

THERMOELECTRIC PROPERTIES OF THE CeBiTe_3 COMPOUND AND ITS RELEVANCE TO SUSTAINABLE ENERGY TECHNOLOGIES

Saba Mammadova, Fuad Sadigov, Gunel Ganbarova, Yegana Jafarova,
Cingiz Abilov, Zakir Ismailov
Baku State University, Baku, Azerbaijan

Received: 09 February 2026

Accepted: 10 April 2026

Published: 13 April 2026

In this study, we investigate the phase equilibrium, synthesis, and thermoelectric properties of the CeBiTe_3 compound. CeBiTe_3 is formed in the quasi-binary Bi_2Te_3 – Ce_2Te_3 section of the Ce–Bi–Te ternary system. Based on the obtained data, a phase diagram of the Bi_2Te_3 – Ce_2Te_3 system was constructed. The temperature dependences of the electrical conductivity and thermoelectric force (Seebeck coefficient) were studied in the temperature range of 300–960 K.

The band gap energy of CeBiTe_3 was estimated from the temperature dependence of electrical conductivity and found to be approximately 0.2 eV. The results demonstrate that CeBiTe_3 exhibits semimetallic behavior and is a promising thermoelectric material for medium- and high-temperature applications. It was found that CeBiTe_3 forms at 950 K in a 1:1 molar ratio and melts incongruently. The system is eutectic, with the eutectic reaction occurring at 800 K and a composition of 80 mol% Bi_2Te_3 .

The solubility limit of the solid solution at room temperature was found to be approximately 97 mol% Bi_2Te_3 .

In addition, the study contributes to the development of sustainable energy technologies through waste heat recovery and improved energy efficiency, in accordance with the United Nations Sustainable Development Goals (SDGs), particularly SDG 7 (Affordable and Clean Energy), SDG 9 (Industry, Innovation and Infrastructure), and SDG 13 (Climate Action).

Keywords: thermoelectric materials, electrical conductivity, system, temperature, phase, diagram

INTRODUCTION

Understanding the phase relationships in this ternary system is crucial for creating materials with optimized properties for specific applications. Furthermore, the coexistence of these phases at different compositions and temperatures provides insight into the stability of complex systems. The goal of this study is to construct a comprehensive phase diagram, identify stable and metastable phases, understand the interactions and compatibility of the components, and examine how thermal and compositional changes affect the system's behavior [1-4]. The results of this work will not only expand our fundamental understanding of complex systems but also provide a valuable foundation for the development of new materials for applications in energy, electronics, and environmental technologies [5-7].

The study of phase equilibria in multicomponent systems is essential for understanding the thermodynamic stability and phase relationships of materials with potential technological applications. This research is particularly important for systems containing selenides and tellurides, which are of significant interest due to their application in promising technologies such as photovoltaics, thermoelectric devices, optoelectronics, and environmental sensors [8-11]. The Ce–Bi–Te system represents a chemically rich area of interest due to the unique properties of its constituent compounds, which are widely known for their use in advanced technologies. The introduction of lanthanide atoms into the crystal lattice of such compounds can improve their properties and create additional functionality. In order to optimize the properties of functional compounds, it is important to develop the physicochemical basis for the synthesis of new inorganic functional materials, which is possible based on studying the phase diagrams of the corresponding systems [12-14].

Most ternary bismuth compounds have been extensively studied for their potential as electronic materials, exhibiting remarkable properties such as high photovoltaic efficiency, radiation detection capabilities, and thermoelectric performance. Their abundance in nature and environmental characteristics have further stimulated recent research into these materials. Bismuth is a p-type semiconductor known for its potential for solar energy applications due to its direct band gap and naturally occurring non-toxic components [15-17].

Therefore, research bismuth telluride (Bi_2Te_3) occupies a special position among semiconductor materials due to its outstanding thermoelectric properties and wide range of applications in electronic devices [18-20]. Moreover, Bi_2Te_3 has attracted significant attention as a topological insulator. However, Bi_2Te_3 and solid solutions based on it possess a layered crystal structure, relatively low melting temperature, and limited mechanical strength, which restrict their practical applications, especially at elevated temperatures [21-23]. To overcome these limitations and to obtain new functional materials with enhanced thermoelectric and electrophysical properties, ternary systems based on bismuth tellurides and rare-earth elements have become an important subject of modern materials science research [24-26]. Among them, the Ce–Bi–Te system is of particular interest due to the high thermoelectric efficiency of both bismuth and cerium tellurides [27-30].

EXPERIMENTAL

For the investigation of electrophysical properties, CeBiTe_3 samples were synthesized by a direct synthesis method in a single-zone furnace at temperatures of 1100–1200 K. High-purity elements were used: tellurium (TB4), bismuth (B4), and cerium (CEM-0). The starting materials were weighed with an accuracy of 10^{-3}g , sealed in evacuated (0.1Pa) quartz ampoules, and annealed for 8 hours.

The CeBiTe_3 compound was identified in the Bi_2Te_3 – Ce_2Te_3 quasi-binary section of the Ce–Bi–Te ternary system. The system was studied using conventional phase–chemical analysis methods, including differential thermal analysis (DTA), and microstructural analysis (MSA).

The DTA and PXRD techniques were employed to verify the purity and identity of the synthesized compounds, as well as to perform experimental investigations. DTA of the samples was conducted in evacuated quartz ampoules using a 404 F1 Pegasus System differential scanning calorimeter. The measurement data were analyzed with the NETZSCH Proteus Software, ensuring a temperature accuracy of $\pm 20\text{C}$. XRD analysis of the annealed alloys was performed at room temperature using a Bruker D2 PHASER diffractometer with $\text{CuK}\alpha_1$ radiation. The diffraction patterns were indexed using the Topas 4.2 Software.

To ensure complete interaction between the components and structural homogeneity, the samples were subjected to prolonged thermal treatment. The chemical stability of CeBiTe_3 was examined, showing that the compound is stable in air, water, and organic solvents, but decomposes under the action of mineral acids (H_2SO_4 , HNO_3 , HCl) and strong alkalis (NaOH , KOH).

RESULTS AND DISCUSSIONS

Based on the results obtained by the above methods, a phase diagram of the Bi_2Te_3 - Ce_2Te_3 system was constructed (Figure 1).

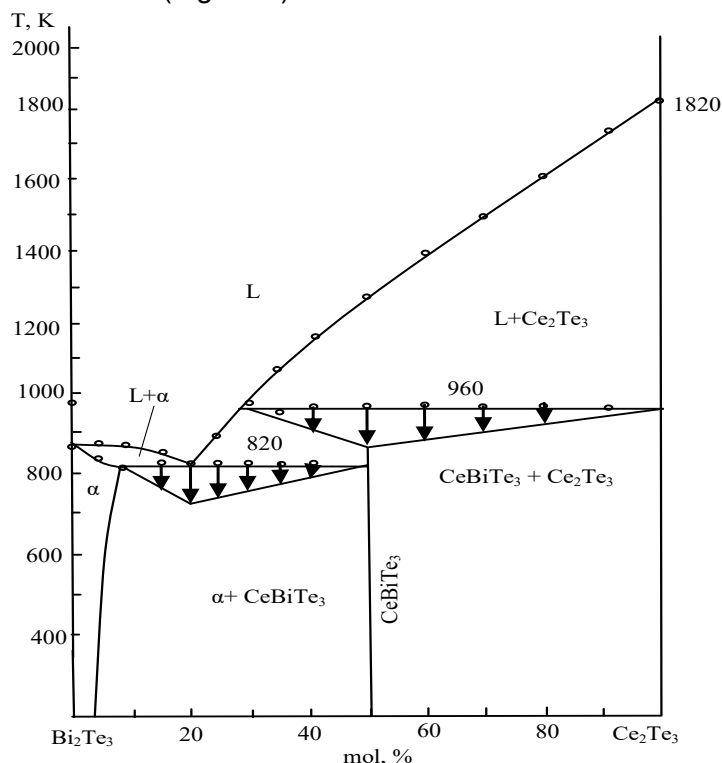


Figure 1. State diagram of the Bi_2Te_3 - Ce_2Te_3 system

According to the phase diagram, CeBiTe_3 forms at 950 K at a 1:1 molar ratio of the components and melts incongruently. The system is of eutectic type, with the eutectic reaction occurring at 800 K and a composition of 80 mol% Bi_2Te_3 . After thermal treatment and quenching in ice water, the solubility limit of the solid solution at room temperature was found to be approximately 97 mol% Bi_2Te_3 .

Thermoelectric measurements were carried out on parallelepiped-shaped polycrystalline samples in the temperature range of 300–960 K using the compensation method described in Ref. [31-33].

The measurement error was estimated to be within 5–7%, mainly due to uncertainties in sample geometry and probe spacing. The electrical conductivity (σ) was calculated using the following expression: where I is the current, U is the potential difference between probes, l is the distance between probes, and S is the cross-sectional area of the sample. The Seebeck coefficient (α) was determined as: where ΔE is the thermoelectric electromotive force and ΔT is the temperature difference between the hot and cold ends of the sample.

$$\sigma = \frac{l_z \cdot I}{U_z \cdot S}$$

The following formula was used to calculate the thermo-e.h.q coefficient:

$$\alpha = \frac{\Delta E}{\Delta T}$$

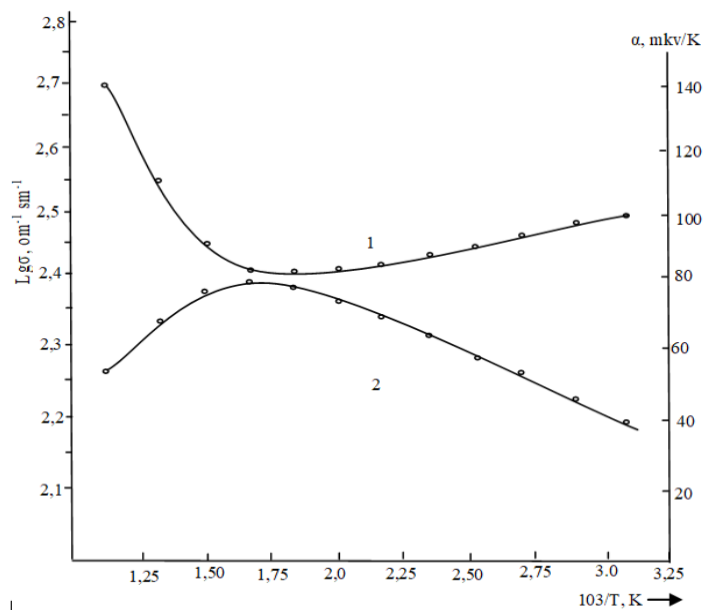


Figure 2. Temperature dependence of the specific electrical conductivity (σ) and thermoelectric coefficient (α) of the BiCeTe_3 compound

The temperature dependence of electrical conductivity reveals semimetallic behavior. From room temperature up to approximately 673 K, the electrical conductivity decreases. With further temperature increase, a sharp rise in conductivity is observed, indicating the onset of intrinsic conduction [34-37].

From the linear region corresponding to intrinsic conductivity, the band gap energy of CeBiTe_3 was estimated and found to be $\Delta E_g \approx 0.2$ eV. The temperature dependence of the Seebeck coefficient exhibits a similar trend: an increase at relatively low temperatures followed by a decrease above 673 K, which is attributed to the dominance of intrinsic charge carriers.

Relevance to Sustainable Development Goals (SDGs). The present study is directly aligned with several United Nations Sustainable Development Goals (SDGs). SDG 7 – Affordable and Clean Energy: CeBiTe_3 -based thermoelectric materials enable direct conversion of waste heat into electrical energy, improving energy efficiency.

SDG 9 – Industry, Innovation and Infrastructure: The development of new functional thermoelectric materials supports innovation in energy and semiconductor technologies.

SDG 12 – Responsible Consumption and Production: Enhanced thermoelectric efficiency contributes to reduced energy losses and more rational use of resources. SDG 13 – Climate Action: Thermoelectric technologies help reduce greenhouse gas emissions by recovering waste heat and decreasing dependence on fossil fuels.

CONCLUSIONS

The phase equilibrium, synthesis, and thermoelectric properties of the CeBiTe_3 compound have been systematically investigated. The compound exhibits semimetallic behavior, a narrow band gap of approximately 0.2 eV, and promising thermoelectric characteristics over a wide temperature range. These properties make CeBiTe_3 a potential candidate for thermoelectric energy conversion applications. Moreover, the results demonstrate the relevance of this material to sustainable energy technologies and global SDG-oriented research.

Based on the obtained data, a phase diagram of the Bi_2Te_3 – Ce_2Te_3 system was constructed. The results of the study show that CeBiTe_3 exhibits semi-metallic behavior and is a promising thermoelectric material. It was found that CeBiTe_3 forms at 950 K in a 1:1 molar

ratio and melts incongruently. The system is eutectic, with the eutectic reaction occurring at 800 K and a Bi_2Te_3 composition of 80 mol%.

REFERENCES

- [1] Goltsman, B.M.; Kidinov, V.A.; Smirnov, I.A. Semiconductor thermoelectric materials based on Bi_2Te_3 , *Nauka, Moscow*, **1972**, 320p, <https://www.scirp.org/reference/referencespapers?referenceid=824182>
- [2] Kost, M.E.; Shilov, A.L.; Mikheeva, V.I. Compounds of rare earth elements, *Nauka, Moscow*, **1983**, 273p, <https://urss.ru/cqibin/db.pl?lang=Ru&blang=ru&page=Book&id=44021>
- [3] Chih-hao, L.; Hsin-jay, W.; Sinn-Wen, C. Liquidus Projection of the Ternary Bi-Sb-Te, *Thermoelectric Material System*, **2013**, v. 44, pp.5424–5433, <https://doi.org/10.1007/s11661-013-1883-8>
- [4] Mammadova, S.H.; Sadigov, F.M.; Ganbarova, G.T.; Cafarova, Y.K.; Abilov, C. Thermoelectric properties of the CeBiTe_3 compound, *Modern problems of theoretical and experimental chemistry Acad. Yusif Mammadaliyev*, **2025**, pp.366-368, <https://mpc2025.bsu.edu.az/>
- [5] Sadiqov, F.M.; Ilyasly, T.M.; Mirzoeva, R.C.; Mamedova, S.M.; Dzhafarova, E.K.; Ismailov, Z.I. Physicochemical study of the $\text{Bi}_2\text{Te}_3\text{-Er}_2\text{Te}_3$ system and properties of the forming phases, *Eurasian Union Scientists*, **2021**, v.10(91), pp.37-40. <https://doi.org/10.31618/ESU.2413-9335.2021.1.91.1488>
- [6] Wu, F.; Song, H.; Jia, J.; Hu, X. Effects of Ce, Y, and Sm doping on the thermoelectric properties of Bi_2Te_3 alloy, *Materials International*, **2013**, v.23(4), pp.408-412, <https://doi.org/10.1016/j.pnsc.2013.06.007>
- [7] Li, J.; Wu, N. Semiconductor-based photocatalysts and photoelectrochemical cells for solar fuel generation, a review, *Catalysis Science & Technology*, **2015**, v.5, pp. 1360-1384, <https://doi.org/10.1039/C4CY00974F>
- [8] Lin, S.; Li, W.; Pei, Y. Thermally insulative thermoelectric argyrodites, *Materials Today*, **2021**, v.48, pp. 198-213, <https://doi.org/10.1016/j.mattod.2021.01.007>
- [9] Babanly, M.B.; Yusibov, Y.A.; Imamaliyeva, S.Z.; Babanly, D.M.; Alverdiyev, I.J. Phase diagrams in the development of the argyrodite family compounds and solid solutions based on them, *Journal of phase equilibria and diffusion*, **2024**, v.45, pp. 228-255, <https://doi.org/10.1007/s11669-024-01088-w>
- [10] Babanly, M.B.; Mashadiyeva, L.F.; Imamaliyeva, S.Z.; Babanly, D.M.; Tagiev, D.B.; Yusibov, Yu.A. Complex copper-based chalcogenides: a review of phase equilibria and thermodynamic properties, *Condensed Matter and Interphases*, **2024**, v.26(4), pp. 579-619, <https://doi.org/10.17308/kcmf.2024.26/12367>
- [11] Alverdiyev, I.J.; Imamaliyeva, S.Z.; Akhmedov, E.I.; Yusibov, Yu.A.; Babanly, M.B. Thermodynamic properties of some ternary compounds of the argyrodite family, *Azerbaijan Chemical Journal*, **2023**, v.4, pp. 21-30, <https://doi.org/10.32737/0005-2531-2023-4-21-30>
- [12] Wang, B.; Li, S.; Luo, Y.; Yang, J.; Ye, H.; Liu, Y.; Jiang, Q. A new thermoelectric Ag_8SiSe_6 argyrodite for room temperature application: sensitivity of thermoelectric performance to cooling conditions, *Material Advances*, **2024**, v.5, pp.3735, <https://doi.org/10.1039/D3MA01190A>
- [13] Chetty, R.; Bali, A. and Mallik, R.C. Tetrahedrites as thermoelectric materials: An overview, *Journal of Materials Chemistry C*, **2015**, v.3(48), 12364-12378. <https://doi.org/10.1039/c5tc02537k>
- [14] Babanly, M.B.; Mashadiyeva, L.F.; Babanly, D.M.; Imamaliyeva, S.Z.; Tagiev, D.B.; Yusibov, Yu.A. Some issues of complex studies of phase equilibria and thermodynamic properties in ternary chalcogenide systems involving EMF measurements (review), *Russian Journal of Inorganic Chemistry*, **2019**, v.64(13), pp1649-1671. <https://doi.org/10.1134/s0036023619130035>

- [15] Babanly, M.B.; Yusibov, Y.A.; Imamaliyeva, S.Z.; Babanly, D.M.; Alverdiyev, I.J. Phase diagrams in the development of the argyrodite family compounds and solid solutions based on them, *Journal of Phase Equilibria and Diffusion*, **2024**, v.45, pp.228-255. <https://doi.org/10.1007/s11669-024-01088-w>
- [16] Ismailov, Z.; Hasanova, Z.; Mirzaeva, R. Character of Chemical Interaction in Bi_2Se_3 - Tb_2Se_3 systems, *Research & Development in Material science*, **2025**, v.21(4), pp.2568-2571, <https://doi.org/10.31031/RDMS.2025.21.001017>
- [17] Sadygov, F.M.; İlyaslı, T.M.; Mammadova, N.Sh.; Huseynov, R.; Aliyev, Y. Study of crystal characterization and chemical interaction in the ternary system Ho-Sb-Te, *East European journal of physics*, **2024**, v.2, pp.297-303, <https://ouci.dntb.gov.ua/en/works/7BYP30Z9/>
- [18] Jeffrey, S. and Eric S. T. Complex Thermoelectric Materials, *Nature Materials*, **2008**, 7(2), pp.105-114, <https://doi.org/10.1038/nmat2090>
- [19] Sadygov, F.M.; İlyasly, T.M.; Ganbarova, G.T.; Zlomanov, V.P.; Aliev, I.I. Physical and chemical study of the Sb_2Se_3 - Nd_2Se_3 system, *Inorganic Materials*, **2017**, v.53(7), pp. 681-685, <https://link.springer.com/journal/10789/volumes-and-issues/53-7>
- [20] Yaprıntsev, M.; Lyubushkin, R.; Soklakova, O.; Ivanov, O. Effects of Lu and Tm doping on thermoelectric properties of Bi_2Te_3 , *Journal of Electronic Materials*, **2018**, v.47, pp.1362–1370, <https://doi.org/10.1007/s11664-017-5940-8>
- [21] Ivanov, O. and Yaprıntsev, M. Mechanisms of thermoelectric efficiency enhancement in Lu-doped Bi_2Te_3 , *Materials Research Express*, **2018**, v.5(1), pp.1-10, <https://doi.org/10.1088/2053-1591/aaa265>
- [22] Yaprıntsev, M.N.; Lyubushkin, R. A.; Soklakova, O.N. Synthesis and electrical properties of Bi_2Te_3 -based thermoelectric materials doped with Er, Tm, Yb, and Lu, *Semiconductors*, **2017**, v.51(6), pp.710-713, https://doi.org/10.1134/S106_3782617060_29X
- [23] B. Cantor. Exploring Multicomponent Phase Space to Discover New Materials, *J. Phase Equilib. Diffus.* 2024, 45, pp.188–218, <https://doi.org/10.1007/s11669-024-01131-w>
- [24] Hagmann, A.J. Chalcogenide topological insulators. In: Chalcogenide From 3D to 2D and Beyond, *Woodhead Publishing Series in Electronic and Optical Materials*, **2020**, pp. 305-337, <https://doi.org/10.1016/B978-0-08-102687-8.00015-4>
- [25] Sadygov, F.M.; İlyasly, T.M.; Ganbarova, G.T.; Ismailov, Z.I.; Mamedova, S.G.; Dzhafarova, E.K.; Mamedov, E.A. Phase equilibria in the Bi_2Se_3 - Nd_3Se_4 system and electrophysical properties of the resulting phases, *Advances in Modern Natural Science*, **2016**, v.4, pp. 53-56, <https://natural-sciences.ru/ru/article/view?id=35861>
- [26] Aliev, Z.S.; İbdova, G.I.; Edenac, J.C.; Babanly, M.B. Phase equilibria in the YbTe- Sb_2Te_3 -Te system, *Journal of Alloys and Compounds*, **2015**, pp.167-171, <https://doi.org/10.1016/j.jallcom.2014.08.102>
- [27] <https://doi.org/10.1016/j.jallcom.2014.08.102>
- [28] Ganbarova, G.T.; Sadıgov, F.M.; İsmayilov, Z.İ.; Mirzayeva, R.C.; Hasanova, Z.T. Phase formation in the ternary system Nd-Bi-Te according to the section Bi_2Se_3 - Nd_2Se_3 , *Journal of Chemistry and Material Sciences*, **2024**, v.1(4), pp.34-39, <https://doi.org/10.30546/209501.201.2024.1.04.035>
- [29] Ganbarova, G.T.; Sadygov, F.M.; İlyasly, T.M. Aliev, I.I.; Mamedova, S.G.; Cafarbayli, S.N. Physicochemical study of the Sb_2Se_3 - Nd_3Se_4 system, *International Journal of Applied and Fundamental Research*, **2016**, v.16(2), pp. 311-313, <https://applied-research.ru/jats.10831.xml>
- [30] Sadiqov, F.M.; Alizade, N.M.; Ismailov, Z.I. Character of chemical interaction in the triple system Er-Bi(Sb)-Se, *Евразийский Союз Ученых*, **2021**, v.1(82), pp.63-67, <https://doi.org/10.31618/ESU.2413-9335.2021.2.82.1213>
- [31] Hasanova, M. Sh.; Abilov, Ch.J.; Kasumova, E. K. Some thermophysical properties of $(\text{In}_2\text{Te}_3)_{1-x}(\text{Cd}_{0.9}\text{Zn}_{0.1}\text{Te})_x$ solid solutions, *Journal of Applied Physics*, **2020**, v.127(12), pp.114-125, <https://doi.org/10.1063/1.5140478>
- [32] Nolas, G.S. and Goldsmid, H.J. Thermal Conductivity of Semiconductors, *Physics of Solids and Liquids*. **2004**, pp.105-121, https://doi.org/10.1007/0-387-26017-X_4
- [33] Paolini, G. V.; Lindan, P. J.; Harding, J. H. The thermal conductivity of defective crystals, *J. Chem. Phys.* **1997**, v.106, pp. 3681–3687, <https://doi.org/10.1063/1.473462>

- [34] Imamaliyeva, S. Z.; Huseynova, I. F.; Daraselia, D.; Japaridze, D.; Shengelaya, A.; Babanly, M. B. Phase Relations in the Tl_2Te - $TlBiTe_2$ - $TlGdTe_2$ Compositions Region of the Tl-Bi-Gd-Te System and Magnetic Properties of the $TlBi_{1-x}GdxTe_2$ Solid Solutions, *Journal of Phase Equilibria and Diffusion*, **2024**, v.45, pp.459– 468, <https://doi.org/10.1007/s11669-024-01096-w>
- [35] Cantor, B. Exploring Multicomponent Phase Space to Discover New Materials, *Journal of Phase Equilibria and Diffusion*, **2024**, v.45, pp.188–218, <https://doi.org/10.1007/s11669-024-01131-w>
- [36] Abilov, Ch.I.; Hasanova, M.Sh.; Huseynova, N.T. Physicochemical properties and thermodynamic functions of alloys of the system $InTe$ - Cr_2Te_3 , *Materials Chemistry and Physics*, **2020**, v.241, pp.122341-122345, <https://doi.org/10.1016/j.matchemphys>
- [37] Bayramova, N.; Huseynova, I.; Melikova, E.; Imamaliyeva, S. Phase relations in the Phase relations in the AgI - Ag_7GeSe_5 - $GeSe_2$ system, *Journal of Chemistry and Material Sciences*, **2025**, v.2(3), pp. 36-42, <https://doi.org/10.30546/209501.201.2025.2.003.012>
- [38] Sadigov, F.M.; Mammadova, S.H.; Abilov, Ch.I.; Ismayilov Z.I. Elektrophysical properties of $ErSbSe_3$ and $ErBiSe_3$ compounds, *Azerbaijan Journal of Physics*, **2025**, v.21(2), pp. 36-40, <https://doi.org/10.70784/azip.1.2025236>