**Brief summary about the project**

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| IRN and project name: | AP08856049 "Metal-organic coordination polymers based on azoles: synthesis, properties research, obtaining new multifunctional materials" |
| Implementation Timeline: | 27.11.2020-31.12.2022 |
| Relevance: | Despite the fundamental interest and wide range of properties of MOCPs, one of the problems in this field of organic synthesis is the limited synthesis methods. The present project aims to address this problem by utilizing the diazotization reaction of aminoheterocycles in the synthesis of ligands. The obtained compounds will be of interest both as ligands and as independent entities due to the high probability of biological activity. |
| Goal: | Synthesis of new metal-organic coordination polymers of carboxylate, azolate and mixed types based on pyridines, triazoles, imidazoles and pyrazoles and study of their properties |
| Expected and achieved results: | **Expected results**a) synthesis, structure and reactivity studies of heteroaromatic diazonium sulfonates;b) synthesis of carboxy-substituted 1,2,3-triazoles from amino derivatives of pyridines, triazoles, imidazoles and pyrazoles by diazotization reaction followed by reactions of nucleophilic substitution of diazo group on azido group and 1,3-dipolar cycloaddition (catalytic variant of Huisgen reaction), proof of structure of the obtained derivatives;c) construction of metal-organic frameworks by two- and three-component reactions of transition metal salts (copper, cobalt, nickel, manganese, zinc, silver, lanthanides in the form of chlorides, nitrates, tetrafluoroborates, acetylacetonates, acetates, perchlorates) with synthesized bitopic and polytopic ligands, proof of the structure of the obtained metal-organic polymer complexes (X-ray structural analysis).d) study of physicochemical properties of the obtained MOCPs (sorption capacity, luminescent activity, reactivity in condensation, oxidation and cross-coupling reactions).**Achieved results**The synthesis, structure and reactivity of heterocyclic diazonium sulfonates have been carried out. New heteroaromatic diazonium salts, their structure and reactivity were studied. Carboxy-substituted 1,2,3-triazoles derivatives from amino derivatives of pyridines, triazoles, imidazoles and pyrazoles were prepared by diazotization reaction followed by nucleophilic substitution of diazo group on azido group and 1,3-dipolar cycloaddition (catalytic variant of Huesgen reaction). The conditions for the effective reaction of azide-alkyne cycloaddition with product yields from 60 to 95% have been selected. The structure of all synthesized compounds was proved by NMR spectroscopy, IR spectroscopy and comparison of melting point depressions for known samples.The first examples of metal-organic frameworks with synthesized bitopic and polytopic ligands were obtained. Their spectral properties (electron spectroscopy and luminescence spectra) have been studied. It is shown that the linker:metal salt ratio affects the structure of the resulting metal-organic polymer.**Approbation of the results of the study**The results of the research were presented at: XVI International Scientific Conference "Gylym zhane bılım - 2021" (Nur-Sultan, diploma of the 2nd degree), International Scientific Conference "Satpayev Readings - 2021" (Almaty, diploma for the best report), as well as in the Republican competition of research works on specialty Chemical Technology (diploma of the 2nd degree).The results of the study were presented at the VI International Symposium "Chemistry of Diazo Compounds and Related Systems Diazo-2021" held in the framework of the XII International Conference of Young Scientists in Chemistry "Mendeleev-2021" (St. Petersburg, Russia). The published works are cited by RINC.1. Aromatic and heteroaromatic diazonium trifluoromethanesulfonates: synthesis and investigation of properties / Estaeva M.T., Kassanova A.Zh. // VI International Symposium `The Chemistry of Diazo compounds and related Systems`. - S-Pb: SPbSU, 2021. - P. 47.2. Preparation of 1.2.3-triazoles by the reaction of azide-alkyne cycloaddition / Kisselev O.V., Snopkov D.I., Kassanova A.Zh. // VI International Symposium `The Chemistry of Diazo compounds and related Systems`. - S-Pb: SPbSU, 2021. - P. 62.2 articles in a peer-reviewed foreign and (or) domestic publication with non-zero impact factor (recommended by the Committee for Quality Assurance in the Sphere of Education of the Ministry of Education of the Republic of Kazakhstan) have been sent for printing. 1 Quantum-chemical study of characteristics of carboxy-containing ligands for metal-organic polymers / Kasanova A.J., Estaeva M.T., Kiselev O.V., Snopkov D.I. // Chemical Journal of Kazakhstan. - In Press. (4 issue) 2 Arenediazonium sulfonates: synthesis, comparison of structural and physico-chemical properties / Kassanova A.Zh., Yestayeva M.T., Turtubayeva M.O. // Bulletin of the University of Karaganda - Chemistry, 105(1), ??-??? https://doi.org/10.31489/2022Ch1/??-??? In Press. (1 issue, 2022). |
| Composition of the research team |
|  | Kassanova Asiya Zhursunovna |
| Position in the project Scientific director of the project |
| Date of birth: 28.01.1990 |
| Candidate of Chemical Sciences, Associate Professor |
| Primary employment: "Toraighyrov University" |
| Research interests: features of disodiumation of aromatic and heteroaromatic amines in the presence of sulfonic acids, preparation of new compounds on the basis of diazotization reaction. |
| Researcher ID \* 12000012195 |
| Scopus Author ID\* 56205473600 |
| ORCID\* <https://orcid.org/0000-0002-9563-5521>  |
| List of publications\*\* and patents \* 1. Kasanova A.J., Krasnokutskaya E.A., Filimonov V.D. Pyridinyltrifluoromethanesulfonates: methods of preparation and use in organic synthesis. Izvestiya Akademiya Nauki. Series Chemical, 2016, 11, 2559-2567. http://portal.tpu.ru:7777/SHARED/a/ASIYAKASS/publications/Tab/IAN2559pdf2. Synthesis, Structure, and Synthetic Potential of Arenediazonium Trifluoromethanesulfonates as Stable and Safe Diazonium Salts / V. D. Filimonov, E. A. Krasnokutskaya, A. Zh. Kassanova, V. A. Fedorova, K. S. Stankevich, N. G. Naumov, V. A. Kataeva // EurJOC. – 2019. – Р. 665–674. https://onlinelibrary.wiley.com/doi/abs/10.1002/ejoc.201800887 (IF 3.09)3. A novel convenient synthesis of pyridinyl and quinolinyltriflates and tosylates via one-pot diazotization of aminopyridines and aminoquinolines in solutions / A. Zh. Kassanova, E. A. Krasnokutskaya, P. S. Beisembai, V. D. Filimonov // Synthesis. – 2016. – № 48. – Р. 256–262. thieme-connect.com/products/ejournals/pdf/10.1055/s-0035-1560394.pdf (IF 2.65)4. One-pot synthesis of chloropyridines from aminopyridines via diazotization / Yu. A. Lesina, A. Zh. Kassanova, P. S. Beysembay // Key Engineering Materials. – 2016. – Vol. 712. – P. 273–276. https://www.scientific.net/KEM.712.273 (IF 0.4)5. Pyridinyl trifluoromethanesulfonates: preparation methods and use in organic synthesis / A. Zh. Kassanova, E. A. Krasnokutskaya, V. D. Filimonov // Russian Chemical Bulletin: Scientific Journal. – 2016. – Vol. 65, iss. 2. – P. 2559–2567. https://link.springer.com/article/10.1007/s11172-016-1619-1 (IF 0.31)6. The first study of the thermal and storage stability of arenediazonium triflates comparing to 4-nitrobenzenediazonium tosylate and tetrafluoroborate by calometric metods / A. A. Bondarev, N. G. Naumov, A. Zh. Kassanova, E. A. Krasnokutskaya, K. S. Stankevich, V. D. Filimonov // Organic Process Research and Development. – 2019. - 23 -11. https://pubs.acs.org/doi/10.1021/acs.oprd.9b00307 (IF 3.3)7. Hydrochemical Research and Geochemical Classification of Salt Lakes in the Pavlodar Region / Ubaskin, A., Kassanova, A., Lunkov, A., K. Ahmetov, K. Almagambetova, Erzhanov, N., Abylkhassanov // IOP Conference Series: Materials Science and Engineering. - 2020. - Vol. 754. https://iopscience.iop.org/article/10.1088/1757-899X/754/1/012009 IF 0.19 |
|  | Andrey Sergeyevich Potapov |
| Position in the project Chief Scientist |
| Date of Birth: 31.12.1981 |
| Doctor of Chemical Sciences, Professor |
| Primary employment: Leading Researcher at the Laboratory of Metal-Organicscoordination polymers, A.V. Nikolaev Institute of Inorganic Chemistry. SB RAS (Novosibirsk) |
| Research interests: synthesis of derivatives of nitrogen-containing heterocyclic compounds - azoles, preparation of coordination compounds, including coordination polymers and metal-organic frameworks, study of their sorption, electrochemical and catalytic properties. |
| Scopus Author ID\* 14033131800 |
| ORCID\* <https://orcid.org/0000-0003-2360-7473>  |
| List of publications\*\* and patents \* 1 Synthesis, Crystal Structure, Thermal Analysis, and DFT Calculations of Molecular Copper(II) Chloride Complexes with Bitopic Ligand 1,1,2,2-tetrakis(pyrazol-1-yl)ethane /Lider, E.; Sukhikh, T.; Smolentsev, A.; Semitut, E.; Filatov, E.; **Potapov, A**. // Crystals. – 2019. – 9. – Р. 222. doi: 10.3390/cryst9040222. (IF 2.144, WoS, Q2)2 Exploring the multifunctionality in metal-organic frameworks materials: how do the stilbenedicarboxylate and imidazolyl ligands tune the characteristics of coordination polymers / Barsukova, M. O.; Sapchenko, S. A.; Kovalenko, K. A.; Samsonenko, D. G.; **Potapov, A**.; Dybtsev, D. N.; Fedin, V. P. // New J. Chem. – 2018. – 42. –Р. 6408-6415. doi: 10.1039/C8NJ00494C (IF 3.269, WoS, Q1)3. Crystal structure of a Zn complex with terephthalate and 1,6-bis(1,2,4-triazol-1-yl)hexane / T.S. Sukhikh, E.Y. Semitut, **A.S. Potapov //** Acta Crystallogr. Sect. E. – 2018. – 74. – Р. 6–9. doi:10.1107/S2056989017017224.4. Synthesis, Crystal Structure, and Luminescent Properties of Novel Zinc Metal–Organic Frameworks Based on 1,3-Bis(1,2,4-triazol-1-yl)propane /Semitut, E. Y.; Sukhikh, T. S.; Filatov, E. Y.; Anosova, G. A.; Ryadun, A. A.; Kovalenko, K. A.; **Potapov, A. S. //** Cryst. Growth Des. – 2017. – 17. – 5559–5567. doi: 10.1021/acs.cgd.7b01133 (IF=4,055, WoS, Q1). |
|  | Turtubaeva Meruert Orazgalievna |
| Position in the project Senior Researcher |
| Date of Birth: 19.05.1988 |
| PhD, Associate Professor |
| Primary employment: "Toraighyrov University" |
| Research interests: X-ray diffraction and thermodynamic studies of new REE-based compounds |
| Scopus Author ID\* 55803859200 |
| List of publications\*\* and patents \*1. New nano-sized (nanocluster) cobalt- cuprate -manganites of lanthane and alkaline metals and their X-ray diffraction study //Investigations of the National Academy of Sciences of the Republic of Kazakhstan. Series "Chemistry and Technology". - Almaty. - 2018. - №3. - С. 67 - 72.2. Synthesis and study of thermodynamic properties of new zincate-manganites NdM2IIznmno6 (MII - Mg, Ca) // [ChemTech](https://www.scopus.com/authid/detail.uri?authorId=55803859200#disabled), 2018, 61(3), pp. 16–20.3. Calorimetric research into the heat capacity of novel nano-sized cobalt(Nickelite)-cuprate-manganites of LaBaMeIICuMnO6 (MeII = Co, Ni) and their thermodynamic properties // [Eurasian Chemico-Technological Journal](https://www.scopus.com/authid/detail.uri?authorId=55803859200#disabled), 2020, 22(1), pp. 27–33.4. Patent for utility model No. 4559. Method of preparation of new semiconductor nanoscale cobalt-cuprato-manganites of lanthanum alkaline-earth metals. 5. Synthesis and x-ray investigation of novel nanostructured copper-zinc manganites of lanthanum and alkali metals // [Eurasian Physical Technical Journal](https://www.scopus.com/authid/detail.uri?authorId=55803859200#disabled)// 2021, 18(1), pp. 2933 |
| D:\с ноута\диас с флешки\Диас данные\фото Диас.jpg | Dias Talgatovich Tolegenov |
| Position in the project Research Associate |
| Date of Birth: 24.03.1992 |
| postgraduate student 2 years |
| Primary employment: "Toraighyrov University" |
| Research interests: building ceramics |
| List of publications\*\* and patents \* 1C25D 3/38 Method of producing a reagent -stabilizer for drilling fluids;2 C25D 3/00 Electrolyte for nickel plating;3 C25D 3/22 Zinc electrolyte. |
|  | Estayeva Makpal Tlemivosovna |
| Project position Junior researcher |
| Date of birth: 22.10.1990 |
| master of engineering and technology |
| Primary employment: "Toraighyrov University" |
| Research interests: aromatic diazonium salts: synthesis, structure and reactivity studies in palladium-catalyzed transformations. |
| ORCID\* 0000-0003-2127-3465 |
| List of publications\*\* and patents \*1. Elena A. Krasnokutskaya, Assiya Zh. Kassanova, Makpal T. Estaeva, Victor D. Filimonov. A new synthesis of pyridinyl trifluoromethanesulfonates via one-pot diazotization of aminopyridines in the presence of trifluoromethanesulfonic acid. Tetrahedron Letters 55 (2014) pp. 3771–3773. (Scopus)2. M.T. Estaeva, A.J. Kasanova, A.G. Fefelova, Synthesis and study of arendiazonium trifluoromethanesulfonates // III International Scientific and Technical Conference of Young Scientists, Postgraduates and Students "High Technology in Modern Science and Technology" March 26-28, 2014 Tomsk - p.250 (Winner of the diploma of 2 degree). 3. A.J. Kasanova, O.V. Kiselev, D.E. Seilkhanova, M.T. Estaeva. Preparation of 1,2,3-triazoles by azide-alkyne cycloaddition reaction. Proceedings of Satpayev Readings "Satpayev Readings -2021", 2021, Almaty - pp. 244-2474 Quantum chemical study of the characteristics of carboxy-containing ligands for metal-organic polymers / Kasanova A.J., Estayeva M.T., Kiselev O.V., Snopkov D.I. // Chemical Journal of Kazakhstan. - In Press. (4 issue)5 Arenediazonium sulfonates: synthesis, comparison of structural and physico-chemical properties / Kassanova A.Zh., Yestayeva M.T., Turtubayeva M.O. // Bulletin of the University of Karaganda - Chemistry, 105(1), ??-??? https://doi.org/10.31489/2022Ch1/??-??? In Press. (1 issue, 2022). |
| C:\Users\erzha\Desktop\Mergalym u4eba\9964408b-d7a2-4742-9220-aaef0307bdc7.jfif | Bayshukir Mergalym Darkhanuly. |
| Project position Lead Engineer |
| Date of birth: 16.09.1996 |
| Master's student of the 1st year of specialty "Chemical Engineering" |
| Primary employment: "Toraighyrov University" |
| Research interests: metal-organic coordination polymers |
|  | Oleg Vasilyevich Kiselev |
| Position in the project laboratory assistant |
| Date of birth: 21.01.2000 |
| 4th year student of the Department of Chemistry and Chemical Technologies |
| Primary employment: "Toraighyrov University" |
| Research interests: preparation of new compounds on the basis of diazotization reaction |
| ORCID\* 0000-0002-4902-8990 |
| Список публикаций\*\* и патентов \* 1 Preparation of 1.2.3-triazoles by the reaction of azide-alkyne cycloaddition / Kisselev O.V., Snopkov D.I., Kassanova A.Zh. // VI International Symposium `The Chemistry of Diazo compounds and related Systems`. - S-Pb: SPbSU, 2021. - P. 62. 2 A.J. Kasanova, O.V. Kiselev, D.E. Seilkhanova, M.T. Estaeva. Preparation of 1,2,3-triazoles by azide-alkyne cycloaddition reaction. Proceedings of Satpayev Readings "Satpayev Readings -2021", 2021, Almaty - pp. 244-2473 Quantum chemical study of the characteristics of carboxy-containing ligands for metal-organic polymers / Kasanova A.J., Estayeva M.T., Kiselev O.V., Snopkov D.I. // Chemical Journal of Kazakhstan. - In Press. (4 issue) |