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| Name      | Development of Novel Metal-Organic Frameworks for Needle Trap Devices to Detect Volatile Organic Pollutants in Environmental Samples                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| Relevance | The relevance of the study is driven by the need to improve the efficiency of environmental pollutant monitoring. The use of MOF sorbents and NTD devices will enhance the accuracy and sensitivity of analysis while simplifying the process. The results will enable the development of modern environmental monitoring tools востребованных in practice.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| Target    | The project aims to develop and synthesize novel MOFs to assemble highly efficient Needle Trap Devices (NTDs) capable of accurately detecting VOC concentrations in environmental objects (air, water, and soil). The project focuses on improving the selectivity and sensitivity of VOC analysis while ensuring the practicality and accessibility of monitoring methods, ultimately enhancing environmental control and human health protection.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| Tasks     | <p>Task 1: Synthesis and characterization of Metal Organic Frameworks (MOFs)</p> <p>Under Task 1, two types of metal organic frameworks will be synthesized: classical ZnMOF-74 and a novel structure ZnMOF-74a. The synthesis will include optimization of conditions for obtaining particles of the desired size (20-250 <math>\mu\text{m}</math>). The physical and chemical properties of the synthesized MOFs, such as structure, morphology, surface area, and thermal stability will be characterized.</p> <p>Task 2: Development and optimization of MOF-Based Needle Trap Devices</p> <p>Under Task 2, novel MOFs will be integrated into the configuration of NTDs, prototypes will be developed and assembled. The influence of configuration parameters on sorption capacity will be studied, and the optimal device parameters will be determined.</p> <p>Task 3: Optimization of VOC Sampling Parameters using MOF-Based NTDs</p> <p>Under Task 3, a study of the impact of temperature and humidity on sampling will be conducted, in order to achieve maximum efficiency. Optimal conditions for active sampling of VOCs will be determined. Sampling protocols will be developed for various environmental samples (air, water, soil), ensuring the technology's adaptability to a wide range of environmental conditions.</p> <p>Task 4: Development of VOC Desorption and Analysis Methods using MOF-Based NTDs.</p> <p>Under Task 4, optimization of VOC thermal desorption conditions (temperature and time) from MOFs and develop a method for analyzing VOCs using gas chromatography-mass spectrometry. The reusability NTDs will be investigated.</p> <p>Task 5: Development of theoretical models for adsorption and desorption of analytes on the MOF surface.</p> |

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|                               | <p>Under Task 5, the competitive adsorption of various analytes will be studied, adsorption isotherms will be obtained and selectivity coefficients will be calculated to understand the mechanisms of interaction between analytes and the MOF surface.</p> <p>Task 6: Validation of VOC Determination Methods using MOF-Based NTDs.</p> <p>Under Task 6 the analytical performance of methods, using MOF-based NTDs (accuracy, sensitivity, selectivity, detection limits) for quantifying VOCs will be evaluated. The effectiveness of MOF-based NTDs will be compared to existing VOC analysis methods in environmental samples.</p> <p>Task 7: Field Testing on Environmental Samples and Development of Operating Procedures for MOF-Based NTDs.</p> <p>Under Task 7, VOC sampling will be conducted in various environmental samples to assess the effectiveness of MOF-based NTDs in real-world conditions. The influence of matrix effects on VOC detection will be analyzed to adapt the devices for use in complex matrices, improving measurement accuracy and robustness. Guidelines for using MOF-based NTDs in environmental sample analysis (air, water, soil) will be developed</p>                                                                                                                                                                                                                                                                     |
| Expected and achieved results | <p>1) During the project implementation, research results will be published according to one of the following options:</p> <ul style="list-style-type: none"> <li>- at least 3 (three) articles and/or reviews in peer-reviewed scientific journals indexed in Science Citation Index Expanded of Web of Science database and/or having a CiteScore percentile in Scopus database of at least 50 (fifty);</li> <li>- at least 1 patent for invention (including positive decision);</li> <li>- at least 2 (two) articles or reviews in a peer-reviewed foreign or domestic journal recommended by CCEQHE; One of the articles must be in the multidisciplinary category (multidisciplinary or interdisciplinary practical application) addressing the needs of enterprises from Kazakhstan's real economy sector.</li> </ul> <p>For domestic journals from CCEQHE list 1, not belonging to the multidisciplinary category, journals from CCEQHE lists 1 and 2 that are indexed in two or more categories are counted.</p> <ul style="list-style-type: none"> <li>- or at least 1 (one) article or review in a peer-reviewed scientific journal that is in the 1st (first) or 2nd (second) quartile by impact factor in Web of Science database and/or has a CiteScore percentile in Scopus database of at least 65 (sixty-five);</li> <li>- at least 1 (one) patent included in the Derwent Innovations Index database (Web of Science, Clarivate Analytics);</li> </ul> |

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|  | <p>- at least 2 (two) articles or reviews in a peer-reviewed foreign or domestic journal recommended by CCEQHE; One of the articles must be in the multidisciplinary category (multidisciplinary or interdisciplinary practical application) addressing the needs of enterprises from Kazakhstan's real economy sector.</p> <p>For domestic journals from CCEQHE list 1, not belonging to the multidisciplinary category, journals from CCEQHE lists 1 and 2 that are indexed in two or more categories are counted.</p> <p>- or at least 1 (one) article or review in a peer-reviewed scientific journal indexed in Science Citation Index Expanded and being in the 1st (first) quartile by impact factor in Web of Science database and/or having a CiteScore percentile in Scopus database of at least 80 (eighty);</p> <p>- at least 1 patent for invention (including positive decision);</p> <p>- at least 1 (one) article or review in a peer-reviewed foreign or domestic journal recommended by CCEQHE; One of the articles must be in the multidisciplinary category (multidisciplinary or interdisciplinary practical application) addressing the needs of enterprises from Kazakhstan real economy sector.</p> <p>For domestic journals from CCEQHE list 1, not belonging to the multidisciplinary category, journals from CCEQHE lists 1 and 2 that are indexed in two or more categories are counted.</p> <p>2) Metal-organic frameworks (MOFs) with optimal characteristics for selective sorption of volatile organic compounds will be synthesized, including controlled particle size and high specific surface area. Based on the synthesized materials, "Needle Trap" devices with optimized design parameters will be developed. Optimal sampling conditions will be determined considering various factors, and protocols for air, water, and soil analysis will be developed. As a result of studying analyte adsorption and desorption processes, a universal method for determining VOCs in environmental objects using gas chromatography with mass spectrometric detection will be created and validated. The methodology will be tested on real environmental objects, and guidelines for using NTD devices will be developed.</p> <p>3) During the project implementation, it is expected that PhD candidate Kan Tatyana will prepare for her doctoral dissertation defense.</p> <p>4) The developed analytical methods and devices will be proposed for implementation in analytical laboratories of major industrial enterprises such as JSC "KazMunayGas", LLP "Tengizchevroil", JSC "ArcelorMittal Temirtau", LLP "Kazzinc", as well as in environmental services of cities with acute environmental situations (Almaty,</p> |
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|                                                                                                                                                               | <p>Astana, Karaganda, Temirtau, Ust-Kamenogorsk, Shymkent).</p> <p>5) The obtained results will be transferred to territorial divisions of the Ministry of Ecology and Natural Resources of the Republic of Kazakhstan to improve the environmental monitoring system and environmental quality control.</p> <p>6) Research results will be presented at two international conferences: EUROMOF 2027 (Greece) and MOF 2027 (USA) with oral presentations and poster presentations. The conferences will demonstrate the project's achievements in synthesizing new materials and developing analytical methods, which will allow establishing new scientific contacts and expanding international cooperation.</p> <p>Results achieved:</p> <p>New ZnMOF-74 and ZnMOF-74a were synthesized, their comprehensive physicochemical characterization was conducted, and preliminary adsorption tests of target analytes on NTD devices under atmospheric conditions were performed.</p> |
| Names and surnames of research group members with their identifiers (Scopus Author ID, Researcher ID, ORCID, if available) and links to the relevant profiles | <p>1. Galeeva Alina Kulbaevna Scopus ID: 56436524000; ORCID: 0000-0001-9303-5277; ResearcherID: A-8292–2015</p> <p>2. Baimatova Nasiba Khikmatullaevna Scopus ID: 56436524000; ORCID: 0000-0001-9303-5277; ResearcherID: A-8292–2015</p> <p>3. Omarova Anara Sagidullaevna – Scopus ID: 57271406600; ORCID: 0000-0002-3990-1952; ResearcherID: P-5606–2017</p> <p>4. Muratuly Aset Scopus Author ID: 57396626800; ResearcherID: ACD-0802-2022; ORCID ID: 0000-0001-6343-988</p> <p>5. Starodubtseva Alena Anatolyevna Scopus Author ID: 57988905100; ORCID ID: 0000-0003-4344-2039</p> <p>6. Sovetova Diana Omirzhanovna ORCID ID: 0000-0003-3199-3845</p> <p>7. Kan Tatyana Viktorovna ORCID ID: 0000-0002-1945-8471</p>                                                                                                                                                                                                                                                           |
| Usage                                                                                                                                                         | <p>This study is devoted to a comprehensive analysis of air, water and soil pollutants, aimed at solving the key state task of improving environmental quality and reducing the negative impact of pollutants on the health of the population of the Republic of Kazakhstan.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| Priority over real analogues                                                                                                                                  | <p>The project plans to develop and implement more effective pollution monitoring methods using ZnMOF-74a and ZnMOF-74 sorbents in an NTD device. Simplifying sample preparation and increasing analytical efficiency will provide accurate data on hazardous substance concentrations, improving the speed and accuracy of health risk assessments and helping develop timely</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |

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|                                         | measures to improve the environmental situation in the country. |
| List of publications with links to them | No                                                              |
| Patent Information                      | No                                                              |
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