Молдова)
Илолов М.И. проф., академик (Тәжікстан),
Леска Богуслава проф. (Польша),
Локшин В.Н. проф. чл.-корр. (Қазақстан)
Нараев В.Н. проф. (Ресей)
Неклюдов И.М. проф., академик (Украина)
Нур Изура Удзир проф. (Малайзия)
Перни Стефано проф. (Ұлыбритания)
Потапов В.А. проф. (Украина)
Прокопович Полина проф. (Ұлыбритания)
Омбаев А.М. проф. (Қазақстан)
Өтелбаев М.О. проф., академик (Қазақстан)
Садыбеков М.А. проф., корр.-мүшесі (Қазақстан)
Сатаев М.И. проф., корр.-мүшесі (Қазақстан)
Северский И.В. проф., академик (Қазақстан)
Сикорски Марек проф. (Польша)
Рамазанов Т.С. проф., корр.-мүшесі (Қазақстан)
Такибаев Н.Ж. проф., академик (Қазақстан), бас ред. орынбасары
Харин С.Н. проф., академик (Қазақстан)
Чечин Л.М. проф., корр.-мүшесі (Қазақстан)
Харун Парлар проф. (Германия)
Энджун Гао проф. (Қытай)
Эркебаев А.Э. проф., академик (Қырғыстан)

«Қазақстан Республикасы Ұлттық ғылым академиясының баяндамалары»
ISSN 2518-1483 (Online),
ISSN 2224-5227 (Print)

Меншіктенуші: «Қазақстан Республикасының Ұлттық ғылым академиясы» Республикалық қоғамдық бірлестігі (Алматы қ.)
Қазақстан республикасының Мәдениет пен ақпарат министрлігінің Ақпарат және мұрағат комитетінде 01.06.2006 ж.
берілген №5540-Ж мерзімдік басылым тіркеуіне қойылу туралы куәлік

Мерзімділігі: жылына 6 рет.
Тиражы: 2000 дана.

Редакцияның мекенжайы: 050010, Алматы қ., Шевченко көш., 28, 219 бөл., 220, тел.: 272-13-19, 272-13-18,
<http://nauka-nanrk.kz>, reports-science.kz

© Қазақстан Республикасының Ұлттық ғылым академиясы, 2017

Типографияның мекенжайы: «Аруна» ЖК, Алматы қ., Муратбаева көш., 75.

Главный редактор
д.х.н., проф., академик НАН РК **М. Ж. Журинов**

Редакционная коллегия:

Адекенов С.М. проф., академик (Казахстан) (зам. гл. ред.)
Боос Э.Г. проф., академик (Казахстан)
Величкин В.И. проф., чл.-корр. (Россия)
Вольдемар Вуйчик проф. (Польша)
Гончарук В.В. проф., академик (Украина)
Гордиенко А.И. проф., академик (Беларусь)
Дука Г. проф., академик (Молдова)
Илолов М.И. проф., академик (Таджикистан),
Леска Богуслава проф. (Польша),
Локшин В.Н. проф. чл.-корр. (Казахстан)
Нараев В.Н. проф. (Россия)
Неклюдов И.М. проф., академик (Украина)
Нур Изура Удзир проф. (Малайзия)
Перни Стефано проф. (Великобритания)
Потапов В.А. проф. (Украина)
Прокопович Полина проф. (Великобритания)
Омбаев А.М. проф. (Казахстан)
Отелбаев М.О. проф., академик (Казахстан)
Садыбеков М.А. проф., чл.-корр. (Казахстан)
Сатаев М.И. проф., чл.-корр. (Казахстан)
Северский И.В. проф., академик (Казахстан)
Сикорски Марек проф., (Польша)
Рамазанов Т.С. проф., чл.-корр. (Казахстан)
Такибаев Н.Ж. проф., академик (Казахстан), зам. гл. ред.
Харин С.Н. проф., академик (Казахстан)
Чечин Л.М. проф., чл.-корр. (Казахстан)
Харун Парлар проф. (Германия)
Энджун Гао проф. (Китай)
Эркебаев А.Э. проф., академик (Кыргызстан)

Доклады Национальной академии наук Республики Казахстан»

ISSN 2518-1483 (Online),

ISSN 2224-5227 (Print)

Собственник: Республиканское общественное объединение «Национальная академия наук Республики Казахстан» (г. Алматы)

Свидетельство о постановке на учет периодического печатного издания в Комитете информации и архивов Министерства культуры и информации Республики Казахстан №5540-Ж, выданное 01.06.2006 г.

Периодичность: 6 раз в год.

Тираж: 2000 экземпляров

Адрес редакции: 050010, г.Алматы, ул.Шевченко, 28, ком.218-220, тел. 272-13-19, 272-13-18

<http://nauka-nanrk.kz> reports-science.kz

©Национальная академия наук Республики Казахстан, 2017 г.

Адрес типографии: ИП «Аруна», г.Алматы, ул.Муратбаева, 75

E d i t o r i n c h i e fdoctor of chemistry, professor, academician of NAS RK **M.Zh. Zhurinov****E d i t o r i a l b o a r d :****Adekenov S.M.** prof., academician (Kazakhstan) (deputy editor in chief)**Boos E.G.** prof., academician (Kazakhstan)**Velichkin V.I.** prof., corr. member (Russia)**Voitsik Valdemar** prof. (Poland)**Goncharuk V.V.** prof., academician (Ukraine)**Gordiyenko A.I.** prof., academician (Belarus)**Duka G.** prof., academician (Moldova)**Ilov M.I.** prof., academician (Tadjikistan),**Leska Boguslava** prof. (Poland),**Lokshin V.N.** prof., corr. member. (Kazakhstan)**Narayev V.N.** prof. (Russia)**Nekludov I.M.** prof., academician (Ukraine)**Nur Izura Udzir** prof. (Malaysia)**Perni Stephano** prof. (Great Britain)**Potapov V.A.** prof. (Ukraine)**Prokopovich Polina** prof. (Great Britain)**Ombayev A.M.** prof. (Kazakhstan)**Otelbayv M.O.** prof., academician (Kazakhstan)**Sadybekov M.A.** prof., corr. member. (Kazakhstan)**Satayev M.I.** prof., corr. member. (Kazakhstan)**Severskiy I.V.** prof., academician (Kazakhstan)**Sikorski Marek** prof., (Poland)**Ramazanov T.S.** prof., corr. member. (Kazakhstan)**Takibayev N.Zh.** prof., academician (Kazakhstan), deputy editor in chief**Kharin S.N.** prof., academician (Kazakhstan)**Chechin L.M.** prof., corr. member. (Kazakhstan)**Kharun Parlar** prof. (Germany)**Endzhun Gao** prof. (China)**Erkebayev A.Ye.** prof., academician (Kyrgyzstan)**Reports of the National Academy of Sciences of the Republic of Kazakhstan.****ISSN 2224-5227****ISSN 2518-1483 (Online),****ISSN 2224-5227 (Print)**

Owner: RPA "National Academy of Sciences of the Republic of Kazakhstan" (Almaty)

The certificate of registration of a periodic printed publication in the Committee of Information and Archives of the Ministry of Culture and Information of the Republic of Kazakhstan N 5540-Ж, issued 01.06.2006

Periodicity: 6 times a year

Circulation: 2000 copies

Editorial address: 28, Shevchenko str., of.219-220, Almaty, 050010, tel. 272-13-19, 272-13-18,
<http://nauka-nanrk.kz / reports-science.kz>

© National Academy of Sciences of the Republic of Kazakhstan, 2017

Address of printing house: ST "Aruna", 75, Muratbayev str, Almaty

REPORTS OF THE NATIONAL ACADEMY OF SCIENCES
OF THE REPUBLIC OF KAZAKHSTAN

ISSN 2224-5227

Volume 3, Number 313 (2017), 11 – 15

UDC 548.735+548.31+577.112.387.2+ 577.112.37+661.8...35

S. B. Berdibay^{1,2,*}, N. A. Paretskaya², A. N. Sabitov², R. A. Islamov²,
R. A. Tamazyan³, S. Zh. Tokmoldin¹, A. I. Ilin², K. S. Martirosyan⁴

¹K. I. Satpayev Kazakh National Research Technical University, Almaty, Kazakhstan,

²Scientific Center for Anti-Infectious Drugs, Almaty, Kazakhstan,

³The foundation "Research Center for Advanced Technologies", Yerevan, Armenia,

⁴The University of Texas Rio Grande Valley, Texas, USA.

*E-mail: sniper_8888@mail.ru

PHENYLALANINE – IODINE COMPLEX AND ITS STRUCTURE

Abstract. This report describes synthesis and structural characterization of the phenylalanine-iodine complex monocrystal in acetone. Crystals of the substance exhibited a rhombic syngony and were stable at a temperature of 25 °C. As a result, a new compound α, α' -di-amino- β, β' -diphenylpropionic acid monoiodide has been obtained. X-ray diffraction analysis showed that dimers of phenylalanine molecules ($C_{18}H_{23}N_2O_4$) are formed due to hydrogen bonds between the oxygen atoms of carboxyl groups. The hydrogen bonds between the amino groups and iodide form the layers parallel to the (001) plane and these molecular layers are bound to a three-dimensional structure via the van der Waals forces.

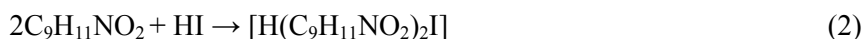
Keywords: phenylalanine, iodine, halogen, hydrogen bonds, amino acid complex with iodine.

Introduction. Iodine, in comparison with other halogens - fluorine, chlorine and bromine, has a number of distinctive properties. First of all, the interatomic distance in the iodine molecule in the solid state is greater than in the gaseous state. This is not observed in either chlorine or bromine. Due to the large size of the iodide anion, the iodide has a small surface charge density, as a result of which the charge distribution can be distorted by the action of certain cations (Li^+ , Mg^{2+} , Fe^{3+} , etc.) and can no longer be regarded as spherically symmetric [1]. In comparison with chlorine and bromine, high iodine polarizability along with low electronegativity makes it possible to form various compounds like charge transfer, donor-acceptor interaction, hydrophobic interaction, hydrogen and halogen bonds [2, 3]. These properties of iodine enable to develop a variety of substances and materials, for example, drugs [2], superconductors [4], nonlinear optical crystals [5]. Iodine forms complex compounds with organic substances and interhalogen compounds, including polyiodides [6-9]. Of particular interest are the compounds of iodine with amino acids [10]. The aim of the study was a synthesis of a complex of phenylalanine and iodine and determination its structure by X-ray diffraction analysis.

Experimental part. Synthesis of the phenylalanine-iodine complex. Acetone (Sigma, USA) and iodine (Reachim, Russia) were mixed in a molar ratio of 34:1 at a temperature of 60-65°C to produce hydrogen iodide:



Then phenylalanine was added and acetone was slowly evaporated. As the acetone evaporates, crystals of black color form for a long time. The obtained crystals had a rhombic syngony and were stable at a temperature of 25°C. The chemical formula of this compound can be represented as: $2C_9H_{11}NO_2 \cdot HI$, and the formation reaction:



X-ray diffraction analysis (XRD). A single-crystal needle-shaped sample of 0.02 x 0.08 x 0.28 mm in size was placed in a glass capillary and fixed with a glass rod. To prevent the destruction of crystals under

the influence of heat and X-rays, diffraction measurements were carried out at low temperatures. Low temperatures on the samples were maintained by a low temperature prefix of the "Enraf-Nonius" firm in pairs of nitrogen with an accuracy of $\pm 1^\circ\text{C}$. Diffraction measurements were carried out at room temperature on an Enraf-Nonius CAD-4 auto-diffractometer (graphite monochromator, Mo- K_α radiation, $\theta/2\theta$ - scanning). The parameters of the rhombic cell are determined and refined by 24 reflections with $12 < \theta < 13$. The absorption was accounted for using the psi-scan method [11]. The structure is deciphered by the direct method. The coordinates of all hydrogen atoms are determined by geometric calculations. The structure is defined by the completely matrix OLS in the anisotropic approximation for non-hydrogen atoms and isotropic for hydrogen atoms. The coordinates of the hydrogen atoms of the NH_3 and OH groups are refined freely, and the coordinates of the remaining hydrogen atoms are refined by the "rider" model with the following conditions: the length of the bonds is $\text{C-H} = 0.98\text{\AA}$, $0.97\text{\AA}$, $0.93\text{\AA}$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for CH , CH_2 and phenyl groups, respectively. All structural calculations were carried out using the SHELXTL program complex [12].

The main crystallographic data and experimental parameters are given in Table 1, and the full crystallographic information of the investigated compound was deposited at the Cambridge structural data bank under the number CCDC 1036670.

Table 1 – Crystallographic data of the complex $2(\text{C}_9\text{H}_{11}\text{NO}_2) \cdot \text{HI}$

Formula	$2(\text{C}_9\text{H}_{11}\text{NO}_2) \cdot \text{HI}$
Molecular weight	458.28
Singonia; Spatial group	Rhombic; $\text{P}2_12_12_1$
Lattice parameters a, b, c [Å]	5.3059(11); 12.265(3); 29.585(6)
alpha, beta, gamma [deg]	90.0; 90.0; 90.0
$V [\text{\AA}]^3$; Z	1925.3(7); 4
$D(\text{calc}) [\text{g}/\text{cm}^3]$; $F(000)$	1.581; 920
$\mu(\text{MoKa}) [\text{mm}^{-1}]$	1.687
Dimensions of the crystal [mm]	0.02 x 0.08 x 0.28
Measuring	
Temperature (K); Radiation [Å]	200; MoKa; $\lambda = 0.71073$
6min; 6max [Deg]	1.4, 30.0
Measurement area	0: 7; -17: 17; 0: 41
Number of reflexes changed, independent, $R(\text{int})$	6498, 5612, 0.048
Observed reflexes [$I > 2.0 \sigma(I)$]	3154
Refinement	
Number of reflexes, Number of parameters	5612, 247
R, wR^2 , S	0.0616, 0.1304, 0.81
Max. and Av. Shift/Error	0.00, 0.00
Flack x	0.00(4)
Min. and Max. Resd. Dens. [$\text{e}/\text{\AA}^3$]	-0.69, 0.85

Results and discussion. The structure of the complex $2(\text{C}_9\text{H}_{11}\text{NO}_2) \cdot \text{HI}$, determined by X-ray diffraction analysis, is shown in Fig. 1. The independent part of the unit cell contains two molecules of phenylalanine ($\text{C}_9\text{H}_{11}\text{NO}_2$), and one anion I^- .

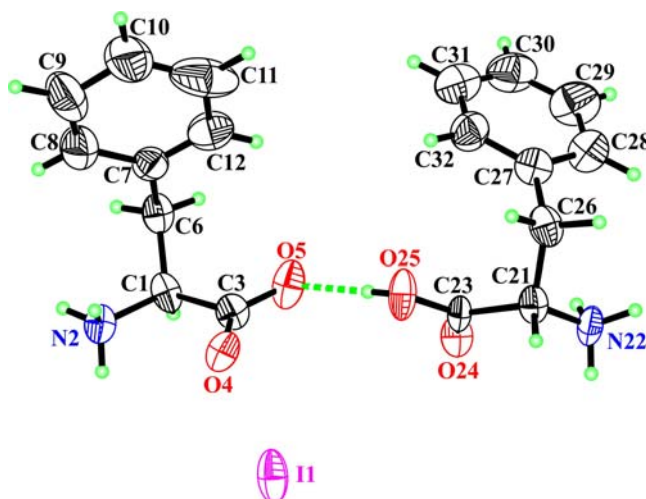


Figure 1 – Atomic model of the structure of $C_{18}H_{23}N_2O_4I$
(ellipsoids of anisotropic thermal oscillations are drawn at the level of 50% probability)

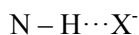
Herewith, two molecules of phenylalanine are bound by the hydrogen bond $O25-H25\cdots O5$ (Table 2) to form a dimer ($C_{18}H_{23}N_2O_4$) (Figure 1).

Table 2 – Hydrogen bonds in structure $2(C_9H_{11}NO_2)\cdot HI$

D	H	A	D-H	H-A	D-A	D-H-A
N2	H2A	O24	0.92(4)	1.87(4)	2.778(7)	168(5)
N2	H2B	I1	0.92(7)	2.81(8)	3.642(6)	151(7)
N2	H2C	I1	0.92(8)	2.79(8)	3.575(6)	144(8)
N22	H22B	O4	0.93(4)	1.83(4)	2.760(7)	173(3)
N22	H22A	I1	0.93(8)	2.77(8)	3.602(6)	149(7)
N22	H22C	I1	0.93(6)	2.75(8)	3.616(6)	158(7)
O25	H25	O5	0.88(9)	1.66(9)	2.423(6)	144(8)

In the three-dimensional packaging of the crystal structure, the dimers ($C_{18}H_{23}N_2O_4$) form an infinite two-dimensional layer parallel to the plane (001) due to the hydrogen bonds between the amino groups and iodide (Figure 2). In the three-dimensional construction of the crystal structure, the interaction between the layers is mainly described by van der Waals forces.

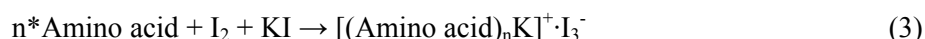
Thus, in the reaction of iodine with phenylalanine in acetone, a complex α,α' -di-amino- β,β' -diphenylpropionic acid monoiodide is formed. Iodine atoms are the acceptors of the hydrogen bond formed with amino groups of phenylalanines of the type:



where, $X = F, Cl, Br$ и I .

The average and normalized length of the hydrogen bond $H\cdots X^-$ is 0.83 and, being less than the mean value 0.873 [13], calculated from known structures, indicates a strong hydrogen bond.

The obtained complex differs from other coordination compounds of iodine with amino acids [10] or other biologically active substances [14] with charge transfer by type:



where, $n \geq 1$.

Iodide promotes the dimerization of phenylalanines, initiating the formation of the hydrogen bond between pairs of amino acid molecules. As it is known, multidimensional structures, formed by hydrogen bonds between biological molecules, play an important role - from metabolic transformations to the realization of genetic information encoded in DNA [15, 16]. The role of halogen ions in the stabilization

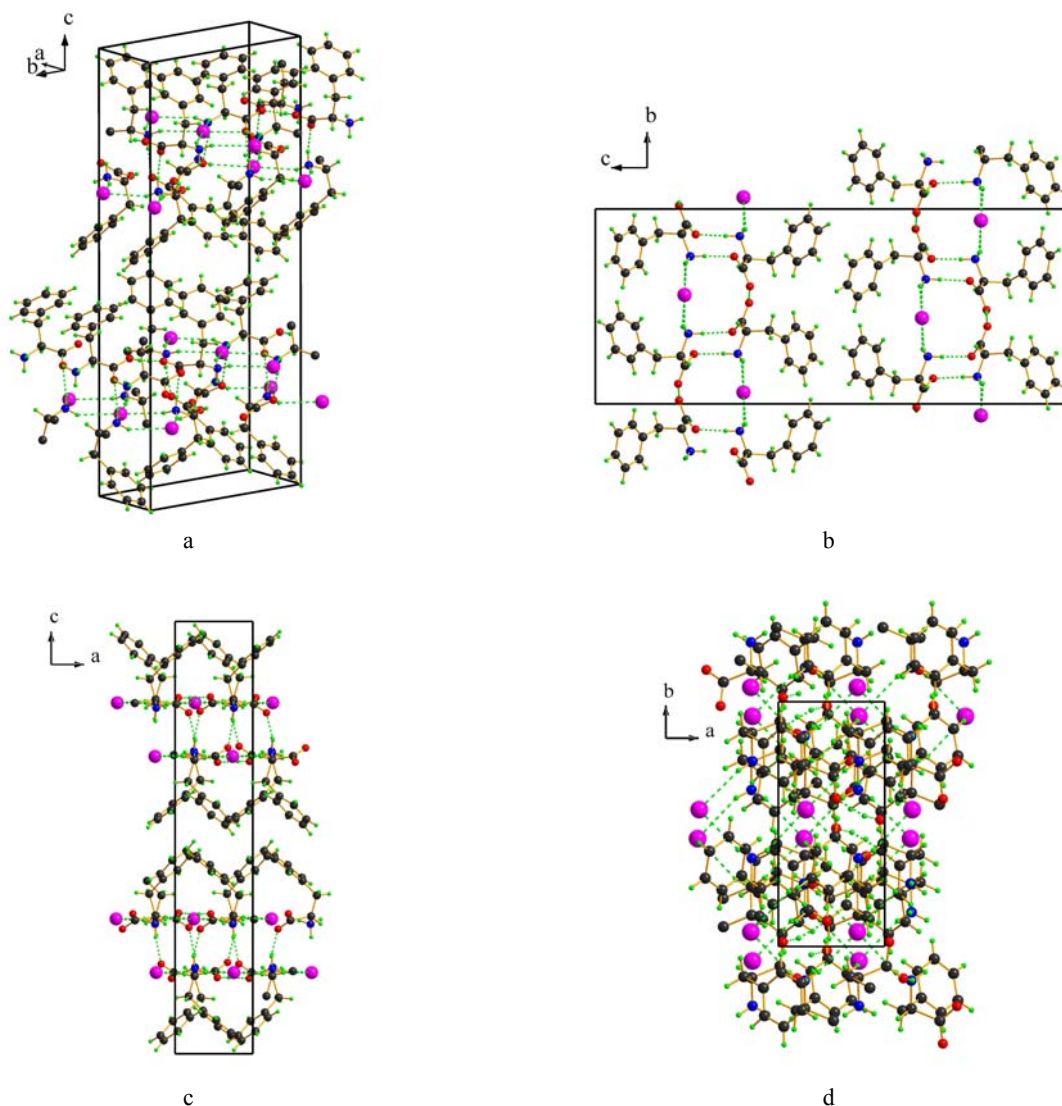


Figure 2 – Crystalline structure $C_{18}H_{23}N_2O_4I$, iodine atoms of magenta colour, carbon - gray, nitrogen - blue, oxygen - red and hydrogen - green, hydrogen bonds are shown in green broken lines:
 (a) - a perspective view of the structure; (b) - the projection of the structure on (100);
 (c) - the projection of the structure on (010); (d) - the projection of the structure on (001)

of the action of the reactive center of enzymes is great. For example, the chlorine anion activates the α -amylase of animals and certain bacteria by forming the hydrogen bond with the amino group of arginine [17]. Similarly, chloride affects cathepsin C [18]. Therefore, interest in halogens as acceptors of the hydrogen bond is very high.

REFERENCES

- [1] Hauskroft K, Konstebl Je. (2002) *Sovremennyy kurs obshhej himii*. Mir, Rossija. ISBN 5-03-003310-6. (In Russian)
- [2] Küpper FC, Feiters MC, Olofsson B, Kaiho T, Yanagida S, Zimmermann MB, Carpenter LJ, Luther GW 3rd, Lu Z, Jonsson M, Kloo L. (2011) Commemorating two centuries of iodine research: an interdisciplinary overview of current research, *Angew Chem Int Ed Engl*, 50:11598-11620. DOI: 10.1002/anie.201100028
- [3] Bartashevich EV, Cirel'son VG. (2014) Vzaimnoe vliyanie nekovalentnyh vzaimodejstvij v kompleksah i kristallah s galogennymi svyazjami, *Uspehi himii*, 83:1181-1203. DOI: 10/RCR4440. (In Russian)
- [4] Mihalache V, Aldica GV, Miu D. (2007) Superconducting properties of iodine-intercalated $Bi_2Sr_2Ca_2Cu_3O_{10+x}$, *J Supercond Nov Magn*, 20:261-272. DOI: 10.1007/s10948-006-0199-y
- [5] Yin Z, Wang QX, Zeng MH. (2012) Iodine release and recovery influence of polyiodide anions on electrical conductivity and nonlinear optical activity in an interdigitated and interpenetrated bipillared-bilayer metal-organic framework, *J Am Chem Soc*, 134:4857-4863. DOI: 10.1021/ja211381e

- [6] Refat MS, Al Didamony H, Abou El-Nour KM, El-Zayat L. (2010) Synthesis and spectroscopic characterization on the tri-iodide charge transfer complex resulted from the interaction between morpholine as donor and iodine sigma-acceptor, *J Saudi Chem Soc*, 14:232-330. DOI: 10.1016/j.jscs.2010.04.004
- [7] Blake AJ, Li WS, Lippolis V, Parsons S, Schröder M. (2007) Extended structures of polyiodide salts of transition metal macrocyclic complexes, *Acta Crystallogr B*, 63:81-92. DOI: 10.1107/S0108768106041668
- [8] Walbaum C, Pantenburg I, Junk P, Deacon GB, Meyer G. (2010) Bulky Cations and Four different Polyiodide Anions in $[\text{Lu}(\text{Db18c6})(\text{H}_2\text{O})_3(\text{thf})_6]_4(\text{I}_3)_2(\text{I}_5)_6(\text{I}_8)(\text{I}_{12})$, *Z Anorg Allg Chem*, 636:1444-1446. DOI: 10.1002/zaac.201000112
- [9] Madhu S, Evans HA, Doan-Nguyen VV, Labram JG, Wu G, Chabinyc ML, Seshadri R, Wudl F. (2016) Infinite polyiodide chains in the pyrroloperylene-iodine complex: insights into the starch-iodine and perylene-iodine complexes, *Angew Chem Int Ed Engl*, 55:8032-8035. DOI: 10.1002/anie.201601585
- [10] Mahmoud KR, Refat MS, Sharshar T, Adam MA, Manaaa El-SA. (2016) Synthesis of amino acid iodine charge transfer complexes in situ methanolic medium: Chemical and physical investigations, *J Mol Liq*, 222:1061-1067. DOI: 10.1016/j.molliq.2016.07.138
- [11] North ACT, Phillips DC, Mathews FS. (1968) *Acta Cryst*, A24:351-359.
- [12] Sheldrick GM. (2008) All programs beginning with SHELX, *Acta Cryst*, A64:112-122
- [13] Brammer L, Bruton EA, Sherwood P. (2001) Understanding the behavior of halogens as hydrogen bond acceptors, *Crystal Growth & Design*, 1:277-290. DOI: 10.1021/cg015522k
- [14] Solanki GK, Amin A, Padhiyar A, Ray AK, Oza AT. (2008) Polaron hopping in some biomolecular solids and their charge transfer complexes, *Indian J Biochem Biophys*, 45:421-429
- [15] Bissantz C, Kuhn B, Stahl M. (2010) A Medicinal Chemist's Guide to Molecular Interactions, *J Med Chem*, 53:5061-5084. DOI: 10.1021/jm100112j
- [16] Scholfield MR, Zanden CMV, Carter M, Ho PS. (2013) Halogen bonding (X-bonding): A biological perspective, *Protein Sci*, 22:139-152. DOI: 10.1002/pro.2201
- [17] Aghajari N, Feller G, Gerday C, Haser R. (2002) Structural basis of α -amylase activation by chloride, *Protein Sci*, 11:1435-1441. DOI: 10.1110/ps.0202602
- [18] Cigic B, Pain RH. (1999) Location of the binding site for chloride ion activation of cathepsin C, *Eur J Biochem*, 264:944-951

С. Б. Бердібай^{1,2}, Н. А. Парецкая², А. Н. Сабитов², Р. А. Исламов²,
Р. А. Тамазян³, С. Ж. Токмолдин¹, А. И. Ильин², К. С. Мартirosян⁴

¹Қ. И. Сәтбаев атындағы Қазақ ұлттық техникалық зерттеу университеті, Алматы, Қазақстан,

²Инфекцияға қарсы препараттар ғылыми орталығы, Алматы, Қазақстан,

³Перспективалық технологиялар зерттеу орталығы фонды, Ереван, Армения,

⁴The University of Texas Rio Grande Valley, Texas, USA

ИОД ЖӘНЕ ОНЫҢ ҚҰРЫЛЫМЫМЕН ФЕНИЛАЛАЛИННІҢ КЕШЕНДІ КОМПЛЕКСІ

Аннотация. Мақалада ацетонда фенилаланин-иод кешенінің монокристаллды алу және синтезі сипатталады. Заттың кристаллы ромбылық сингониясы болды және 25 °C температурада тұрақты болды. Нәтижесінде α, α' -ди-амино- β, β' -моноиодид дифенилпропиониды қышқылының жаңа қосылысы алынды. Рентгендік құрылымдық зерттеулерімен фенилаланиннің молекула диметрлері ($\text{C}_{18}\text{H}_{23}\text{N}_2\text{O}_4$) карбоксил топтарының оттегі атомдар арасындағы сутектік байланыс салдарынан пайда болатынын көрсетті. Амин топтары мен иодид арасындағы сутектік байланыс параллель жазықтық қатпары пайда болып, осы молекулалар қатпарлары Ван-дер-Ваальс арқылы үш өлшемді құрылысын байланыстырады.

Түйін сөздер: фенилаланин, иод, галоген, сутектік байланыстар, иодпен амин қышқылы кешені.

С. Б. Бердібай^{1,2,*}, Н. А. Парецкая², А. Н. Сабитов², Р. А. Исламов²,
Р. А. Тамазян³, С. Ж. Токмолдин¹, А. И. Ильин², К. С. Мартirosян⁴

¹Казахский национальный исследовательский технический университет им. К. И. Сатпаева, Алматы, Казахстан,

²Научный центр противоинфекционных препаратов, Алматы, Казахстан,

³Фонд «Центр исследования перспективных технологий», Ереван, Армения,

⁴The University of Texas Rio Grande Valley, USA

КОМПЛЕКС ФЕНИЛАЛАНИНА С ИОДОМ И ЕГО СТРУКТУРА

Аннотация. В статье описывается синтез и структурный анализ монокристалла комплекса фенилаланин-иод в ацетоне. Кристаллы вещества имели ромбическую сингонию и были стабильны при температуре 25 °C. В результате получено новое соединение α, α' -ди-амино- β, β' -дифенилпропионовой кислоты моноиодид. Рентгенструктурными исследованиями показано, что димеры молекул фенилаланина ($\text{C}_{18}\text{H}_{23}\text{N}_2\text{O}_4$) образуются за счёт водородных связей между атомами кислорода карбоксильных групп. Водородные связи между аминогруппами и иодидом образуют слои параллельно плоскости (001) и эти слои молекул связываются в трехмерную постройку силами Ван-дер-Ваальса.

Ключевые слова: фенилаланин, иод, галоген, водородные связи, комплекс аминокислоты с иодом.

CONTENT

<i>Berdibay S.B., Paretskaya N.A., Sabitov A.N., Islamov R.A., Tamazyan R.A., Tokmoldin S.Zh., Ilin A.I., Martirosyan K.S.</i> Phenylalanine – iodine complex and its structure.....	11
<i>Ruzuddinov S., Amiraev U.A., Karkabayeva K.U., Tuhvatshin R.R.</i> Change in cellular and humoral immunity in patients with metallic dentures.....	16
<i>Kabyshv A.M., Kuterbekov K.A., Penionzhkevich Yu.E., Maslov V.A., Mendibayev K., Sobolev Yu.G., Lukyanov S.M., Kabdrakhimova G.D., Aznabayev D.T., Kurmanzhanov A.T.</i> Errors in the total reaction cross sections and energies of incident particles measured using modified transmission technique.....	20
<i>Berdenova B., Kaltayev A.</i> Review of adsorption and thermal characteristics of activated carbon and its application in ang storage and acs systems.....	28
<i>Sotnikov Y.V., Ibraimov V.M.</i> Calculated water demand as the main factor influencing the reliability of hydrogeological forecasts at the evaluation of groundwater elastic reserves..	39
<i>Batpenov N., Ospanov K., Jaxybekova G.</i> Endoprosthesis replacement in deforming arthrosis of the hip joint.....	47
<i>Koigeldina A., Nikolova A., Vassilev A.</i> Drought-induced acclimation changes in young castor (<i>Ricinus communis</i> L.) plants.....	56

Publication Ethics and Publication Malpractice in the journals of the National Academy of Sciences of the Republic of Kazakhstan

For information on Ethics in publishing and Ethical guidelines for journal publication see <http://www.elsevier.com/publishingethics> and <http://www.elsevier.com/journal-authors/ethics>.

Submission of an article to the National Academy of Sciences of the Republic of Kazakhstan implies that the work described has not been published previously (except in the form of an abstract or as part of a published lecture or academic thesis or as an electronic preprint, see <http://www.elsevier.com/postingpolicy>), that it is not under consideration for publication elsewhere, that its publication is approved by all authors and tacitly or explicitly by the responsible authorities where the work was carried out, and that, if accepted, it will not be published elsewhere in the same form, in English or in any other language, including electronically without the written consent of the copyright-holder. In particular, translations into English of papers already published in another language are not accepted.

No other forms of scientific misconduct are allowed, such as plagiarism, falsification, fraudulent data, incorrect interpretation of other works, incorrect citations, etc. The National Academy of Sciences of the Republic of Kazakhstan follows the Code of Conduct of the Committee on Publication Ethics (COPE), and follows the COPE Flowcharts for Resolving Cases of Suspected Misconduct (http://publicationethics.org/files/u2/New_Code.pdf). To verify originality, your article may be checked by the originality detection service Cross Check <http://www.elsevier.com/editors/plagdetect>.

The authors are obliged to participate in peer review process and be ready to provide corrections, clarifications, retractions and apologies when needed. All authors of a paper should have significantly contributed to the research.

The reviewers should provide objective judgments and should point out relevant published works which are not yet cited. Reviewed articles should be treated confidentially. The reviewers will be chosen in such a way that there is no conflict of interests with respect to the research, the authors and/or the research funders.

The editors have complete responsibility and authority to reject or accept a paper, and they will only accept a paper when reasonably certain. They will preserve anonymity of reviewers and promote publication of corrections, clarifications, retractions and apologies when needed. The acceptance of a paper automatically implies the copyright transfer to the National Academy of sciences of the Republic of Kazakhstan.

The Editorial Board of the National Academy of sciences of the Republic of Kazakhstan will monitor and safeguard publishing ethics.

Правила оформления статьи для публикации в журнале смотреть на сайте:

www.nauka-nanrk.kz

ISSN 2518-1483 (Online), ISSN 2224-5227 (Print)

<http://www.reports-science.kz/index.php/ru/>

Редакторы М. С. Ахметова, Д. С. Аленов, Т.А. Апендиев
Верстка на компьютере А.М. Кульгинбаевой

Подписано в печать 01.06.2017.
Формат 60x881/8. Бумага офсетная. Печать – ризограф.
4,0 п.л. Тираж 2000. Заказ 3.