

**O‘ZBEKISTON RESPUBLIKASI OLIY VA O‘RTA MAXSUS
TA‘LIM VAZIRLIGI**

BUXORO DAVLAT UNIVERSITETI

**“KOORDINATSION BIRIKMALAR KIMYOSINING
HOZIRGI ZAMON MUAMMOLARI”
MAVZUSIDA XALQARO ILMIY-AMALIY
KONFERENSIYA
MATERIALLARI TO‘PLAMI**



**2022-yil 22-23-dekabr
Buxoro**

**МИНИСТЕРСТВО ВЫСШЕГО И СРЕДНЕГО
СПЕЦИАЛЬНОГО ОБРАЗОВАНИЯ РЕСПУБЛИКИ
УЗБЕКИСТАН**

БУХАРСКИЙ ГОСУДАРСТВЕННЫЙ УНИВЕРСИТЕТ

**«СОВРЕМЕННЫЕ ПРОБЛЕМЫ ХИМИИ
КООРДИНАЦИОННЫХ СОЕДИНЕНИЙ»**

Материалы международной научно-практической
конференции



22-23 декабря 2022 г.
г. Бухара, Республика Узбекистан

**MINISTRY OF HIGHER AND SECONDARY SPECIAL
EDUCATION OF THE REPUBLIC OF UZBEKISTAN**

BUKHARA STATE UNIVERSITY

**INTERNATIONAL SCIENTIFIC AND PRACTICAL
CONFERENCE ON
"CURRENT PROBLEMS OF THE CHEMISTRY OF
COORDINATION COMPOUNDS"**



**22-23-december
Bukhara, Uzbekistan – 2022**

“Koordinatsion birikmalar kimyosining hozirgi zamon muammolari” mavzusida xalqaro ilmiy-amaliy anjumani materiallari. Buxoro – 2022. - 734 bet

Buxoro davlat universitetida O'zbekiston Respublikasi Vazirlar Mahkamasining 2022 yil 7 martdagi 101-f-sonli farmoyishi bilan tasdiqlangan O'zbekiston Respublikasida 2022 yilda xalqaro va respublika miqyosida o'tkaziladigan ilmiy va ilmiy-texnik tadbirlar rejasida belgilangan tadbirlarning bajarilishi maqsadida 2022 yil 22-23 dekabr kunlari **“Koordinatsion birikmalar kimyosining hozirgi zamon muammolari”** mavzusidagi xalqaro ilmiy-amaliy anjumani bo'lib o'tadi.

Mas`ul muharrir:

Umarov Baqo Bafayevich – kimyo fanlari doktori, professor

Tahrir hayati:

O`M. Mardonov, M.Ya. Ergashov, H.T. Avezov, N.G. Sevinchov, E.D. Niyozov, Q.G`Avezov, M.A. Tursunov, S.F. Abduraxmonov, Z.A. Sulaymonova, F.M. Nurutdinova, D.A. Hazratova, Sh.Sh. Xudoyberdiyev, Z.K. Qodirova, E.A. Xudoyorova, D.B. Mutalipova, G.Q. Xoliqova, S.A. Karomatov

Maqolalarni to'plovchi va nashrga tayyorlovchilar Organik va fizkolloid kimyo kafedrasini mudiri, k.f.f.d. S.F. Abduraxmonov, kafedra o`qituvchisi B.Sh. Ganiyev.

Ushbu xalqaro ilmiy-amaliy konferensiya materiallari to'plamiga bakalavr va magistrantlar, ilmiy tadqiqot ishlarini olib borayotgan izlanuvchi va tadqiqotchilar, katta ilmiy xodim-izlanuvchilar, ilmiy-tadqiqot institutlari olimlari va oliy o'quv yurtlari professor-o'qituvchilari hamda kimyo sohalari xususan koordinatsion birikmalar kimyosi sohasida tadqiqot olib borayotgan mutaxassislarning ilmiy ishlari kiritilgan.

Mazkur to'plamga kiritilgan materiallarning mazmuni, undagi statistik ma'lumotlar va me'yoriy hujjatlar sanasining to'g'riligiga hamda tanqidiy fikr mulohazalarga mualliflarning o'zlari mas'uldir.

“Koordinatsion birikmalar kimyosining hozirgi zamon muammolari”

“Koordinatsion birikmalar kimyosining hozirgi zamon muammolari” mavzusidagi xalqaro ilmiy-amaliy anjumanining tashkiliy va dasturiy qo‘mita a‘zolari

Obidjon Xafizovich Xamidov	Buxoro davlat universiteti rektori, i.f.d., prof.
To‘lqin Husenovich Rasulov	Buxoro davlat universiteti ilmiy ishlar va innovatsiyalar bo‘yicha prorektori, f-m.f.d., prof.
Abdulahat Turobovich Djalilov	TKTITI direktori, k.f.d., akademik.
Sayyora Shrofovna Rashidova	O‘zR FA Polimerlar kimyosi va fizikasi instituti direktori, k.f.d., akademik.
Abbasxan Sobirxanovich To‘rayev	O‘zR FA BKI direktori, k.f.d., akademik.
Baxtiyor Sobirjonovich Zokirov	O‘zR FA UNKI professori, k.f.d., akademik.
Quvondiq Sanoqulovich Sanoqulov	NKMK direktori, t.f.d., prof.
Aziz Baxtiyarovich Ibragimov	O‘zR FA UNKI direktor o‘rinbosari, k.f.d., prof.
Shaxnoza Abduxalilovna Kadirova	O‘zMU Kimyo fakulteti dekani, k.f.d., prof.
Sergey Zubarovich Vatsadze	M.V. Lomonosov nomidagi MDU professori, k.f.d., prof.
Vadim Viktorovich Minin	Rossiya FA N.S. Kurnakov nomidagi UNKI yetakchi ilmiy xodimi, k.f.d., prof.
Vadim Vitalievich Negrebetsky	N.I.Pirogov nomidagi Rossiya MTTU Kimyo kafedrası mudiri, k.f.d., prof.
Suriya Irekovna Gilmanshina	Qozon federal universiteti professori, p.f.d., prof.
Savash Kaya	Sivas davlat universiteti professori
Mohd Nadeem Bukhari	Handwara davlat kolleji, PhD, associate professor.
Xamdani Ikromovich Akbarov	O‘zMU professori, k.f.d., prof.
Abdullo Murodovich Nasimov	SamDU professori, k.f.d., prof.
Xayit Xudonazarovich To‘rayev	TerDU Kimyo fakulteti dekani, k.f.d., prof.
Shaxobiddin Xasanboyevich Avdullayev	ADU professori, k.f.d., prof.
Shavkat Vohidovich Avdullayev	NamDU professori, k.f.d., prof.
Zuxra Chingizovna Kadirova	O‘zbekiston – Yaponiya yoshlar innovatsiya markazi, k.f.d., prof.
Olim Ruzimuradov	Toshkent shahridagi Turin politexnika universiteti professori, k.f.d., prof.
Jamshid Mengnorovich Ashurov	O‘zR FA BKI yetakchi ilmiy xodimi, k.f.d., prof.
Baqo Bafoevich Umarov	BuxDU professori, k.f.d., prof.
Muxtar Raxmatovich Amonov	BuxDU professori, t.f.d., prof.
MansurYarashevich Ergashev	BuxDU professori, k.f.n., prof.
Murod Amonovich Tursunov	BuxDU O‘quv-uslubiy departament boshlig‘i, k.f.f.d., PhD, dots.
Erkin Dilmurodovich Niyozov	BuxDU Tabiiy fanlar fakulteti dekani, t.f.n., dots.
O‘ktam Mardonovich Mardonov	BuxDU dotsenti, k.f.n., dots.
Hasan Tillayevich Avezov	BuxDU dotsenti, k.f.n., dots.
Qahramon Shayimovich Husenov	NDKTU dotsenti, k.f.n., dots.
Nemat Gulboyevich Sevinchov	BuxDU dotsenti, k.f.n., dots.
Qozoqmurod Asadovich Ravshanov	BuxDU dotsenti, k.f.n., dots.
Hasan Qalandarovich Razzoqov	BuxDU dotsenti, t.f.n., dots.
Sayfullo Ibodulloevich Nazarov	BuxDU Umumiy va noorganik kimyo kafedrası mudiri, t.f.n., dots.
Sayfiddin Fayzullayevich Abduraxmonov	BuxDU Organik va fizkolloid kimyo kafedrası mudiri, k.f.f.d., PhD.
Quvondiq G‘iyosovich Avezov	BuxDU dotsenti, k.f.f.d., PhD, dots.
Gulbahor Akiyevna Xudonazarova	BuxDU dotsenti, k.f.n., dots.
Muzaffar Samandarovich Sharipov	BuxDU dotsenti, n.f.n., dots.
Shuxrat Shamsiddinovich Xudoyberdiyev	BuxDU dotsenti, k.f.f.d., PhD.

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UDK 546.302+ 547.466 + 547.415.1

SYNTHESIS AND PHYSICO-CHEMICAL PROPERTIES OF BENZOIC ACID DERIVATIVES WITH 3d-METALS WITH MIXED LIGAND COMPLEXES

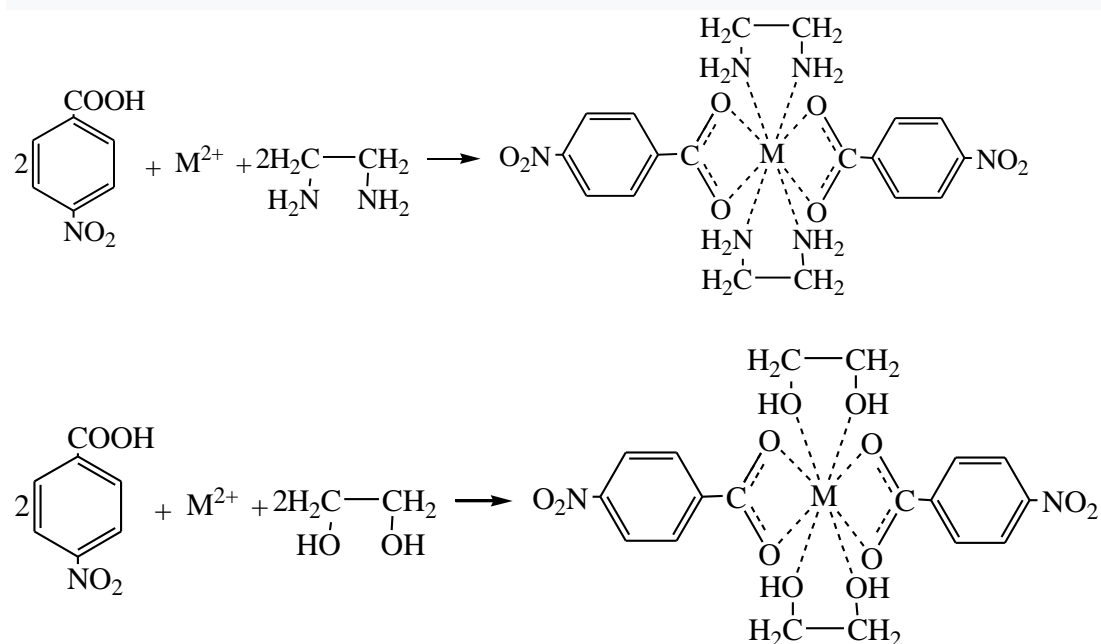
Tursunov M.A., professor, Boltayev R.O'., student
Bukhara State University

Abstract: In this article, the structure and properties of complex compounds with mixed ligands of Ni(II), Cu(II), Zn(II) ions from various 3d metals based on benzoic acid derivatives were studied using modern physical and chemical research methods. Complex formation properties, geometry and physicochemical properties of various mono- and bidentate ligands obtained were studied.

Key words: benzoic acid, benzoic acid derivatives, mixed ligand, monodentate ligand, bidentate ligand, complex compound, infrared spectroscopy, symmetric and asymmetric vibrational frequency, valence vibration, quantum chemical calculation, molecular orbital, relaxation molecular orbital energy.

Today, chemical scientists are interested in the synthesis and research of complex compounds of intermediate 3d metals such as Ni(II), Cu(II), Zn(II) with para-nitrobenzoic acid with mixed ligands such as diethylamine or ethanediol. Because such substances are widely used as fungicides, biocatalysts, medicinal substances in medicine, antimicrobial agents and plant growth stimulants, biologically active substances in agriculture. Intermediate metal ions researchers are paying attention to researching the dependence of centers of formation of complexes with ligands, energy parameters, electron density and coordination with 3d-central ion on various factors.

The reaction scheme for the formation of a complex compound can be expressed as follows:



M=Ni(II), Cu(II), Zn(II).

As a result of determining the "composition-structure-property" system in complex compounds, it is possible to predict the composition and properties of complex compounds, as well as the structure and electron distribution of the molecule. Based on this information, it is possible to

“Koordinatsion birikmalar kimyosining hozirgi zamon muammolari”

draw preliminary conclusions and plan the synthesis of complex compounds. Quantum-chemical calculations of the synthesized complexes were carried out.

The coordination of monodentate and diethylamine or ethanediols through nitrogen and oxygen atoms was determined through the oxygen of the carboxyl group of para-Nitrobenzoic acid.

According to the results of the chemical analysis of the complex compound, it was determined that the metal ion is a substance with a unique complex composition consisting of molecules of a double core, mixed ligand (anions of para-nitrobenzoic acid and dimethyl amine or ethanediol). Also, in order to study the method of coordination of ligands in each inner and outer sphere and the surrounding of the central ion, the IR-spectrum of the ligands in the complex and free state was compared and studied. The IR spectrum has the following absorption lines (cm⁻¹): 3090 (C-H, Ar), 2510–2995 (OH), 1660-1690 (C=O), 1600, 1575 (Ar), 1515, 1340 (para-NO₂), 1290 (C-O, COOH). Absorption lines (1525, 1350 cm⁻¹) characteristic of the valence vibrations of the nitro group in the ligand were shifted to a lower frequency region (1515, 1340 cm⁻¹) in the obtained complex, and absorption lines in the region 1660-1690 cm⁻¹ belonging to the C–O group are not present in the spectrum of the complex compound.

In the molecular orbitals of the complex compound (para-nitrobenzoic acid) (8) the share of r-orbitals of oxygen atoms is 36.12% and 37.03%, respectively. It was found that in the second band MO ($E_{\text{HOMO}-1} = -6.6$ eV) the share of d-electrons of Ni(II) atoms is large (54.92%). However, the second empty MO ($E_{\text{LUMO}+1} = -3.12$ eV) is composed mainly of the relaxation orbitals of the para-nitrobenzoic acid molecule. The analysis of the energy of the frontier molecular orbitals and the electron density of states diagram showed that the energy of the lower relaxing molecular orbitals and the energy gap are very small. The lower relaxing molecular orbital energy has a small value (-3.98 eV), which indicates that the complex has a high electron affinity and the molecule is prone to nucleophilic reactions.

In the charge distribution of atoms in the para-nitrobenzoic acid, dimethylamine and copper(II) complex, we can see that the lowest negative charges are localized in the carboxylate group of oxygen atoms, and the highest positive charge is localized in carbon atoms. At the same time, the negative charge on the oxygen atoms of the carboxylate group is 0.38-0.42 units, and the nitrogen group attached to the carbon of the aromatic ring in the para position has a negative charge of 0.34 units. Considering the para-nitrobenzoic acid molecule as a ligand, the coordination capabilities of the oxygen of the carboxyl group are higher compared to the competing oxygen atoms of the -NO₂ group, and coordination is carried out at the expense of -COO⁻.

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xalqaro ilmiy-amaliy anjumani materiallari

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МУАЛЛИФЛАР КЎРСАТКИЧИ

A		B	
Abdisamatov E.D.	662	Babaev B.N.	80, 152
Abdisamatova O.A.	662	Babamuratov B.E.	333
Abdugalilova S.A.	689	Babayev B.N.	101, 144, 180
Abdukarimov A.G'.	354	Baqoyeva M.A.	353
Abdukarimova D.N.	403	Barkamoljon V.	525
Abdulazizov A.A.	523	Batirbay Torambetov	54
Abdullajonov X.	667	Baxriddinov A.X.	202
Abdullayev A.X.,	78	Bazarov A.A.	525, 680
Abdullayeva N.S.	214	Bazarov A.A.	526
Abdulxafizov G'.A.	212	Bekchanov D.	532
Abdunazarov A.A.	523	Bekchanov D.J.	554
Abdunazzarov A.T.	380	Beknazarov H.S.	353
Abduraximov A.A.	664	Beknazarov X.S.	477
Abduraxmonov S.F. 16, 18, 83, 84, 124, 208, 515		Berdiyev J.O'.	416
Abduraxmonov S.T.	544	Bobilova Ch.H.	273
Abduraxmonova T.	359	Bobojon O.S.	512
Abduraxmonova T.R.	696	Boltaboyev Z.Z.	388
Abdusharipova O.S.	360	Boltaeva Z.A.	81
Abjalov A.	631	Boltayev R.O'	280
Ahrorova D.,	655	Boltayev R.O'.	286
Akbarov X.I.	162	Botirova S.A.	133, 213
Akramjonov A.A.	550		
Akramov M.	438, 440	C	
Alieva G.K.	169	Chalaboyeva Z.M	111
Alikabulova H.	631	Садуллаева С.А.	191
Alikulov R.V.	474	Сиддикова К.Т.	219
Alimova N.M.	736		
Aliqulov R.V.	477	D	
Aliyev S.G.	267	Daminbek Ziyatov	54
Aliyeva F.A.	483	Davlatboyev M.O.	224
Aminjonov J.	440	Davronbekov A.A.	380
Aminova H.S.	124, 208	Djalilov A.T.	333, 467
Amirov A.O'.	529	Dmitry Tarasenko	11
Amrilloev A.A.	652	Do'smatova A.D.	656
Asadov J.I.	83, 515	Doniyorov K.A.	133, 213
Asgerova Z.G.	265		
Ashurov J.M.	81, 96, 164, 224	E	
Askarova G.A.	362	Ergashev I.M.	678
Aslanov A.Q.	131	Ergashev M.I.	303
Aslonova F.S.	356	Ergashev N.A.	547
Asrorova Z.	631	Ergashev Q.X.	162
Atoeva M.O.	251	Ergasheva M.I.	685
Avezov H.T.	229, 231	Ergasheva M.J.	662
Axmedov O'.Ch.	429, 431	Ergasheva Z.B.	685
Axmedova N.X.	432, 680	Ergashov M.Y.	90
Aziz Atashov	54	Ergashova Sh.I.	678
Azizjanov X.M.	14		



O‘ZBEKISTON RESPUBLIKASI OLIY VA O‘RTA MAXSUS TA‘LIM VAZIRLIGI
BUXORO DAVLAT UNIVERSITETI REKTORINING
BUYRUG‘I

2022-yil “ 21 ” dekabr

№ 578-U

Buxoro sh.

Ilmiy-amaliy anjuman
o‘tkazish to‘g‘risida

O‘zbekiston Respublikasi Vazirlar Mahkamasining 2022-yil 7-martdagi 101-F-sonli Farmoyishi hamda Oliy va o‘rta maxsus talim vazirligining 2022-yil 14-martdagi 97-sonli buyrug‘i asosida universitetda 2022-yil 23-24-dekabr kunlari **“Zamonaviy koordinatsion birikmalar kimyosining muammolari”** mavzusida xalqaro miqyosidagi ilmiy-amaliy anjumanni o‘tkazish maqsadida

BUYURAMAN:

1. Quyidagi tarkibdan iborat dasturiy qo‘mita tuzilsin:

1.	O.X. Xamidov	–	Universitet rektori, rais;
2.	T.H. Rasulov	–	Ilmiy ishlar va innovatsiyalar bo‘yicha prorektor, rais muovini;
3.	G.T. Zaripov	–	IT, I va IPKTB bo‘limi boshlig‘i, a‘zo;
4.	E.D. Niyozov	–	Tabiiy fanlar fakulteti dekani, a‘zo;
5.	B.B. Umarov	–	Organik va fizkolloid kimyo kafedrasida professori a‘zo;
6.	M.Ya.Ergashov	–	Organik va fizkolloid kimyo kafedrasida professori, a‘zo;
7.	H.T.Avezov	–	Organik va fizkolloid kimyo kafedrasida dotsenti, a‘zo;
8.	M.A.Tursunov	–	Organik va fizkolloid kimyo kafedrasida dotsenti, a‘zo;
9.	S.F.Abduraxmonov	–	Organik va fizkolloid kimyo kafedrasida dotsenti, a‘zo;
10.	Sh. Xudoyberdiyev	–	Organik va fizkolloid kimyo kafedrasida dotsenti, a‘zo;
11.	F.M.Nuritdinova	–	Organik va fizkolloid kimyo kafedrasida dotsenti, kotib;

2. Tashkiliy qo'mita.

1.	O.X. Xamidov	–	Universitet rektori, rais;
2.	T.H. Rasulov	–	Ilmiy ishlar va innovatsiyalar bo'yicha prorektor, rais muovini;
3.	O'.U. Rashidov	–	Moliya va iqtisod ishlari bo'yicha prorektor, a'zo;
4.	G.T. Zaripov	–	IT, I va IPKTB bo'limi boshlig'i, a'zo;
5.	E.D. Niyozov	–	Tabiiy fanlar fakulteti dekani, a'zo;
4.	Z.A. Sulaymonova	–	Organik va fizkolloid kimyo kafedrası dotsenti, a'zo;
5.	D.A. Hazratova	–	Organik va fizkolloid kimyo kafedrası dotsenti, a'zo;
6.	O'.M. Mardonov	–	Organik va fizkolloid kimyo kafedrası dotsenti, a'zo;
7.	N.G. Sevinchov	–	Organik va fizkolloid kimyo kafedrası dotsenti, a'zo;
8.	Q.G'. Avezov	–	Organik va fizkolloid kimyo kafedrası dotsenti, a'zo;
9.	Z.K. Qodirova	–	Organik va fizkolloid kimyo kafedrası dotsenti, a'zo;
10.	E.A. Xudoyorova	–	Organik va fizkolloid kimyo kafedrası o'qituvchisi a'zo;
11.	D.B. Mutalipova	–	Organik va fizkolloid kimyo kafedrası o'qituvchisi a'zo;
12.	G.Q. Xoliqova	–	Organik va fizkolloid kimyo kafedrası o'qituvchisi a'zo;
13.	S.A. Karomatov	–	Organik va fizkolloid kimyo kafedrası o'qituvchisi a'zo;

3.Organik va fizkolloid kimyo kafedrası mudiri v.v.b. S.F. Abduraxmonovga:

- anjuman dasturini ishlab chiqish, anjuman yakuni bo'yicha qabul qilingan tavsiyalarni iqtisodiyotning tegishli tarmoq va sohalariga tatbiq etish bo'yicha chora-tadbirlar dasturini manfaatdor tashkilotlar bilan kelishish;

- anjumanlar o'tkazilgandan so'ng 3 kun muddatda anjuman yakuni bo'yicha qabul qilingan tavsiyalarni amaliyotga tatbiq etish bo'yicha chora-tadbirlar dasturining bajarilishi hamda anjumanlarning ilmiy, ijtimoiy va iqtisodiy samaradorligi to'g'risidagi hisobotni Ilmiy tadqiqot, innovatsiyalar va ilmiy pedagogik kadrlarni tayyorlash bo'limiga taqdim etilishini ta'minlash vazifasi yuklatilsin.

4. Moliya va iqtisod ishlari bo'yicha prorektor O'.U. Rashidovga:

- ilmiy anjumanni tashkil etish va o'tkazish bilan bog'liq xarajatlarni tegishli smeta asosida amalga oshirish vazifasi yuklatilsin.

5. Ilmiy tadqiqot, innovatsiyalar va ilmiy pedagogik kadrlarni tayyorlash bo'limi boshlig'i G.T. Zaripovga:

- anjumanni tashkil etish va o'tkazish bilan bog'liq bo'lgan ishlarni amalga oshirish;
- anjumanni yakuniy hisobotini tayyorlab Oliy va o'rta maxsus ta'lim vazirligiga taqdim etish vazifasi yuklatilsin.

6. Ushbu buyruq ijro nazorati Ilmiy ishlar va innovatsiyalar bo'yicha prorektor T.H. Rasulov zimmasiga yuklatilsin.

Asos: O'zbekiston Respublikasi Vazirlar Mahkamasining 2022-yil 7-martdagi 101-f-sonli Farmoyishi, Oliy va o'rta maxsus talim vazirligining 2022-yil 14-martdagi 97-sonli buyrug'i hamda Organik va fizkolloid kimyo kafedrasini mudiri bildirishnomasi

Rektor



O.X. Xamidov

“Koordinatsion birikmalar kimyosining hozirgi zamon muammolari”
mavzusidagi xalqaro ilmiy-amaliy anjumanining tashkiliy va dasturiy qo‘mita
a‘zolari

Obidjon Xafizovich Xamidov	Buxoro davlat universiteti rektori, i.f.d., prof.
To‘lqin Husenovich Rasulov	Buxoro davlat universiteti ilmiy ishlar va innovatsiyalar bo‘yicha prorektori, f-m.f.d., prof.
Abdulohat Turobovich Djalilov	TKTITI direktori, k.f.d., akademik.
Sayyora Shrofovna Rashidova	O‘zR FA Polimerlar kimyosi va fizikasi instituti direktori, k.f.d., akademik.
Abbasxan Sobirxanovich To‘rayev	O‘zR FA BKI direktori, k.f.d., akademik.
Baxtiyor Sobirjonovich Zokirov	O‘zR FA UNKI professori, k.f.d., akademik.
Quvondiq Sanoqulovich Sanoqulov	NKMK direktori, t.f.d., prof.
Aziz Baxtiyarovich Ibragimov	O‘zR FA UNKI direktor o‘rinbosari, k.f.d., prof.
Shaxnoza Abduxalilovna Kadirova	O‘zMU Kimyo fakul’teti dekani, k.f.d., prof.
Sergey Zubarovich Vatsadze	M.V. Lomonosov nomidagi MDU professori, k.f.d., prof.
Vadim Viktorovich Minin	Rossiya FA N.S. Kurnakov nomidagi UNKI yetakchi ilmiy xodimi, k.f.d., prof.
Vadim Vitalievich Negrebetsky	N.I.Pirogov nomidagi Rossiya MTTU Kimyo kafedrasini mudiri, k.f.d., prof.
Suriya Irekovna Gilmanshina	Qozon federal universiteti professori, p.f.d., prof.
Savash Kaya	Sivas davlat universiteti professori
Mohd Nadeem Bukhari	Handwara davlat kolleji, PhD, associate professor.
Xamdani Ikromovich Akbarov	O‘zMU professori, k.f.d., prof.
Abdullo Murodovich Nasimov	SamDU professori, k.f.d., prof.
Xayit Xudonazarovich To‘rayev	TerDU Kimyo fakul’teti dekani, k.f.d., prof.
Shaxobiddin Xasanboyevich Avdullayev	ADU professori, k.f.d., prof.
Shavkat Vohidovich Avdullayev	NamDU professori, k.f.d., prof.
Zuxra Chingizovna Kadirova	O‘zbekiston – Yaponiya yoshlar innovatsiya markazi, k.f.d., prof.
Olim Ruzimuradov	Toshkent shahridagi Turin politexnika universiteti professori, k.f.d., prof.
Jamshid Mengnorovich Ashurov	O‘zR FA BKI yetakchi ilmiy xodimi, k.f.d., prof.
Baqo Bafoevich Umarov	BuxDU professori, k.f.d., prof.
Muxtar Raxmatovich Amonov	BuxDU professori, t.f.d., prof.
Mansur Yarashevich Ergashev	BuxDU professori, k.f.n., prof.
Murod Amonovich Tursunov	BuxDU O‘quv-uslubiy departament boshlig‘i, k.f.f.d., PhD, dots.
Erkin Dilmurodovich Niyozov	BuxDU Tabiiy fanlar fakul’teti dekani, t.f.n., dots.
O‘ktam Mardonovich Mardonov	BuxDU dotsenti, k.f.n., dots.
Hasan Tillayevich Avezov	BuxDU dotsenti, k.f.n., dots.
Qahramon Shayimovich Husenov	NDKTU dotsenti, k.f.n., dots.
Nemat Gulboyevich Sevinchov	BuxDU dotsenti, k.f.n., dots.
Qozoqmurod Asadovich Ravshanov	BuxDU dotsenti, k.f.n., dots.
Hasan Qalandarovich Razzoqov	BuxDU dotsenti, t.f.n., dots.
Sayfullo Ibdulloyevich Nazarov	BuxDU Umumiy va noorganik kimyo kafedrasini mudiri, t.f.n., dots.
Sayfiddin Fayzullayevich Abduraxmonov	BuxDU Organik va fizkolloid kimyo kafedrasini mudiri, k.f.f.d., PhD.
Quvondiq G‘iyosovich Avezov	BuxDU dotsenti, k.f.f.d., PhD, dots.
Gulbahor Akiyevna Xudonazarova	BuxDU dotsenti, k.f.n., dots.
Muzaffar Samandarovich Sharipov	BuxDU dotsenti, n.f.n., dots.
	BuxDU dotsenti, k.f.f.d., PhD.

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mavzusidagi xalqaro ilmiy-amaliy anjumanida ishtirok etuvchi universitet
professor-o‘qituvchilar va talabalar ro‘yxati**

Professor-o‘qituvchilar ro‘yxati

- 1 Sayfiddin Fayzullayevich Abduraxmonov – Tabiiy fanlar fakulteti
- 2 Baqo Bafoyeovich Umarov – Tabiiy fanlar fakulteti
- 3 Mansur Yarashevich Ergashev – Tabiiy fanlar fakulteti
- 4 Hasan Tillayevich Avezov – Tabiiy fanlar fakulteti
- 5 Quvondiq G‘iyosovich Avezov – Tabiiy fanlar fakulteti
- 6 Feruza Muidinovna Nurutdinova – Tabiiy fanlar fakulteti
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- 8 Shuxrat Shamsiddinovich Xudoyberdiyev – Tabiiy fanlar fakulteti
- 9 Zulfiya Kobilovna Qodirova – Tabiiy fanlar fakulteti
- 10 Zilola Abduraxmonovna Sulaymonova – Tabiiy fanlar fakulteti
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- 13 Sardor Aminovich Karomatov – Tabiiy fanlar fakulteti
- 14 Gulyayra Qo‘ldoshevna Xoliqova – Tabiiy fanlar fakulteti
- 15 Baxtiyor Shukurulloevich Ganiyev – Tabiiy fanlar fakulteti
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- 17 Muxtar Raxmatovich Amonov – Tabiiy fanlar fakulteti
- 18 Qozoqmurod Asadovich Ravshanov – Tabiiy fanlar fakulteti
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- 20 Gulbahor Akiyevna Xudoynazarova – Tabiiy fanlar fakulteti
- 21 Muzaffar Samandarovich Sharipov – Tabiiy fanlar fakulteti
- 22 Nurullo Ibodulloyevich Nazarov – Tabiiy fanlar fakulteti
- 23 Maxbuba Kamolovna Ochilova – Tabiiy fanlar fakulteti
- 24 Sherzod Sharof o‘g‘li Ortiqov – Tabiiy fanlar fakulteti
- 25 Ilg‘or Ilhom o‘g‘li Norov – Tabiiy fanlar fakulteti
- 26 Lobar Olimovna Sharipova – Tabiiy fanlar fakulteti
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- 28 Anvar Nusratovich Nematov – Tabiiy fanlar fakulteti
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- 33 Mahliyo Aliyevna Muhammedova – Tabiiy fanlar fakulteti
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- 36 Alisher Latipovich Shirinov – Tasviriy va amaliy san‘at kafedrası
- 37 Farmonov Ikrom – Tasviriy va amaliy san‘at kafedrası
- 38 Saidov Javlon – Tasviriy va amaliy san‘at kafedrası
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- 42 Nafisa Mukhammadovna Aslonova - Tabiiy fanlar fakulteti
- 43 Nurbibi Raximovna Ochilova - Tabiiy fanlar fakulteti
- 44 G‘ayratjon Qodirjonovich Shirinov - Tabiiy fanlar fakulteti

44	Usmonov Javohir Ubayd o'g'li	10.2KIM-21
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51	Anvarova Zarina Anvar qizi	10.2KIM-21
52	Amonova Nargiza Muxtorovna	10.2KIM-21

Talabalar ro'yxati

1	Bozorova Nargiza Izzat qizi	2-1KIM-20
2	Baqoyeva Marjona Adiz qizi	2-1KIM-20
3	Ochilova Munisa Jonibek qizi	2-1KIM-20
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5	Tursunov Mirshod Ixtiyorovich	2-1KIM-20
6	Temirova Zebiniso Amon qizi	2-1KIM-20
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8	Sayfullayeva Dilbar Shavkat qizi	2-1KIM-20
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