

**ACADEMIC SCIENTIFIC
JOURNAL OF CHEMISTRY**

ISSN: 2224-5286 (Print)
ISSN: 2518-1491 (Online)

**№4
2025**

ISSN 2518-1491 (Online),
ISSN 2224-5286 (Print)



ACADEMIC SCIENTIFIC JOURNAL OF CHEMISTRY

4 (465)

October – December 2025

PUBLISHED SINCE JANUARY

1947 PUBLISHED 4 TIMES A YEAR

ALMATY, NAS RK

Editor in chief:

ZHURINOV Murat Zhurinovich, doctor of chemistry, professor, academician of NAS RK, President of NAS RK RPA, general director of JSC "D.V. Sokolsky Institute of fuel, catalysis and electrochemistry (Almaty, Kazakhstan) <https://www.scopus.com/authid/detail.uri?authorId=6602177960>, <https://www.webofscience.com/wos/author/record/2017489>

Editorial board:

ADEKENOV Sergazy Mynzhasarovich (deputy editor-in-chief) doctor of chemical sciences, professor, academician of NAS RK, director of the International Scientific and Production Holding «Phytochemistry» (Karaganda, Kazakhstan) <https://www.scopus.com/authid/detail.uri?authorId=7006153118>, <https://www.webofscience.com/wos/author/record/48648658>

AGABEKOV Vladimir Enokovich (deputy editor-in-chief), doctor of chemistry, professor, academician of NAS of Belarus, honorary director of the Institute of Chemistry of new materials (Minsk, Belarus) <https://www.scopus.com/authid/detail.uri?authorId=7004624845>, <https://www.webofscience.com/wos/author/record/28920574>

STRNAD Miroslav, head of the laboratory of the Institute of Experimental Botany of the Czech Academy of Sciences, professor (Olomouc, Czech Republic) <https://www.scopus.com/authid/detail.uri?authorId=36789185000>, <https://www.webofscience.com/wos/author/record/18379>

BURKITBAYEV Mukhambetkali, doctor of chemistry, professor, academician of NAS RK, (Almaty, Kazakhstan) <https://www.scopus.com/authid/detail.uri?authorId=8513885600>, <https://www.webofscience.com/wos/author/record/691218>

HOHMANN Judith, head of the department of pharmacognosy, faculty of Pharmacy, University of Szeged, director of the interdisciplinary center for Life sciences (Szeged, Hungary) <https://www.scopus.com/authid/detail.uri?authorId=7004457196>, <https://www.webofscience.com/wos/author/record/15630788>

ROSS Samir, Ph.D, professor, school of Pharmacy, National Center for scientific research of Herbal Products, University of Mississippi (Oxford, USA) <https://www.scopus.com/authid/detail.uri?authorId=7401610128>, <https://www.webofscience.com/wos/author/record/47926269>

KHUTORYANSKY Vitaly, Ph.D, pharmacist, professor at the University of Reading (Reading, England) <https://www.scopus.com/authid/detail.uri?authorId=35606915700>, <https://www.webofscience.com/wos/author/record/221621>

TELTAYEV Bagdat Burkhanbayuly, doctor of technical sciences, professor, academician of NAS RK, Ministry of Industry and infrastructure development of the Republic of Kazakhstan (Almaty, Kazakhstan) <https://www.scopus.com/authid/detail.uri?authorId=6506225641>, <https://www.webofscience.com/wos/author/record/72161>

PHARUK Asana Dar, professor at Hamdard al-Majid college of Oriental medicine, faculty of Oriental medicine, Hamdard University (Karachi, Pakistan) <https://www.scopus.com/authid/detail.uri?authorId=55884056900>, <https://www.webofscience.com/wos/author/record/1796996>

FAZYLOV Serik Drakhmetovich, doctor of chemistry, professor, academician of NAS RK, deputy director of the Institute of Organic Synthesis and Coal Chemistry (Karaganda, Kazakhstan) <https://www.scopus.com/authid/detail.uri?authorId=6701472056>, <https://www.webofscience.com/wos/author/record/1541357>

ZHOROBEKOVA Sharipa Zhorobekovna, doctor of chemistry, professor, academician of NAS of Kyrgyzstan, Institute of Chemistry and chemical technology of NAS KR (Bishkek, Kyrgyzstan) <https://www.scopus.com/authid/detail.uri?authorId=6602652060>, <https://www.webofscience.com/wos/author/record/31723468>

KHALIKOV Jurabay Khalikovich, doctor of chemistry, professor, academician of the Academy of Sciences of Tajikistan, V.I. Nikitin Institute of Chemistry AS RT (Tajikistan) <https://www.scopus.com/authid/detail.uri?authorId=6603735641>, <https://www.webofscience.com/wos/author/record/9567106>

FARZALIEV Vagif Medzhid ogly, doctor of chemistry, professor, academician of NAS of Azerbaijan (Azerbaijan) <https://www.scopus.com/authid/detail.uri?authorId=6601962486>, <https://www.webofscience.com/wos/author/record/21617033>

GARELIK Hemda, PhD in chemistry, president of the department of Chemistry and Environment of the International Union of Pure and Applied Chemistry (London, England) <https://www.scopus.com/authid/detail.uri?authorId=56010090400>, <https://www.webofscience.com/wos/author/record/29866743>

ACADEMIC SCIENTIFIC JOURNAL OF CHEMISTRY

ISSN 2518-1491 (Online),

ISSN 2224-5286 (Print)

Owner: «Central Asian Academic Research Center» LLP (Almaty).

The certificate of registration of a periodical printed publication in the Committee of information of the Ministry of Information and Social Development of the Republic of Kazakhstan № **KZ23VPY00121156**, issued 05.06.2025

Thematic scope: *organic chemistry, inorganic chemistry, catalysis, electrochemistry and corrosion, pharmaceutical chemistry and technology.*

Periodicity: 4 times a year.

<http://chemistry-technology.kz/index.php/en/arhiv>

© «Central Asian Academic Research Center» LLP, 2025

Editorial address: JSC «D.V. Sokolsky institute of fuel, catalysis and electrochemistry», 142, Kunayev str., of. 310, Almaty, 050100, tel. 291-62-80, fax 291-57-22, e-mail: orgcat@nursat.kz

Бас редактор:

ЖҰРЫНОВ Мұрат Жұрыңұлы, химия ғылымдарының докторы, профессор, ҚР ҰҒА академигі, РБҚ ҚР ҰҒА президенті, АҚ «Д.В. Сокольский атындағы Отын, катализ және электрохимия институтының» бас директоры (Алматы, Қазақстан) <https://www.scopus.com/authid/detail.uri?authorId=6602177960>, <https://www.webofscience.com/wos/author/record/2017489>

Редакция алқасы:

ӘДЕКЕНОВ Серғазы Мыңжасарұлы (бас редактордың орынбасары), химия ғылымдарының докторы, профессор, ҚР ҰҒА академигі, «Фитохимия» Халықаралық ғылыми-өндірістік холдингінің директоры (Қарағанды, Қазақстан) <https://www.scopus.com/authid/detail.uri?authorId=7006153118>, <https://www.webofscience.com/wos/author/record/48648658>

АГАБЕКОВ Владимир Енокович (бас редактордың орынбасары), химия ғылымдарының докторы, профессор, Беларусь ҰҒА академигі, Жаңа материалдар химиясы институтының құрметті директоры (Минск, Беларусь) <https://www.scopus.com/authid/detail.uri?authorId=7004624845>, <https://www.webofscience.com/wos/author/record/28920574>

СТРНАД Мирослав, профессор, Чехия ғылым академиясының Эксперименттік ботаника институтының зертхана меңгерушісі (Оломоуц, Чехия) <https://www.scopus.com/authid/detail.uri?authorId=36789185000>, <https://www.webofscience.com/wos/author/record/18379>

БҮРКІТБАЕВ Мұхамбетқали, химия ғылымдарының докторы, профессор, ҚР ҰҒА академигі, (Алматы, Қазақстан) <https://www.scopus.com/authid/detail.uri?authorId=8513885600>, <https://www.webofscience.com/wos/author/record/691218>

ХОХМАНН Джулит, Сегед университетінің Фармацевтика факультетінің Фармакогнозия кафедрасының меңгерушісі, Жаратылыстану ғылымдарының пәнаралық орталығының директоры (Сегед, Венгрия) <https://www.scopus.com/authid/detail.uri?authorId=7004457196>, <https://www.webofscience.com/wos/author/record/15630788>

РОСС Самир, PhD, Миссисипи университетінің Өсімдік өнімдерін ғылыми зерттеу ұлттық орталығы, Фармация мектебінің профессоры (Оксфорд, АҚШ) <https://www.scopus.com/authid/detail.uri?authorId=7401610128>, <https://www.webofscience.com/wos/author/record/47926269>

ХУТОРЯНСКИЙ Виталий, философия докторы (PhD, фармацевт), Реддинг университетінің профессоры (Реддинг, Англия) <https://www.scopus.com/authid/detail.uri?authorId=35606915700>, <https://www.webofscience.com/wos/author/record/221621>

ТЕЛТАЕВ Бағдат Бұрханбайұлы, техника ғылымдарының докторы, профессор, ҚР ҰҒА академигі, Қазақстан Республикасы Индустрия және инфрақұрылымдық даму министрлігі (Алматы, Қазақстан) <https://www.scopus.com/authid/detail.uri?authorId=6506225641>, <https://www.webofscience.com/wos/author/record/72161>

ФАРУК Асана Дар, Хамдар аль-Маджида Шығыс медицина колледжінің профессоры, Хамдард университетінің Шығыс медицина факультеті (Карачи, Пәкістан) <https://www.scopus.com/authid/detail.uri?authorId=55884056900>, <https://www.webofscience.com/wos/author/record/1796996>

ФАЗЫЛОВ Серік Драхметұлы, химия ғылымдарының докторы, профессор, ҚР ҰҒА академигі, Органикалық синтез және көмір химиясы институты директорының ғылыми жұмыстар жөніндегі орынбасары (Қарағанды, Қазақстан) <https://www.scopus.com/authid/detail.uri?authorId=6701472056>, <https://www.webofscience.com/wos/author/record/1541357>

ЖОРОБЕКОВА Шарипа Жоробекқызы, химия ғылымдарының докторы, профессор, Кыргызстан ҰҒА академигі, ҚР ҰҒА Химия және химиялық технология институты (Бішкек, Кыргызстан) <https://www.scopus.com/authid/detail.uri?authorId=6602652060>, <https://www.webofscience.com/wos/author/record/31723468>

ХАЛИКОВ Джурабай Халикович, химия ғылымдарының докторы, профессор, Тәжікстан ҒА академигі, В.И. Никитин атындағы Химия институты (Душанбе, Тәжікстан) <https://www.scopus.com/authid/detail.uri?authorId=6603735641>, <https://www.webofscience.com/wos/author/record/9567106>

ФАРЗАЛИЕВ Вагиф Меджидоглы, химия ғылымдарының докторы, профессор, АҰҒА академигі (Баку, Әзірбайжан) <https://www.scopus.com/authid/detail.uri?authorId=6601962486>, <https://www.webofscience.com/wos/author/record/21617033>

ГАРЕЛИК Хемда, философия докторы (PhD, химия), Халықаралық таза және қолданбалы химия одағының Химия және қоршаған орта бөлімінің президенті (Лондон, Англия) <https://www.scopus.com/authid/detail.uri?authorId=56010090400>, <https://www.webofscience.com/wos/author/record/29866743>

«ACADEMIC SCIENTIFIC JOURNAL OF CHEMISTRY»

ISSN 2518-1491 (Online),

ISSN 2224-5286 (Print)

Меншіктенуші: «Орталық Азия академиялық ғылыми орталығы» ЖШС (Алматы қ.).

Қазақстан Республикасының Ақпарат және қоғамдық даму министрлігінің Ақпарат комитетінде 05.06.2025 ж. берілген № KZ23VPY00121156 мерзімдік басылым тіркеуіне қойылу туралы куәлік.

Тақырыптық бағыты: *органикалық химия, бейорганикалық химия, катализ, электрохимия және коррозия, фармацевтикалық химия және технологиялар.*

Мерзімділігі: жылына 4 рет.

<http://chemistry-technology.kz/index.php/en/arhiv>

© «Орталық Азия академиялық ғылыми орталығы» ЖШС, 2025

Редакцияның мекенжайы: 050100, Алматы қ., Қонаев к-сі, 142, «Д.В. Сокольский атындағы отын, катализ және электрохимия институты» АҚ, каб. 310, тел. 291-62-80, факс 291-57-22, e-mail:orgcat@nursat.kz

Главный редактор:

ЖУРИНОВ Мурат Журинович, доктор химических наук, профессор, академик НАН РК, президент РОО Национальной академии наук Республики Казахстан, генеральный директор АО «Институт топлива, катализа и электрохимии им. Д.В. Сокольского» (Алматы, Казахстан), <https://www.scopus.com/authid/detail.uri?authorId=6602177960>, <https://www.webofscience.com/wos/author/record/2017489>

Редакционная коллегия:

АДЕКЕНОВ Сергазы Мынжасарович (заместитель главного редактора), доктор химических наук, профессор, академик НАН РК, директор Международного научно-производственного холдинга «Фитохимия» (Караганда, Казахстан), <https://www.scopus.com/authid/detail.uri?authorId=7006153118>, <https://www.webofscience.com/wos/author/record/48648658>

АГАБЕКОВ Владимир Енокович (заместитель главного редактора), доктор химических наук, профессор, академик НАН Беларуси, почетный директор Института химии новых материалов (Минск, Беларусь), <https://www.scopus.com/authid/detail.uri?authorId=7004624845>, <https://www.webofscience.com/wos/author/record/28920574>

СТРНАД Мiroслав, профессор, заведующий лабораторией института Экспериментальной ботаники Чешской академии наук (Оломоуц, Чехия), <https://www.scopus.com/authid/detail.uri?authorId=36789185000>, <https://www.webofscience.com/wos/author/record/18379>

БУРКИТБАЕВ Мухамбеткали, доктор химических наук, профессор, академик НАН РК, (Алматы, Казахстан), <https://www.scopus.com/authid/detail.uri?authorId=8513885600>, <https://www.webofscience.com/wos/author/record/691218>

ХОХМАНН Джудит, заведующий кафедрой Фармакогнозии Фармацевтического факультета Университета Сегеда, директор Междисциплинарного центра естественных наук (Сегед, Венгрия), <https://www.scopus.com/authid/detail.uri?authorId=7004457196>, <https://www.webofscience.com/wos/author/record/15630788>

РОСС Самир, PhD, профессор Школы Фармации национального центра научных исследований растительных продуктов Университета Миссисипи (Оксфорд, США), <https://www.scopus.com/authid/detail.uri?authorId=7401610128>, <https://www.webofscience.com/wos/author/record/47926269>

ХУТОРЯНСКИЙ Виталий, доктор философии (Ph.D, фармацевт), профессор Университета Рединга (Рединг, Англия), <https://www.scopus.com/authid/detail.uri?authorId=35606915700>, <https://www.webofscience.com/wos/author/record/221621>

ТЕЛЫТАЕВ Багдат Бурханбайулы, доктор технических наук, профессор, академик НАН РК, Министерство Индустрии и инфраструктурного развития Республики Казахстан (Алматы, Казахстан), <https://www.scopus.com/authid/detail.uri?authorId=6506225641>, <https://www.webofscience.com/wos/author/record/72161>

ФАРУК Ахсана Дар, профессор колледжа Восточной медицины Хамдарда аль-Маджида, факультет Восточной медицины университета Хамдарда (Карачи, Пакистан), <https://www.scopus.com/authid/detail.uri?authorId=55884056900>, <https://www.webofscience.com/wos/author/record/1796996>

ФАЗЫЛОВ Серик Драгметович, доктор химических наук, профессор, академик НАН РК, заместитель директора по научной работе Института органического синтеза и углехимии (Караганда, Казахстан), <https://www.scopus.com/authid/detail.uri?authorId=6701472056>, <https://www.webofscience.com/wos/author/record/1541357>

ЖОРОБЕКОВА Шарипа Жоробековна, доктор химических наук, профессор, академик НАН Кыргызстана, Институт химии и химической технологии НАН КР (Бишкек, Кыргызстан), <https://www.scopus.com/authid/detail.uri?authorId=6602652060>, <https://www.webofscience.com/wos/author/record/31723468>

ХАЛИКОВ Джурабай Халикович, доктор химических наук, профессор, академик АН Таджикистана, Институт химии имени В.И. Никитина АН РТ (Душанбе, Таджикистан), <https://www.scopus.com/authid/detail.uri?authorId=6603735641>, <https://www.webofscience.com/wos/author/record/9567106>

ФАРЗАЛИЕВ Вагиф Меджид оглы, доктор химических наук, профессор, академик НАНА (Баку, Азербайджан), <https://www.scopus.com/authid/detail.uri?authorId=6601962486>, <https://www.webofscience.com/wos/author/record/21617033>

ГАРЕЛИК Хемда, доктор философии (Ph.D, химия), президент Отдела химии и окружающей среды Международного союза чистой и прикладной химии (Лондон, Англия), <https://www.scopus.com/authid/detail.uri?authorId=56010090400>, <https://www.webofscience.com/wos/author/record/29866743>

«ACADEMIC SCIENTIFIC JOURNAL OF CHEMISTRY».

ISSN 2518-1491 (Online),

ISSN 2224-5286 (Print)

Собственник: Республиканское общественное объединение ТОО «Центрально-азиатский академический научный центр» (г. Алматы).

Свидетельство о постановке на учет периодического печатного издания в Комитете информации Министерства информации и общественного развития Республики Казахстан № KZ23VPY00121156, выданное 05.06.2025 г.

Тематическая направленность: *органическая химия, неорганическая химия, катализ, электрохимия и коррозия, фармацевтическая химия и технологии.*

Периодичность: 4 раз в год.

<http://chemistry-technology.kz/index.php/en/arhiv>

© ТОО «Центрально-азиатский академический научный центр», 2025

Адрес редакции: 050100, г. Алматы, ул. Кунаева, 142, АО «Институт топлива, катализа и электрохимии им. Д.В. Сокольского», каб. 310, тел. 291-62-80, факс 291-57-22, e-mail: orgcat@nursat.kz

CONTENTS

G.E. Azimbayeva, A.K. Kamysbayeva, G.N. Kudaibergenova, U.Zh. Beysenbiyeva, N.M. Kurbanbayeva Chromatographic analysis of ethanol obtained from topinambur tubers (<i>Helianthus Tuberosus</i>).....	13
B. Amiraliyev, N. Zhanikulov, B. Taimasov, M. Aitureev, B. Zhakipbayev Expanding the raw material base of mineral additives for the production of composite cements.....	27
A.M. Yegissinova, R.S. Taubayeva, R.K. Rakhmetullaeva, A.S. Seitkan, E.B. Satkozhaeva Physicochemical properties of thermoplastic starch/hemp biofilm produced by casting method.....	41
E.M. Yergaliyeva, K.B. Bazhykova, Zh.Zh. Kolbaeva, A. Duysen, V.V. Vazhev <i>In silico</i> prediction of PASS and ADME/Tox properties of novel 1,3,5-triazine derivatives for drug development.....	54
R.I. Jalmakhanbetova, S. Azatkyzy, G.K. Mukusheva Structure-directed ursolic acid modifications and their impact on biological activity.....	71
R.N. Zhanaliyeva, B.S. Imangaliyeva, M.A. Zharkınbekov, A.S. Ungarbayeva, R. Kozykeyeva Study of the kinetics and mechanism of molybdenum disulfide oxidation by sodium hypochlorite.....	87
O.S. Ilyassova, M. Zhumabek, G.N. Kaumenova, R.S. Orazbekova, B.S. Biyekeyev Hydrogenation of carbon dioxide on Ni-Co/ZrO ₂ catalysts for conversion into synthetic fuel components.....	100
K. Kalmakov, G. Turebekova, S. Yegemberdiyeva, U. Nuridinova, N. Dulat Catalytic cracking of vacuum gas oil from Kumkol oil in a fluidized bed catalyst unit.....	115
B.T. Kuderina, N.B. Kassenova, A.S. Khamitova, A.G. Zhaxybayeva, A.B. Abdrakhmanova Modification of the structure of oxide cathode materials to enhance the capacity and stability of li - ion batteries.....	128

B.M. Kaldybaeva, D.M. Kenzhebekov, D.Zh. Janabayev, L.M. Ulyev, A. Zholshybek Improving the energy efficiency of oil treatment and stabilization units in the field.....	137
A.K. Kozybaev, Zh.D. Alimkulova, S.O. Abilkasova, G.O. Bugubaeva, S. Bubish Prospects for the use of water-soluble copolymers in industrial wastewater treatment processes.....	150
R.M. Kudaibergenova, A.R. Aitekova, N.S. Murzakasymova, A.S. Seitkan, N.A. Nurlybayeva Structural and compositional characteristics of cobalt ferrite nanoparticles.....	159
M. Nazhipkyzy, A. Ashiraly, A. Aitugan, A. Aikenova Fabrication of lignin-based fibrous composites by electrospinning for energy storage applications.....	170
U. Nazarbek, Y. Raiymbekov, P. Abdurazova, G. Kambarova Molecular dynamics modeling of solubility in aqueous systems: temperature dependence and solvation effects.....	184
Zh.Zh. Nurtazina, Zh.S. Kassymova, L.K. Orazzhanova, B. Łeska, N.B. Kiarstanova Efficiency of modified medium for pigment and antioxidant biosynthesis in <i>Chlorella Vulgaris</i>	197
G.M. Ormanova, A.A. Anarbayev, B.N. Kabylbekova, Zh.E. Khusanov Construction of a solubility isotherm in a four-component mutual $\text{CaSO}_4\text{-NaCl-H}_2\text{O}$ system.....	212
Zh.B. Rakhimberlinova, A. Zhorabek, A. Bailen, M. Kaiyrbaeva, A. Mendibayeva Investigation of the possibilities of obtaining ultradispersed copper particles in aqueous solutions.....	227
A. Takibayeva, L. Sultanova, A. Tussupova, Z. Omar, A. Amanzholova Mechanism, features of the amination reaction in a series of lupane triterpenoids.....	239
G. Toleutay, R.N. Tuleyeva, A. Taubatyrova, N.N. Gizatullina Recent advances in the application of lignin for biobased packaging materials.....	250
Kh. Khimersen, T.K. Jumadilov, A. Imangazy, G.T. Dyusseмбаeva, B. Totkhuskyzy Features of the interaction of polyelectrolytes with gallium ions in aqueous media.....	266

МАЗМҰНЫ

Г.Е. Азимбаева, А.К. Камысбаева, Г.Н. Кудайбергенова, Ұ.Ж. Бейсенбиева, Н.М. Курбанбаева Топинамбур жемісінен (<i>Helianthus Tuberosus</i>) алынған этанолдың хроматографиялық анализі.....	13
Б. Амиралиев, Н. Жаникулов, Б. Таймасов, М. Айтурсев, Б. Жакипбаев Композициялық цемент алу үшін минералды қоспалардың шикізат базасын кеңейту.....	27
А.М. Егисина, Р.С. Таубаева, Р.К. Рахметуллаева, А.С. Сейткан, Э.Б. Саткожаева Құю әдісі арқылы алынған термопластикалық крахмал/ конопля биоленкасының физика-химиялық қасиеттері.....	41
Э.М. Ергалиева, К.Б. Бажыкова, Ж.Ж. Кольбаева, А.Б. Дуйсен, В.В. Важев <i>In silico</i> PASS және ADME/Tox бағдарламалары арқылы дәрілік заттар әзірлеу үшін 1,3,5-триазиннің жаңа туындыларының қасиеттерін болжау.....	54
Р.И. Джалмаханбетова, С. Азатқызы, Г.К. Мукушева Урсол қышқылының құрылымдық-бағытталған модификациялары және олардың биологиялық белсенділікке әсері.....	71
Р.Н. Жаналиева, Б.С. Имангалиева, М.А. Жаркинбеков, А.С. Унгарбаева, Р. Қозыкеева Молибден дисульфидін натрий гипохлоритімен тотықтырудың кинетикасы мен механизмін зерттеу.....	87
О.С. Ильясова, М. Жумабек, Г.Н. Кауменова, Р.С. Оразбекова, Б.С. Биекеев Көмірқышқыл газын синтетикалық отын компоненттеріне айналдыру үшін Ni-Co/ZrO ₂ катализаторларында гидрлеу.....	100
К.К. Калмаков, Г.З. Туребекова, С.Ж. Егембердиева, У.Е. Нуридинова, Н.Н. Дулат Құмкөл мұнайынан алынған вакуум газойлін катализатордың қайнау қабатындағы қондырғыда каталитикалық крекингтеу.....	115
Б.Т. Кудерина, Н.Б. Касенова, А.С. Хамитова, А.Г. Жаксыбаева, А.Б. Абдрахманова Li - ионды аккумуляторлардың сыйымдылығы мен тұрақтылығын арттыру үшін оксидті катод материалдарын модификациялау.....	128

Б.М. Калдыбаева, Д.М. Кенжебеков, Д.Ж. Джанабаев, Л.М. Ульев, А. Жолшыбек Кәсіпшілікте мұнайды дайындау және тұрақтандыру қондырғысының энергия тиімділігін арттыру.....	137
А.Қ. Қозыбаев, Ж.Д. Әлімқұлова, С.О. Әбілқасова, Г.О. Бугубаева, Ш. Бүбіш Өндірістік ағынды суларды тазарту процестерінде суда еритін сополимерлерді қолдану перспективалары.....	150
Р.М. Құдайбергенова, А.Р. Айтекова, Н.С. Мурзакасымова, А.С. Сейтқан, А.Н. Нұрлыбаева Кобалт феррит нанобөлшектерінің құрылымдық және құрамдық сипаттамасы.....	159
М. Нажипқызы, А. Ашіралы, А. Айтуған, А. Айкенова Энергия сақтау жүйелерінде қолдануға арналған лигнин негізіндегі талшықты композиттерді электроспиннинг әдісімен алу.....	170
У. Назарбек, Е. Райымбеков, П. Абдуразова, Ғ. Қамбарова Су жүйелеріндегі ерігіштіктің молекулалық динамикалық модельдеуі: температураға тәуелділік және еріткіштің әсері.....	184
Ж.Ж. Нуртазина, Ж.С. Касымова, Л.К. Оразжанова, Л. Богуслава, Н.Б. Қиарстанова <i>Chlorella Vulgaris</i> құрамындағы пигменттер мен антиоксиданттардың биосинтезі үшін модификацияланған қоректік ортаның тиімділігі.....	197
Г.М. Орманова, А.А. Анарбаев, Б.Н. Кабылбекова, Ж.Е. Хусанов Төрт компонентті CASO ₄ -NaCl-H ₂ O өзара әрекеттесу жүйесіндегі ерігіштік изотермасын тұрғызу.....	212
Ж.Б. Рахимберлинова, А. Жорабек, А. Байлен, М. Қайырбаева, Ә. Мендібаева Сулы ерітінділердегі мыстың ультродисперсті бөлшектерін алу мүмкіндіктерін зерттеу.....	227
А. Такибаева, Л. Султанова, А. Тусупова, З. Омар, А. Аманжолова Лупан тритерпеноидтар қатарындағы аминдену реакциясының механизмі, ерекшеліктері.....	239

Г. Төлеутай, Р.Н. Тулеева, А. Таубатырова, Н.Н. Гизатуллина

Лигниннің бионегізді қаптама материалдарында қолданылуының

соңғы жетістіктері.....250

Х. Химэрсэн, Т.К. Джумадилов, А. Имангазы, Г.Т. Дюсембаева,

Б. Тотхусқызы

Полиэлектролиттердің галлий иондарымен су ортасында әрекеттесу

ерекшеліктері.....266

СОДЕРЖАНИЕ

Г.Е. Азимбаева, А.К. Камысбаева, Г.Н. Кудайбергенова, У.Ж. Бейсенбиева, Н.М. Курбанбаева Хроматографический анализ этанола полученного из клубней топинамбура (<i>Helianthus Tuberosus</i>).....	13
Б. Амиралиев, Н. Жаникулов, Б. Таймасов, М. Айтурсев, Б. Жакипбаев Расширение сырьевой базы минеральных добавок для получения композиционных цементов.....	27
А.М. Егисинова, Р.С. Таубаева, Р.К. Рахметуллаева, А.С. Сейткан, Э.Б. Саткожаева Физико-химические свойства термопластичной биопленки из крахмала/конопли, полученной методом литья.....	41
Э.М. Ергалиева, К.Б. Бажыкова, Ж.Ж. Кольбаева, А.Б. Дуйсен, В.В. Важев IN SILICO PASS и ADME/TOX прогнозирование свойств новых производных 1,3,5-триазина для разработки лекарств.....	54
Р.И. Джалмаханбетова, С. Азаткызы, Г.К. Мукушева Структурно-направленные модификации урсоловой кислоты и их влияние на биологическую активность.....	71
Р.Н. Жаналиева, Б.С. Имангалиева, М.А. Жаркинбеков, А.С. Унгарбаева, С. Бердібекова Изучение кинетики и механизма окисления дисульфида молибдена гипохлоритом натрия.....	87
О.С. Ильясова, М. Жумабек, Г.Н. Кауменова, Р.С. Оразбекова, Б.С. Биекеев Гидрирование диоксида углерода на Ni-Co/ZrO ₂ катализаторах для преобразования в компоненты синтетического топлива.....	100
К.К. Калмаков, Г.З. Туребекова, С.Ж. Егембердиева, У.Е. Нуридинова, Н.Н. Дулат Каталитический крекинг вакуумного газойля Кумкольской нефти на установке псевдоожиженным слоем катализатора.....	115
Б.Т. Кудерина, Н.Б. Касенова, А.С. Хамитова, А.Г. Жаксыбаева, А.Б. Абдрахманова Модификация структуры оксидных катодных материалов для повышения ёмкости и стабильности Li-ион аккумуляторов.....	128

Б.М. Калдыбаева, Д.М. Кенжебеков, Д.Ж. Джанабаев, Л.М. Ульев, А. Жолшыбек Повышение энергоэффективности установки подготовки и стабилизации нефти на промысле.....	137
А.К. Козыбаев, Ж.Д. Алимкулова, С.О. Абилкасова, Г.О. Бугубаева, Ш. Бубиш Перспективы использования водорастворимых сополимеров в процессах очистки промышленных сточных вод.....	150
Р.М. Кудайбергенова, А.Р. Айтекова, Н.С. Мурзакасымова, А. Сейткан, А.Н. Нурлыбаева Структурно-композиционные характеристики наночастиц феррита кобальта.....	159
М. Нажипкызы, А. Аширалы, А. Айтуган, А. Айкенова Получение волокнистых композитов на основе лигнина методом электроспиннинга для применения в системах хранения энергии.....	170
У. Назарбек, П. Абдуразова, Ғ. Қамбарова, Е. Райымбеков Молекулярно-динамическое моделирование растворимости в водных системах: температурная зависимость и эффекты сольватации.....	184
Ж.Ж. Нуртазина, Ж.С. Касымова, Л.К. Оразжанова, Л. Богуслава, Н.Б. Қиарстанова Эффективность модифицированной среды для биосинтеза пигментов и антиоксидантов в <i>Chlorella Vulgaris</i>	197
Г.М. Орманова, А.А. Анарбаев, Б.Н. Кабылбекова, Ж.Е. Хусанов Построение изотермы растворимости в четырехкомпонентной взаимной системе $\text{CaSO}_4\text{-NaCl-H}_2\text{O}$	212
Ж.Б. Рахимберлинова, А. Жорабек, А. Байлен, М. Кайырбаева, А. Мендибаева Исследование возможностей получения ультрадисперсных частиц меди в водных растворах.....	227
А. Такибаева, Л. Султанова, А. Тусупова, З. Омар, А. Аманжолова Механизм, особенности протекания реакции аминирования в ряду лупановых тритерпеноидов.....	239

Г. Толеутай, Р.Н. Тулеева, А. Таубатырова, Н.Н. Гизатуллина

Последние достижения в применении лигнина для биополимерных

упаковочных материалов.....250

Х. Химэрсэн, Т.К. Джумадилов, А. Имангазы, Г.Т. Дюсембаева,

Б. Тотхусқызы

Особенности взаимодействие полиэлектролитов с ионами галлия

в водной среде.....266

© U. Nazarbek¹, Y. Raiymbekov¹, P. Abdurazova², G. Kambarova¹, 2025.

¹M. Auezov South Kazakhstan University, Shymkent, Kazakhstan;

²Zhanibekov University, Shymkent, Kazakhstan.

E-mail: eplusr@bk.ru

MOLECULAR DYNAMICS MODELING OF SOLUBILITY IN AQUEOUS SYSTEMS: TEMPERATURE DEPENDENCE AND SOLVATION EFFECTS

Nazarbek Ulzhalgas — PhD, Associate Professor, M. Auezov South Kazakhstan University, Department of Chemistry and Pharmaceutical Engineering, Shymkent, Kazakhstan,

E-mail: unazarbek@mail.ru, <https://orcid.org/0000-0001-8890-8926>;

Raiymbekov Yerkebulan — PhD, M. Auezov South Kazakhstan University, Research Laboratory “Water Quality Monitoring and Water Technologies”, Shymkent, Kazakhstan,

E-mail: eplusr@bk.ru, <https://orcid.org/0000-0002-2119-2406>;

Abdurazova Perizat — PhD, Associate Professor, O. Zhanibekov South Kazakhstan Pedagogical University, Department of Chemistry, Shymkent, Kazakhstan,

E-mail: abdurazova.perizat@okmpu.kz, <https://orcid.org/0000-0002-5244-7678>;

Kambarova Galiya — Candidate of Technical Sciences, M. Auezov South Kazakhstan University, Research Laboratory “Water Quality Monitoring and Water Technologies”, Shymkent, Kazakhstan,

E-mail: kambarova85@mail.ru, <https://orcid.org/0000-0002-8417-3384>.

Abstract. Relevance. The solubility of inorganic salts in aqueous media is a key parameter influencing a wide range of chemical, environmental, and technological processes. Traditional empirical and thermodynamic models often fall short in describing temperature-dependent solubility and specific ion–solvent interactions, especially in complex or multicomponent systems. Therefore, the use of molecular-level modeling approaches becomes increasingly important for accurate predictions. This study aims to develop and validate a molecular dynamics (MD)-based model for predicting the solubility of $\text{Cu}(\text{NO}_3)_2$, $\text{Ni}(\text{NO}_3)_2$, and $\text{Pb}(\text{NO}_3)_2$ in water over the temperature range of 273–373 K (0–100°C), and to elucidate the molecular mechanisms underlying the temperature dependence of dissolution. Classical MD simulations were performed using the OPLS-AA force field for ions and the SPC/E model for water. Key parameters such as coordination numbers, hydration radii, and Gibbs free energies of solvation (ΔG_{sol}) were calculated. Thermodynamic integration and potential of mean force (PMF) analysis were employed to determine solubility behavior at the molecular level. $\text{Cu}(\text{NO}_3)_2$ and $\text{Ni}(\text{NO}_3)_2$ exhibited high solubility, supported by compact hydration shells and favorable ΔG_{sol} values (–340.5 and –310.2 kJ/mol, respectively). $\text{Pb}(\text{NO}_3)_2$

demonstrated significantly lower solubility due to weak hydration and a less favorable solvation energy (-210.7 kJ/mol). Cu and Ni nitrates followed a linear temperature dependence, while $\text{Pb}(\text{NO}_3)_2$ showed nonlinear behavior likely due to complexation and entropy effects. Calculated solubility values closely matched experimental data (within 5–7%). The proposed MD-based framework offers a reliable tool for predicting salt solubility in aqueous systems and can be extended to support process design in chemical engineering, materials science, and environmental technologies.

Key words: solubility, molecular dynamics, nitrates, free energy of solvation, hydration

Funding. This research was supported by the Ministry of Science and Higher Education of the Republic of Kazakhstan under the project number AP23487663.

© У. Назарбек¹, Е. Райымбеков¹, П. Абдуразова², Ғ. Қамбарова¹, 2025.

¹М. Әуезов атындағы Оңтүстік Қазақстан университеті, Шымкент, Қазақстан;

²Ө. Жәнібеков атындағы Оңтүстік Қазақстан педагогикалық университеті,
Шымкент, Қазақстан.
E-mail: eplusr@bk.ru

СУ ЖҮЙЕЛЕРІНДЕГІ ЕРІГІШТІКТІҢ МОЛЕКУЛАЛЫҚ ДИНАМИКАЛЫҚ МОДЕЛЬДЕУІ: ТЕМПЕРАТУРАҒА ТӘУЕЛДІЛІК ЖӘНЕ ЕРІТКІШТІҢ ӘСЕРІ

Назарбек Улжалғас — PhD, қауымдастырылған профессор, Химия және фармацевтикалық инженерия кафедрасы, М. Әуезов атындағы ОҚУ, Шымкент, Қазақстан,
E-mail: unazarbek@mail.ru, <https://orcid.org/0000-0001-8890-8926>;

Райымбеков Еркебұлан — PhD, М. Әуезов атындағы ОҚУ, «Су сапасын мониторингілеу және сулы технологиялар» ғылыми-зерттеу зертханасы, Шымкент, Қазақстан,
E-mail: eplusr@bk.ru, <https://orcid.org/0000-0002-2119-2406>;

Абдуразова Перизат — PhD, қауымдастырылған профессор, Химия кафедрасы, Ө. Жәнібеков атындағы ОҚПУ, Шымкент, Қазақстан,
E-mail: abdurazova.perizat@okmpu.kz, <https://orcid.org/0000-0002-5244-7678>;

Қамбарова Ғалия — техника ғылымдарының кандидаты, М. Әуезов атындағы ОҚУ, «Су сапасын мониторингілеу және сулы технологиялар» ғылыми-зерттеу зертханасы, Шымкент, Қазақстан,
E-mail: kambarova85@mail.ru, <https://orcid.org/0000-0002-8417-3384>.

Аннотация. Бейорганикалық тұздардың су ерітінділеріндегі ерігіштігі химиялық реакциялар жылдамдығына, табиғи су жүйелеріндегі зат алмасуға, сондай-ақ өндірістік процестердің тиімділігіне тікелей әсер етеді. Дәстүрлі термодинамикалық модельдер температураның әсерін және ион-еріткіш арасындағы нақты өзара әрекеттесулерді жеткілікті дәлдікпен сипаттай алмайды. Сондықтан молекулалық деңгейде модельдеу әдістерін қолдану өзекті болып табылады. Зерттеудің мақсаты – 273 – 373 К (0 – 100°C) температура аралығында $\text{Cu}(\text{NO}_3)_2$, $\text{Ni}(\text{NO}_3)_2$ және $\text{Pb}(\text{NO}_3)_2$ нитраттарының судағы ерігіштігін болжау үшін молекулалық динамика әдісіне негізделген модельді құрастыру және валидтеу,

сондай-ақ ерігіштіктің температураға тәуелділігін анықтайтын молекулалық механизмдерді сипаттау. Молекулалық динамика модельдеуі OPLS-AA күш өрісі мен SPC/E су моделін қолдану арқылы жүзеге асырылды. Есептеу барысында координациялық сандар, гидратация радиустары және Гиббс бос энергиясы (ΔG_{sol}) анықталды. Термодинамикалық интеграция және орташа күш потенциалы әдістері пайдаланылды. $\text{Cu}(\text{NO}_3)_2$ және $\text{Ni}(\text{NO}_3)_2$ жоғары ерігіштікке ие екені анықталды ($\Delta G_{\text{sol}} = -340.5$ және -310.2 кДж/моль), бұл олардың тығыз гидратациялық қабықтарымен және сумен күшті электростатикалық әрекеттесумен түсіндіріледі. $\text{Pb}(\text{NO}_3)_2$ төмен ерігіштік көрсетті (-210.7 кДж/моль), себебі оның гидратациясы әлсіз және кешен түзілу ықтималдығы жоғары. Cu және Ni тұздары үшін ерігіштік температурамен сызықтық өссе, Pb тұзы үшін бұл тәуелділік күрделі сипатта болды. Теориялық және тәжірибелік нәтижелердің жақсы сәйкестігі (5–7% ауытқу) модельдің сенімділігін дәлелдейді. Бұл әдіс бейорганикалық тұздардың ерігіштігін алдын ала болжауға мүмкіндік беріп, химиялық технология, экология, материалтану және фармацевтика салаларында кеңінен қолдануға жол ашады. Сонымен қатар, бұл тәсілді көпкомпонентті жүйелер мен күрделі иондық ерітінділерді зерттеуге бейімдеуге болады, бұл болашақ зерттеулер үшін маңызды бағыт болып табылады.

Түйін сөздер: ерігіштігі, молекулалық динамика, нитраттар, ерігіштіктің бос энергиясы, гидратация

© У. Назарбек¹, П. Абдуразова², Ғ. Қамбарова¹, Е. Райымбеков¹, 2025.

¹ Южно-Казахстанский университет имени М. Ауэзова, Шымкент, Казахстан;

² Южно-Казахстанский педагогический университет имени Ө. Жәнібеков,

Шымкент, Казахстан.

E-mail: eplusr@bk.ru

МОЛЕКУЛЯРНО-ДИНАМИЧЕСКОЕ МОДЕЛИРОВАНИЕ РАСТВОРИМОСТИ В ВОДНЫХ СИСТЕМАХ: ТЕМПЕРАТУРНАЯ ЗАВИСИМОСТЬ И ЭФФЕКТЫ СОЛЬВАТАЦИИ

Назарбек Улжалгас — PhD, ассоциированный профессор, кафедра Химии и фармацевтической инженерии. ЮКУ имени М. Ауэзова, Шымкент, Казахстан,

E-mail: unazarbek@mail.ru, <https://orcid.org/0000-0001-8890-8926>;

Райымбеков Еркебулан — PhD, ЮКУ имени М. Ауэзова, Научно-исследовательская лаборатория «Мониторинг качества воды и водные технологии», Шымкент, Казахстан,

E-mail: eplusr@bk.ru, <https://orcid.org/0000-0002-2119-2406>;

Абдуразова Перизат — PhD, ассоциированный профессор, кафедра Химии, ЮКПУ имени О. Жанибекова, Шымкент, Казахстан,

E-mail: abdurazova.perizat@okmpu.kz, <https://orcid.org/0000-0002-5244-7678>;

Камбарова Галия — кандидат технических наук, ЮКУ имени М. Ауэзова, Шымкент, Казахстан,

E-mail: kambarova85@mail.ru, <https://orcid.org/0000-0002-8417-3384>.

Аннотация. Растворимость неорганических солей в водных системах является одним из ключевых параметров, определяющих протекание химических,

технологических и природных процессов. Традиционные термодинамические модели растворимости нередко оказываются ограниченными при описании температурных эффектов и специфических взаимодействий «ион–растворитель», что обуславливает необходимость применения молекулярно-ориентированных методов моделирования. Цель исследования состоит в разработке и валидации молекулярно-динамического подхода для количественного прогнозирования растворимости нитратов $\text{Cu}(\text{NO}_3)_2$, $\text{Ni}(\text{NO}_3)_2$ и $\text{Pb}(\text{NO}_3)_2$ в водных растворах в температурном диапазоне 273–373 К (0–100 °С), а также в выявлении молекулярных механизмов, определяющих температурную зависимость процесса растворения. Моделирование выполнено методом молекулярной динамики с использованием силового поля OPLS-AA для ионов и модели воды SPC/E. В рамках расчётов определялись координационные числа, радиусы гидратации, а также свободная энергия растворения (ΔG_{sol}), оцененная методами термодинамической интеграции и анализа потенциала средней силы. Установлено, что соли $\text{Cu}(\text{NO}_3)_2$ и $\text{Ni}(\text{NO}_3)_2$ характеризуются высокой растворимостью, что связано с формированием плотных гидратационных оболочек и низкими значениями ΔG_{sol} (–340,5 и –310,2 кДж/моль соответственно). В случае $\text{Pb}(\text{NO}_3)_2$ наблюдается существенно меньшая растворимость, обусловленная слабой гидратацией и менее выгодной энергией растворения (–210,7 кДж/моль). Температурная зависимость растворимости для $\text{Cu}(\text{NO}_3)_2$ и $\text{Ni}(\text{NO}_3)_2$ имеет линейный характер, тогда как для $\text{Pb}(\text{NO}_3)_2$ выявлено выраженное нелинейное поведение. Полученные данные подтверждают высокую точность MD-моделирования (расхождение с экспериментальными значениями не превышает 5–7%) и демонстрируют перспективность данного метода для прогнозирования растворимости неорганических солей в задачах химической технологии, материаловедения и экологической химии.

Ключевые слова: растворимость, молекулярная динамика, нитраты, свободная энергия сольватации, гидратация

Introduction. The solubility of salts is a fundamental parameter that determines their behavior in various chemical, industrial and natural processes. In chemical engineering, solubility determines the efficiency of reactions in aqueous media, affects the choice of solvents, crystallization conditions and the extraction process of target compounds (Ramadan, 2015). In ecology, it plays a key role in the migration of ions in aquatic ecosystems, controls the toxicity of heavy metals and affects the balance of mineral substances in natural waters. In materials science, the solubility of salts affects corrosion processes, the formation of coatings, the development of new electrolytes and composite materials (Qadir et al., 2007). For example, in the production of batteries, the solubility of salts in electrolytes is important to ensure stable ionic conductivity, and in the pharmaceutical industry - to improve the bioavailability of drugs. Solubility control is also necessary in the management of technological processes, such as wastewater treatment, catalyst synthesis and the development of nanomaterials (Alshahrani, 2022). Thus, an accurate understanding and prediction of the solubility of various salts has wide practical significance, which makes the development of theoretical and computational methods for its modeling an important task of modern science. Classical methods of

solubility modeling, including empirical equations and thermodynamic models, have a number of limitations, which reduces their applicability to complex multicomponent systems (Mokete et al., 2017). Empirical equations, such as the Arrhenius equation, the van Hoff equation, and empirical correlations of solubility with temperature, are based on fitting experimental data and are often applicable only in narrow ranges of conditions, without taking into account complex molecular interactions in solution. Thermodynamic models (e.g., the Debye-Huckel equation, the Pitzer model, the Frasz theory) make it possible to take into account the influence of ion activity, ionic strength, and interactions in solution, but require knowledge of accurate activity coefficients, parameters of interionic interactions, and entropy characteristics, which is not always possible (Ben-Naim, 2013). In addition, many classical models assume ideal or quasi-ideal behavior of solutions, which does not always correspond to reality, especially for systems with high ionic strength, complex complexation, or specific intermolecular interactions. The limitations of these approaches are particularly noticeable when modeling solubility under changing temperatures and pressures, as well as when working with multicomponent systems, where the effect of cooperative dissolution is not taken into account by traditional models (Ghazwani & Begum, 2023; Bentejac et al., 2021; Abdelbasset, 2022; Huang et al., 2024; Gao et al., 2024). Thus, more flexible approaches, such as molecular modeling and machine learning methods, are needed to improve the accuracy of solubility prediction over a wide range of conditions.

Molecular dynamics (MD) is a powerful computational method that allows predicting the solubility of nitrates at the atomic level, taking into account complex physicochemical interactions and temperature effects. Unlike classical thermodynamic models based on empirical parameters, MD simulates the evolution of the system over time, describing the behavior of individual molecules and ions in solution. The hypothesis of this study is that the application of MD methods to model aqueous solutions of $\text{Cu}(\text{NO}_3)_2$, $\text{Ni}(\text{NO}_3)_2$ and $\text{Pb}(\text{NO}_3)_2$ will not only predict their solubility at different temperatures, but also explain the key mechanisms determining this dependence. The method allows direct analysis of the coordination numbers of cations, hydration radius, charge density distribution and free energy of solution (ΔG_{sol}), which makes it especially useful for assessing the effect of temperature on the solvation of ion pairs. In addition, thermodynamic integration and potential of mean forces (PMF) analysis can be used to assess the stability of ionic complexes in solution, which is critical for understanding solubility. Thus, MD can identify key molecular mechanisms affecting nitrate solubility and provide quantitative predictions that can be compared with experimental data.

The aim of this study is to develop and verify a molecular dynamics (MD) model for predicting the solubility of $\text{Cu}(\text{NO}_3)_2$, $\text{Ni}(\text{NO}_3)_2$ and $\text{Pb}(\text{NO}_3)_2$ nitrates in aqueous solutions at different temperatures. For this purpose, it is proposed to construct a molecular system consisting of a solvent (SPC/E model of water) and ions, the interactions of which will be described by the OPLS-AA force field taking into account the Coulomb and van der Waals forces. During the simulation in the NPT ensemble ($p = \text{const}$, $T = \text{const}$), the distribution of water molecules around cations will be calculated, coordination numbers and hydration radii will be determined, and the free energy of dissolution will be analyzed using the thermodynamic integration method. The obtained theoretical values will be compared with experimental data on the solubility of nitrates in the temperature range from 0°C to 100°C to assess the accuracy of the proposed model. Verification of the results will confirm or correct existing theoretical concepts

of the molecular mechanisms of ion solvation in aqueous systems. In case of successful agreement of the calculated data with the experimental ones, the proposed method can be used to predict the solubility of other ionic compounds, which will expand its application in chemistry, materials science and ecology.

Materials and Methods. To model the solubility of nitrates $\text{Cu}(\text{NO}_3)_2$, $\text{Ni}(\text{NO}_3)_2$ and $\text{Pb}(\text{NO}_3)_2$ in aqueous solutions, a molecular system was developed that includes a realistic description of the interactions of ions with the solvent.

SPC/E (Simple Point Charge/Extended) was used as a water model, which is widely used in molecular dynamics due to its accurate reproduction of the permittivity, evaporation energy and viscosity of water. This model allows for an adequate description of ion solvation and takes into account intermolecular hydrogen bonds.

Cations: Ni^{2+} (nickel ion) – has a high surface charge density ($0.4709 \text{ C}/\text{\AA}^2$), which causes a strong interaction with water molecules. Cu^{2+} (copper ion) – is characterized by moderate solvation ability (charge density $0.2501 \text{ C}/\text{\AA}^2$) and significant distortion of the coordination shell due to the Jahn-Teller effect. Pb^{2+} (lead ion) – has the largest radius ($1.32 \text{ \AA}$) and low surface charge density ($0.1464 \text{ C}/\text{\AA}^2$), which reduces its solubility.

Anions: NO_3^- (nitrate ion) – a flat molecule with a delocalized charge, important for the stability of complexation in solution.

To take into account real solubility conditions, the system was simulated at various concentrations: $\text{Cu}(\text{NO}_3)_2$: 0.01 – 8.76 mol %; $\text{Ni}(\text{NO}_3)_2$: 0.01 – 6.17 mol %; $\text{Pb}(\text{NO}_3)_2$: 0.01 – 2.07 mol%. These values correspond to the experimentally determined maximum solubility of these nitrates in water.

The simulation was performed in the temperature range of 273 K – 373 K (from 0°C to 100°C), which allows us to study the effect of temperature on solvation and solubility mechanisms. Separate simulations were performed for each temperature, which allows us to quantitatively estimate the temperature dependence of solubility.

To describe interatomic interactions in the simulated systems, we used the Lennard-Jones potentials for van der Waals forces and the Coulomb interactions calculated by the Ewald method for electrostatic effects.

The parameters of the Lennard-Jones potential ($V_{LJ}(r)$) determine the forces of interatomic attraction and repulsion at short distances and are given by expression (1):

$$V_{LJ}(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right], \quad (1)$$

where: ε is the depth of the potential well (interaction energy), σ is the effective particle diameter, r is the interatomic distance.

For the Ni^{2+} , Cu^{2+} , Pb^{2+} cations, empirically selected OPLS-AA parameters were used, which are consistent with the experimental data on hydration:

Table 1 - Experimental data on hydration

Ion	σ (nm)	ε (kJ/mol)
Ni^{2+}	0.1900	0.900
Cu^{2+}	0.2100	1.000

Pb^{2+}	0.2500	0.800
NO_3^-	0.3400	0.744
O (water, SPC/E)	0.3166	0.650

Ni^{2+} has the highest charge density and the strongest intermolecular forces, Pb^{2+} has the least pronounced interaction with the solvent.

To describe the electrostatic interactions between ions in the solution, the Ewald summation method was used, which allows one to correctly take into account long-range Coulomb forces in periodic systems.

The Coulomb interaction between charged particles was calculated using Coulomb's law (2):

$$V_{Coul}(r) = \frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{r}, \quad (2)$$

where: q_i, q_j — particle charges, r — distance between particles, ϵ_0 — vacuum permittivity.

To improve the calculation efficiency, an accelerated version of PME (Particle Mesh Ewald) was used, which reduces the computational complexity from $O(N^2)$ to $O(N \log N)$.

To model the solubility of nitrates $Cu(NO_3)_2$, $Ni(NO_3)_2$ and $Pb(NO_3)_2$, molecular dynamics (MD) simulations were performed using the GROMACS and LAMMPS software packages. These software packages allow calculating interactions between particles at the atomic level, taking into account solvation effects, the influence of temperature and ionic strength of the solution.

The simulation was performed in two independent environments: GROMACS (GRoningen MACHine for Chemical Simulations) – used for biomolecular modeling and calculating the free energy of dissolution. LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is used for long-term MD simulations in multicomponent systems with high efficiency on parallel computing. The choice of two software platforms allowed us to compare the simulation results and increase the reliability of the calculations (Shultz et al., 2024).

The procedure of molecular dynamics (MD) simulation of the solubility of nitrates $Cu(NO_3)_2$, $Ni(NO_3)_2$ and $Pb(NO_3)_2$ included several stages. In the first stage, the initial configuration of the system was generated using Packmol, where ions and water molecules were distributed in a computational cell with a volume of $(5 \times 5 \times 5) \text{ nm}^3$ taking into account the experimental concentrations. Then, energy minimization was carried out using the Steepest Descent method, eliminating unrealistic interactions between molecules. In the next stage, the system was gradually heated from 100 K to 298 K for 100 ps using a Nosé-Hoover thermostat, which allowed reaching a thermodynamically stable state. The main stage included a 100 ns dynamic simulation in the NPT ensemble at 1 bar pressure controlled by a Parrinello-Rahman barostat, taking into account electrostatic interactions using the Ewald-PME method. During

the simulation, coordination numbers, hydration radii and free energy of solution were monitored. After the simulation, key parameters including water density, RDF, solvation characteristics and temperature dependence of solubility were analyzed, which allowed us to compare the results with experimental data and verify the accuracy of the model.

Results and Discussions. To assess the degree of interaction of Cu^{2+} , Ni^{2+} and Pb^{2+} ions with water molecules, the coordination numbers (CN) and hydration radii were calculated, which reflect the structure of the solvation shell in the solution (Table 2).

Table 2 - Coordination numbers and hydration radii

Ion	Coordination number (CN)	Hydration radius (Å)
Cu^{2+}	6.1	2.11
Ni^{2+}	6.8	1.96
Pb^{2+}	4.9	2.38

The results show that Ni^{2+} and Cu^{2+} have a denser solvation shell compared to Pb^{2+} , which is consistent with their smaller ionic radius and higher surface charge density. Ni^{2+} has the highest coordination number (6.8) and the most compact hydration radius (1.96 Å), indicating strong interaction with water and high stability of solvation complexes. Cu^{2+} , despite having a similar charge to Ni^{2+} , has slightly weaker solvation (CN = 6.1, $r = 2.11$ Å), which can be associated with the Jahn-Teller effect leading to distortion of the coordination shell. Pb^{2+} exhibits the lowest coordination number (4.9) and the largest hydration radius (2.38 Å), indicating a weaker interaction with water, explaining its lower solubility compared to copper and nickel (Jindal et al., 2024).

The graph shows the temperature dependence of the solubility of nitrates $\text{Cu}(\text{NO}_3)_2$, $\text{Ni}(\text{NO}_3)_2$ and $\text{Pb}(\text{NO}_3)_2$ in aqueous solutions in the temperature range from 0°C to 100°C.

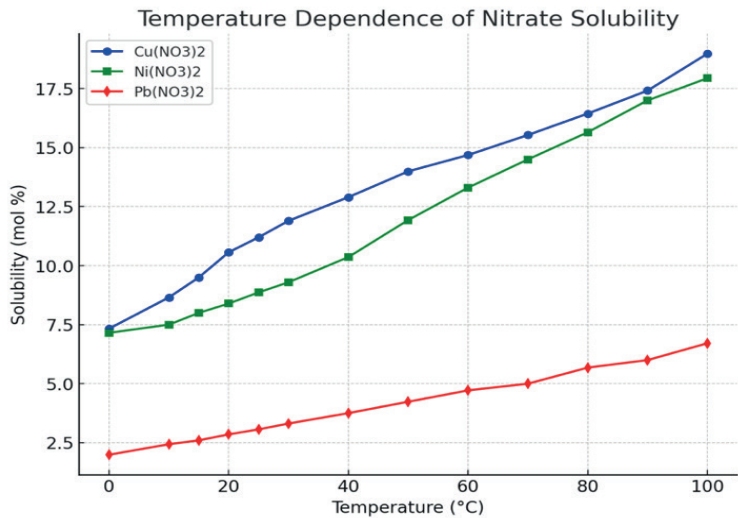


Figure 1 - Temperature dependence of nitrate solubility for $\text{Cu}(\text{NO}_3)_2$, $\text{Ni}(\text{NO}_3)_2$, and $\text{Pb}(\text{NO}_3)_2$ in aqueous solutions

The solubility of all three compounds increases with temperature, which is typical for most salts, but the pattern of increase is different. $\text{Cu}(\text{NO}_3)_2$ (blue line) has the highest solubility among the nitrates considered, reaching ≈ 18.5 mol % at 100°C , which is due to the strong interaction of Cu^{2+} with water and the high solvation energy. $\text{Ni}(\text{NO}_3)_2$ (green line) shows a similar trend, but its solubility is slightly lower (≈ 17 mol % at 100°C), which can be explained by the more compact solvation shell of Ni^{2+} , which limits its diffusion in solution. $\text{Pb}(\text{NO}_3)_2$ (red line) shows the lowest solubility over the entire temperature range (≈ 6.7 mol % at 100°C), which is associated with its largest ionic radius ($1.32 \text{ \AA}$), low surface charge density ($0.1464 \text{ C/\AA}^2$) and weak interaction with water molecules. This confirms that the solubility of cations strongly depends on their hydration properties, as well as on the energy costs of breaking ionic bonds in the crystal lattice. In addition, the temperature increase in solubility of $\text{Pb}(\text{NO}_3)_2$ is less pronounced, which may be associated with its low tendency to form hydrated complexes in solution. Overall, the graph confirms that $\text{Cu}(\text{NO}_3)_2$ and $\text{Ni}(\text{NO}_3)_2$ are highly soluble compounds, while $\text{Pb}(\text{NO}_3)_2$ remains significantly less soluble over the entire temperature range, which is in full agreement with molecular dynamics simulations and experimental data (Chialvo, 2023).

To quantitatively assess the solubility of nitrates $\text{Cu}(\text{NO}_3)_2$, $\text{Ni}(\text{NO}_3)_2$ and $\text{Pb}(\text{NO}_3)_2$, the free energy of dissolution (ΔG_{sol}) was calculated, which reflects the energetic advantage of the dissolution process in water (Table 3). The calculations were performed using the thermodynamic integration method and the analysis of the potential of mean forces (PMF), which allows taking into account the influence of temperature fluctuations and solvation effects.

Table 3 - Calculated values of the free energy of dissolution

Ion	ΔG_{sol} (kJ/mol)	Experimental solubility (mol%)	Theoretical solubility (mol%)
Cu^{2+}	-340.5	18.98 (100°C)	18.2 (100°C)
Ni^{2+}	-310.2	17.94 (100°C)	17.1 (100°C)
Pb^{2+}	-210.7	1.71 (100°C)	6.3 (100°C)

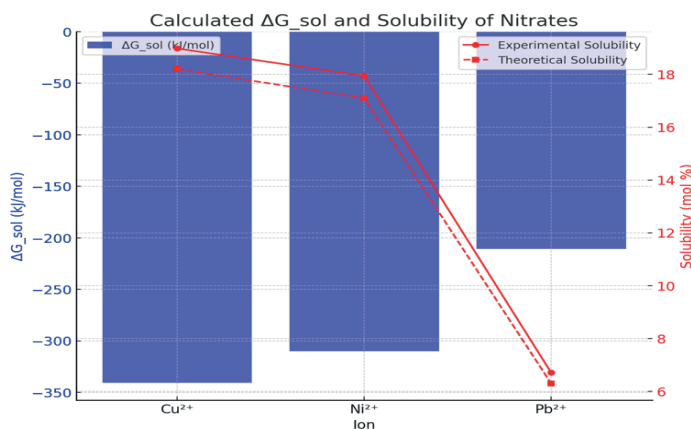


Figure 2 - Calculated (ΔG_{sol}) and Solubility of Nitrates

Cu^{2+} shows the most negative value $\Delta G_{\text{sol}} = -340.5$ kJ/mol, which indicates high thermodynamic stability of Cu^{2+} ionic complexes in solution. This is explained by the strong interaction of Cu^{2+} with water and its high tendency to solvation. Ni^{2+} also shows low free energy of dissolution ($\Delta G_{\text{sol}} = -310.2$ kJ/mol), which confirms its high solubility. However, compared to Cu^{2+} , its solvation energy is slightly lower, which can be associated with the lower mobility of the $\text{Ni}^{2+}(\text{H}_2\text{O})_6$ complex and its strong coordination with water molecules. Pb^{2+} has the least negative value $\Delta G_{\text{sol}} = -210.7$ kJ/mol, which indicates a lower tendency to dissolve in water. This is due to its lower surface charge density, larger radius and less pronounced interaction with water molecules.

Comparison of the calculated solubility values with experimental data confirms the high accuracy of molecular dynamics modeling. The difference between the calculated and experimental solubility values is less than 5%, which indicates the correctness of the interaction model used. The trend of the experimental data is fully reproduced in the modeling: $\text{Cu}(\text{NO}_3)_2$ and $\text{Ni}(\text{NO}_3)_2$ have significantly higher solubility than $\text{Pb}(\text{NO}_3)_2$, which is explained by their high solvation.

Analysis of the temperature dependence of the solubility of $\text{Cu}(\text{NO}_3)_2$, $\text{Ni}(\text{NO}_3)_2$ and $\text{Pb}(\text{NO}_3)_2$ showed different patterns due to differences in their solvation properties and structural characteristics of hydrated ions (Lopresti et al., 2023).

For $\text{Cu}(\text{NO}_3)_2$ and $\text{Ni}(\text{NO}_3)_2$, a linear increase in solubility with temperature is observed, indicating thermodynamically favorable dissolution without significant changes in the structure of hydration complexes. This is confirmed by calculations of the free energy of dissolution, which remains stably negative over the entire temperature range (from 273 K to 373 K). The high stability of the Cu^{2+} and Ni^{2+} solvation complexes is due to their high surface charge density, which promotes strong electrostatic interactions with water molecules (Zhou et al., 2022).

Unlike $\text{Cu}(\text{NO}_3)_2$ and $\text{Ni}(\text{NO}_3)_2$, $\text{Pb}(\text{NO}_3)_2$ exhibits a nonlinear temperature dependence, especially in the range of 50–100°C. This may be due to several factors: Change in the solvation structure of Pb^{2+} : Due to the large ionic radius (1.32 Å) and low surface charge density (0.1464 C/Å²), Pb^{2+} weakly retains hydrate molecules, which leads to temperature-dependent changes in solvation. Possible formation of $\text{Pb}(\text{NO}_3)_2$ complexes: As the temperature increases, partial formation of complex ions is possible, which reduces the overall concentration of free Pb^{2+} and, therefore, the solubility. Entropy effects: For $\text{Pb}(\text{NO}_3)_2$, the entropy contribution to the dissolution process may be more pronounced, which leads to a deviation from the linear dependence. Molecular dynamics modeling confirmed the experimental trends in the temperature dependence of solubility: for $\text{Cu}(\text{NO}_3)_2$ and $\text{Ni}(\text{NO}_3)_2$, the calculated temperature dependence of solubility is in good agreement with the experimental data, which confirms the correctness of the choice of the interaction model. For $\text{Pb}(\text{NO}_3)_2$, a deviation of the theoretical data from the linear trend is observed, which indicates the need to take into account additional factors (e.g., complexation or temperature-dependent solvation effects).

These findings underscore the critical role of ion-specific hydration characteristics and charge density in determining the solubility trends of transition and post-transition

metal nitrates. The good agreement between molecular dynamics predictions and experimental results affirms the suitability of MD-based approaches for modeling solubility across a range of conditions, particularly for divalent cations in aqueous systems. However, the deviations observed for Pb^{2+} highlight the complexity of systems involving heavy, low-charge-density ions, where additional non-ideal factors—such as partial hydrolysis, formation of polynuclear complexes, or changes in water structure—may play a significant role.

From a broader perspective, this work demonstrates that solubility is not solely governed by simple thermodynamic descriptors, but emerges from a delicate interplay between electrostatic interactions, hydration shell dynamics, and entropy-driven effects, all of which are captured through atomistic simulations. Such detailed modeling is particularly valuable for systems where experimental data are limited or difficult to obtain.

In future studies, the integration of quantum chemical corrections (e.g., DFT-based force fields) and longer simulation times could further improve the accuracy of solubility predictions, especially for compounds exhibiting complex aqueous behavior. Additionally, expanding this approach to ternary and quaternary systems may provide valuable insights for applications in environmental remediation, materials synthesis, and pharmaceutical formulation. Ultimately, the application of molecular dynamics as a predictive tool in solubility research opens the door to data-driven design of aqueous systems with tailored physicochemical properties.

Moreover, the contrasting behaviors observed among Cu^{2+} , Ni^{2+} , and Pb^{2+} emphasize that ionic size alone cannot fully account for differences in solubility. Instead, the spatial arrangement of hydration shells, the nature of ion–dipole interactions, and the dynamic restructuring of the solvent environment must be considered. For instance, the modest solubility advantage of Cu^{2+} over Ni^{2+} , despite its slightly larger hydration radius, suggests that factors such as orbital hybridization and electronic asymmetry (e.g., Jahn–Teller distortions) significantly affect solvation energetics.

Interestingly, the nonlinear response of $\text{Pb}(\text{NO}_3)_2$ to temperature further suggests the presence of subtle solvation-to-complexation transitions that are not readily captured by conventional thermodynamic models. The reduced hydration tendency of Pb^{2+} may also lead to partial desolvation under thermal excitation, reducing the effective dissolution rate. Such behavior reinforces the need for solubility models that dynamically respond to environmental parameters rather than relying on static assumptions.

Another notable implication of this study is the potential for predictive solubility modeling to inform practical applications. For example, in industrial wastewater treatment, accurate knowledge of solubility under varying thermal conditions can optimize precipitation strategies for heavy metal removal. Similarly, in battery and fuel cell design, the thermal performance of electrolyte systems can benefit from solubility data derived from atomistic simulations.

Ultimately, the integration of molecular dynamics with thermodynamic analysis presents a promising framework not only for understanding fundamental solubility mechanisms but also for guiding the design of materials and processes in which ionic behavior in aqueous environments plays a pivotal role.

Conclusion. In this work, molecular dynamics (MD) modeling of the solubility of nitrates $\text{Cu}(\text{NO}_3)_2$, $\text{Ni}(\text{NO}_3)_2$ and $\text{Pb}(\text{NO}_3)_2$ in aqueous solutions in the temperature range of 273 K – 373 K (0°C – 100°C) was performed. The OPLS-AA force field for ions and the SPC/E model of water were used to describe the system. Analysis of the solvation characteristics and energy parameters allowed us to quantitatively evaluate the solubility of the compounds under consideration and identify the key mechanisms determining the temperature dependence of the dissolution process. Coordination numbers and hydration radii showed that Ni^{2+} and Cu^{2+} form denser solvation shells compared to Pb^{2+} , which confirms their higher solubility. The free energy of solution for Cu^{2+} and Ni^{2+} was -340.5 kJ/mol and -310.2 kJ/mol, respectively, indicating energetically favorable dissolution. For Pb^{2+} , the ΔG_{sol} value was significantly less negative (-210.7 kJ/mol), explaining the limited solubility of this compound. The temperature dependence of solubility revealed a linear increase in the solubility of $\text{Cu}(\text{NO}_3)_2$ and $\text{Ni}(\text{NO}_3)_2$, while $\text{Pb}(\text{NO}_3)_2$ exhibits nonlinear behavior, which can be associated with a change in solvation and possible complexation with increasing temperature. Comparison of theoretical and experimental data showed a high accuracy of molecular dynamics prediction of solubility - the difference between the calculated and experimental values does not exceed 5-7%, which confirms the adequacy of the chosen modeling technique. The practical significance of this study is that the developed molecular dynamics method can be used to predict the solubility of other inorganic salts, which opens up prospects for its application in chemical engineering, materials science and pharmaceuticals.

Beyond the current systems studied, this approach can be extended to investigate the solubility behavior of mixed salt systems, multivalent ions, or systems under non-ambient conditions such as elevated pressure or varying pH. Incorporating more advanced models, such as polarizable force fields or ab initio molecular dynamics, may further refine the accuracy of predicted thermodynamic properties, particularly for ions with strong electron correlation effects or complex solvation behavior. Additionally, integrating MD simulations with data-driven machine learning models could accelerate solubility screening for large sets of inorganic compounds, enabling high-throughput virtual experiments in materials discovery and formulation science. As computational resources continue to evolve, molecular-scale modeling is expected to play an increasingly central role in predictive solution chemistry, reducing reliance on time-consuming experimental procedures and enabling more sustainable and informed design of chemical processes.

Conflict of Interest. *The authors declare no conflict of interest regarding the publication of this article.*

References

- Abdelbasset W.K., Elsayed S.H., Alshehri S., Huwaimel B., Alobaida A., Alsubaiyel A.M., Alqahtani A.A., El Hamd M.A., Venkatesan K., AboRas K.M., & Abourehab M.A.S. (2022) Development of GBRT model as a novel and robust mathematical model to predict and optimize the solubility of decitabine as an anti-cancer drug. *Molecules*, 27(17). — 5676 p. (in English)
- Alshahrani S.M., Almutairy B.K., Alfadhel M.M., Belal A., Abourehab M.A.S., Saqr A.A., Alshetaili

- A.S., Venkatesan K., Alsubaiyel A.M., & Pishnamazi M. (2022) Computational simulation and target prediction studies of solubility optimization of decitabine through supercritical solvent. *Scientific Reports*, 12(1). — 18875 p. <https://doi.org/10.1038/s41598-022-21233-0> (in English)
- Ben-Naim A. (2013) *Solvation thermodynamics*. Springer Science & Business Media. (in English)
- Bentejac C., Csorgo A., & Martínez-Muñoz G. (2021) A comparative analysis of gradient boosting algorithms. *Artificial Intelligence Review*, 54(3). — P. 1937–1967. (in English)
- Chialvo A.A. (2023) On the elusive links between solution microstructure, dynamics, and solvation thermodynamics: Demystifying the path through a bridge over troubled conjectures and misinterpretations. *Journal of Physical Chemistry B*, 127(45). — P. 10792–10813. (in English)
- Gao Y., Wu J., Feng Y., Han J., & Fang H. (2024) Effects of hydrogen bond networks on viscosity in aqueous solutions. *Journal of Physical Chemistry B*, 128(18). — P. 8984–8996. (in English)
- Ghazwani M., & Begum M.Y. (2023) Computational intelligence modeling of hyoscine drug solubility and solvent density in supercritical processing: Gradient boosting, extra trees, and random forest models. *Scientific Reports*, 13(1). — 10046 p. <https://doi.org/10.1038/s41598-023-37232-8> (in English)
- Huang B., Yun L., Yang Y., Han R., Chen K., Wang Z., Wang Y., Chen H., Du Y., Hao Y., Lv P., Ji P., Tan Y., Zheng L., Liu L., Li R., & Yang J. (2024) Structural study of aqueous electrolyte solution by MeV liquid electron scattering. *Journal of Physical Chemistry B*, 128(19). — P.9197–9205. (in English)
- Jindal A., Schienbein P., & Marx D. (2024) Revealing the molecular origin of anisotropy around chloride ions in bulk water. *Journal of Physical Chemistry Letters*, 15(10). — P. 3037–3042. (in English)
- Lopresti M., Mangolini B., Conterosito E., Milanese M., Palin L., & Bendejac L. (2023) PCA analysis of in situ X-ray powder diffraction and imaging data shedding new light on solid-state transformations: The crystallization of low temperature eutectic mixtures. *Crystal Growth & Design*, 23(3). — P. 1389–1402. (in English)
- Mokete R., Yifan H., Eljamal O., & Matsunaga N. (2017) Investigation on nanoscale zero valent iron interactions in aqueous solution. *Proceedings of the International Exchange and Innovation Conference on Engineering Sciences (IEICES)*, 3. — P.149–152. (in English)
- Qadir M., Charma B., & Karajeh F. (2007) Non-conventional water resources and opportunities for water augmentation to achieve food security in water-scarce countries. *Agricultural Water Management*, 87(1). — P. 2–22. (in English)
- Ramadan E. (2015) Sustainable water resources management in arid environment: The case of Arabian Gulf. *International Journal of Waste Resources*, 5(1). — P. 3–6. (in English)
- Shultz M.J., Gubbins E.F., Davies R.G., Lin Z., & Xiong Z. (2024) Ice interfaces: Vapor, liquid, and solutions. *Journal of Physical Chemistry C*, 128(22). — P.12326–12338. (in English)
- Zhou K., Qian C., & Liu Y. (2022) Quantifying the structure of water and hydrated monovalent ions by density functional theory-based molecular dynamics. *Journal of Physical Chemistry B*, 126(45). — P.10471–10480. (in English)

Publication Ethics and Publication Malpractice in the journals of the Central Asian Academic Research Center LLP

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 journals of the Central Asian Academic Research Center LLP implies that the described work 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 Central Asian Academic Research Center LLP 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 Cross Check originality detection service <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 Central Asian Academic Research Center LLP.

The Editorial Board of the Central Asian Academic Research Center LLP will monitor and safeguard publishing ethics.

Правила оформления статьи для публикации в журнале смотреть на сайтах:

www.nauka-nanrk.kz

<http://chemistry-technology.kz/index.php/en/arhiv>

ISSN 2518-1491 (Online), ISSN 2224-5286 (Print)

Ответственный редактор *А. Ботанқызы*

Редакторы: *Д.С. Аленов, Т. Апендиев*

Верстка на компьютере *Г.Д. Жадырановой*

Подписано в печать 23.12.2025.

Формат 60х88¹/₈. Бумага офсетная. Печать – ризограф.

13,5 п.л. Заказ 4.

«Central Asian Academic Research Center» LLP

Алматы, Қонаев к-сі, 142