

CHARACTERIZATION OF ELECTRIC FIELD GRADIENT
ANISOTROPY AND INTERNAL MAGNETIC FIELDS IN BISMUTH-
CONTAINING COMPOUNDS**Qayumov Oybek Azamat ugli***PhD, Associate Professor Karshi State Technical University**Uzbekistan, Karshi**Email: oybekqayumov@mail.ru*

Abstract: *This study investigates the anisotropy of electronic density and local magnetic fields in bismuth oxide and bismuth oxyhalide compounds using nuclear quadrupole resonance (NQR) spectroscopy of the ^{209}Bi nucleus. Although these materials are conventionally classified as diamagnetic, the experimental results reveal the presence of ordered internal magnetic fields reaching up to 250 Gs. NQR spectra obtained from $\alpha\text{-Bi}_2\text{O}_3$, $\text{Bi}_5\text{O}_4\text{Br}$, $\text{Bi}_4\text{Al}_4\text{O}_9$, $\text{Bi}_4\text{Ge}_3\text{O}_{12}$, and $\text{Bi}_2\text{Ge}_3\text{O}_9$ were analyzed through spectral processing, mathematical modeling, and evaluation of quadrupole interactions. The influence of electric field gradient anisotropy and Zeeman splitting on resonance line structure was examined in detail. The results demonstrate that nonequivalent crystallographic positions of bismuth atoms lead to significant variations in quadrupole parameters and local magnetic environments. Comparative analysis of spectral line broadening and splitting confirms the sensitivity of the NQR method to subtle electronic and magnetic interactions. The obtained findings provide valuable information about the electronic structure of bismuth-containing functional materials and establish a basis for further investigations of local magnetic ordering and crystal-field effects.*

Keywords: *bismuth oxide, nuclear quadrupole resonance, electronic density anisotropy, electric field gradient, Zeeman splitting, local magnetic field, functional materials.*

INTRODUCTION

Bismuth oxide ($\alpha\text{-Bi}_2\text{O}_3$) and related bismuth-containing compounds have attracted significant scientific interest due to their unique structural, electronic, optical, and magnetic properties. These materials serve as important components in high-temperature superconductors, ferroelectric devices, electro-optical systems, ion-conducting materials, and advanced functional ceramics. The performance of such materials is strongly influenced by the local electronic environment and the distribution

of electric and magnetic fields within the crystal lattice. Therefore, understanding the microscopic mechanisms governing these properties is essential for both fundamental research and technological applications.

One of the most informative approaches for investigating local electronic structure is nuclear quadrupole resonance (NQR) spectroscopy. The method is highly sensitive to variations in the electric field gradient (EFG) surrounding quadrupolar nuclei and provides direct information about electron density distribution, crystallographic symmetry, and local magnetic interactions. In bismuth-containing compounds, the ^{209}Bi nucleus is particularly suitable for NQR studies because of its large nuclear quadrupole moment and high sensitivity to changes in the local crystal environment.

Although bismuth oxides are generally considered diamagnetic materials, previous studies have reported the presence of internal magnetic fields and unusual spectral splitting phenomena in their NQR spectra. Such observations suggest the existence of complex local interactions that cannot be fully explained by conventional diamagnetic behavior. The occurrence of Zeeman-type splittings, line broadening, and multiplet structures indicates that local magnetic ordering and anisotropic electron density distributions may play an important role in determining the physical properties of these compounds.

The electric field gradient at the bismuth nucleus is directly related to the spatial distribution of valence electrons and the symmetry of the surrounding crystal lattice. Consequently, any distortion of the electron cloud or crystallographic environment can significantly affect the NQR spectrum. Detailed analysis of quadrupole interactions therefore provides valuable information regarding electronic density anisotropy, magnetic nonequivalence of atomic positions, and local structural disorder in bismuth-based materials.

The aim of this study is to investigate the anisotropy of electronic density and local magnetic fields in $\alpha\text{-Bi}_2\text{O}_3$ and related bismuth oxide compounds using ^{209}Bi nuclear quadrupole resonance spectroscopy. Through experimental spectral analysis and theoretical interpretation of quadrupole and Zeeman interactions, the work seeks to determine the characteristics of internal magnetic fields, evaluate electric field gradient anisotropy, and provide a deeper understanding of the electronic structure of functional bismuth-containing materials.

RESEARCH METHODOLOGY

The investigation of electronic density anisotropy and local magnetic fields in bismuth oxide compounds was carried out using nuclear quadrupole resonance (NQR) spectroscopy of the ^{209}Bi nucleus. The study focused on $\alpha\text{-Bi}_2\text{O}_3$ and several related bismuth-containing compounds, including $\text{Bi}_5\text{O}_4\text{Br}$, $\text{Bi}_4\text{Al}_4\text{O}_9$, $\text{Bi}_4\text{Ge}_3\text{O}_{12}$, and $\text{Bi}_2\text{Ge}_3\text{O}_9$. These materials were selected because of their structural diversity and the presence of nonequivalent crystallographic positions of bismuth atoms, which make them suitable for investigating electric field gradient anisotropy and local magnetic interactions.

NQR measurements were performed on both powdered and single-crystal samples over a temperature range of 77–300 K. The resonance spectra of the ^{209}Bi nucleus were recorded in the absence of an external magnetic field and under the influence of controlled magnetic fields. Particular attention was given to the analysis of resonance frequencies, spectral line broadening, line splitting, and quadrupole spin echo signals.

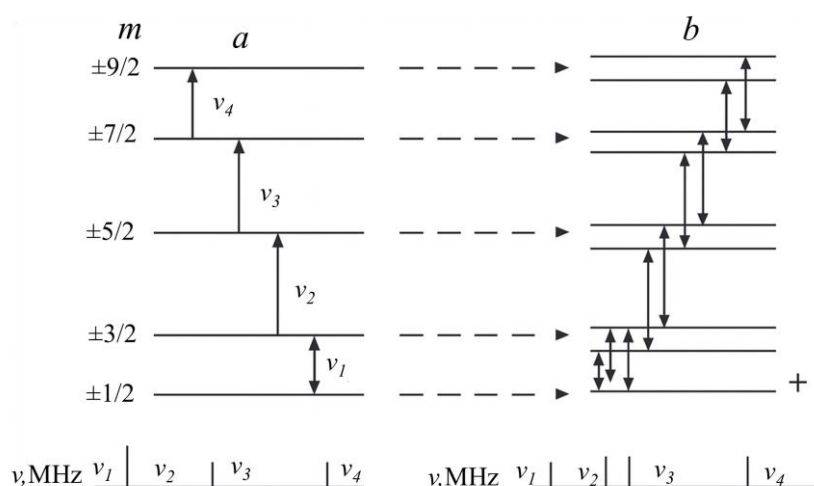


Figure 1. Quadrupole energy levels of the ^{209}Bi nucleus and the transitions between them: (a) in the absence of an external magnetic field, (b) under the influence of an external magnetic field of the Zeeman type.

The experimental data were interpreted using the nuclear quadrupole interaction Hamiltonian, which describes the interaction between the electric quadrupole moment of the nucleus and the electric field gradient generated by the surrounding crystal lattice. The influence of external magnetic fields was evaluated through the Zeeman interaction, allowing the determination of additional energy-level splitting and transition frequencies.

$$q_{ij} = \frac{\partial E_i}{\partial j} = -\frac{\partial^2 U}{\partial ij}$$

Here, E_i represents the strength of the electric field, while U denotes the potential of this field at the point where the nucleus is located. The indices $i, j = x, y, z$ correspond to the spatial axes. The main experimentally measurable quantity in NQR studies is the nuclear quadrupole interaction constant, which characterizes the strength of the interaction between the nuclear quadrupole moment and the electric field gradient at the nucleus.

To characterize the local electronic environment, the quadrupole coupling constant (eQq/h), asymmetry parameter (η), and local magnetic field strength (H_{loc}) were calculated from the measured spectra. Mathematical spectral analysis and computer modeling were employed to determine the magnitude and orientation of internal magnetic fields and to evaluate the anisotropy of the electric field gradient. Comparative analysis of spectral parameters obtained from different compounds enabled the identification of correlations between crystal structure, electron density distribution, and local magnetic ordering.

The obtained results were used to assess the magnetic nonequivalence of bismuth atomic sites, evaluate the anisotropic distribution of electron density, and establish the relationship between crystal symmetry and local magnetic field formation in bismuth-containing functional materials.

RESULTS AND DISCUSSION

The NQR spectra obtained for α - Bi_2O_3 and related bismuth-containing compounds revealed significant information about the local electronic structure and magnetic environment of the ^{209}Bi nucleus. Analysis of the recorded resonance lines demonstrated that the electric field gradient (EFG) at the bismuth sites is strongly influenced by crystallographic symmetry and electron density distribution. As a consequence, noticeable differences in quadrupole interaction parameters were observed among the investigated compounds.

The quadrupole energy level scheme of the ^{209}Bi nucleus is presented in Figure 1. In the absence of an external magnetic field, the observed resonance transitions are determined solely by the interaction between the nuclear quadrupole moment and the electric field gradient. However, when a magnetic field is applied, additional Zeeman splitting occurs, resulting in the appearance of multiple resonance transitions. This behavior confirms the high sensitivity of the NQR method to local magnetic interactions and provides a basis for identifying nonequivalent atomic positions within the crystal lattice.

The experimental NQR spectra recorded for $\text{Bi}_5\text{O}_4\text{Br}$ and α - Bi_2O_3 are shown in Figure 2. The spectra of $\text{Bi}_5\text{O}_4\text{Br}$ exhibit relatively narrow and symmetric resonance

lines, indicating a more ordered electric field distribution and higher crystallographic symmetry. In contrast, the α - Bi_2O_3 spectra display broader and partially split resonance lines, suggesting the presence of multiple nonequivalent bismuth positions and significant anisotropy of the local electric field gradient. These observations demonstrate that structural complexity directly affects the electronic environment surrounding the bismuth nuclei.

The quantitative spectral parameters obtained from the NQR measurements are summarized in Table 1. The values of the quadrupole coupling constant (eqQ/h), asymmetry parameter (η), and local magnetic field strength (H_{loc}) vary considerably among the investigated compounds. In α - Bi_2O_3 , two crystallographically distinct bismuth positions were identified, exhibiting local magnetic fields of 171 Gs and 136 Gs, respectively. The highest internal magnetic field, approximately 250 Gs, was detected in $\text{Bi}_5\text{O}_4\text{Br}$, whereas $\text{Bi}_4\text{Ge}_3\text{O}_{12}$ exhibited significantly lower values, indicating weaker local magnetic interactions.

Comparison of the spectral parameters reveals a clear correlation between crystal symmetry and electric field gradient anisotropy. Compounds possessing higher structural symmetry generally exhibit lower asymmetry parameters and narrower resonance lines. Conversely, structures containing multiple nonequivalent bismuth sites produce larger spectral splitting and broader resonance features. These results indicate that the electronic density around the bismuth nucleus is highly anisotropic and strongly dependent on the local crystal environment.

Table 1. NQR spectra of the ^{209}Bi nucleus and values of the internal magnetic field H_{loc} : measured in bismuth oxide compounds under conditions of zero external magnetic field $H_0=0$ (the frequency values are averaged over the atomic lattice sites).

Compound	T, K	Transition frequencies, MHz				eqQ/h , MHz	η , %	H_{loc},Gs
		ν_1	ν_2	ν_3	ν_4			
α -Bi ₂ O ₃								
Bi(1)	77	25.2	45.8	69.4	92.8	556.7	0.13	171
Bi(2)		39.2	37.2	58.3	79.4	482.6	0.40	136
Bi ₅ O ₄ Br								
Bi(1)	77	21.6	25.1	39.6	53.3	322.6	0.31	-
Bi(2)		58	43.4	61.9	86.6	536.9	0.62	250
Bi ₄ Al ₄ O ₉	77	33.15	50.5	78	104.1	626.4	0.19	150
Bi ₄ Ge ₃ O ₁₂	300	20.4	40.9	61.3	81.7	490.3	0	25
	300	25.25	50.5	75.7	101	605.9	0	-

Bi ₂ Ge ₃ O ₉	77	25.7	51.6	77.35	103.2	618.8	0	60
--	----	------	------	-------	-------	-------	---	----

The observed multiplet structure of the NQR spectra further confirms the magnetic nonequivalence of bismuth atomic positions. Although the investigated materials are conventionally classified as diamagnetic, the presence of internal magnetic fields detected through NQR measurements suggests the existence of complex local magnetic ordering mechanisms. The obtained results demonstrate that the interaction between the electric field gradient and local magnetic fields plays a decisive role in determining the spectral characteristics of bismuth-containing compounds.

REFERENCES

1. Блюм Г., Мюссе Х., Шлихтинг Ф. Ядерный квадрупольный резонанс. — М.: Мир, 1967. — 456 с.
2. Khasanov, A. S., Eshonqulov, U. X., & Khojiev Sh, T. (2022). Technology for the Reduction of Iron Oxides in Fluidized Bed Furnaces. *Technology*, 6(12), 23-29.
3. Djurayevich, K. K., Kxudoynazar O'g'li, E. U., Sirozhevich, A. T., & Abdurashidovich, U. A. (2020). Complex Processing Of Lead-Containing Technogenic Waste From Mining And Metallurgical Industries In The Urals. *The American Journal of Engineering and Technology*, 2(09), 102-108.
4. Pines A., Wemmer D. Nuclear Quadrupole Resonance Spectroscopy in Solids // *Annual Review of Physical Chemistry*. — 1986. — Vol. 37. — P. 415–448.
5. Pinheiro C.B., Pertierra J.M. Structural and Electronic Properties of α -Bi₂O₃: A Review // *Materials Research Bulletin*. — 2007. — Vol. 42, No. 6. — P. 1073–1081.
6. Misra S.K. Multifrequency Electron Paramagnetic Resonance: Theory and Applications. — Weinheim: Wiley-VCH, 2014. — 620 p.
7. Khojakulov, A., Ruziyev, U., Boymurodov, N., Shernazarov, I., Mashaev, E., & Shoyimova, K. (2024). Research and determination of parameters for extracting valuable components from technological waste. In *BIO Web of Conferences* (Vol. 149, p. 01049). EDP Sciences.
8. Abdisamievich, S. A., Mamarasulovich, R. U., & Azamatugli, K. O. (2025). DEVELOPMENT OF TECHNOLOGY FOR OBTAINING ALUMINA FROM LOCAL RAW MATERIALS. *Sanoatda raqamli texnologiyalar/Цифровые технологии в промышленности*, 3(2), 105-111.
9. Petroff T.E., Norberg R.E. Quadrupole Interactions in Bismuth Compounds // *Physical Review*. — 1962. — Vol. 125, No. 6. — P. 1865–1875.

10. Kay M.I., Glasser R.M. Crystal Chemistry and Bonding in Bismuth Oxides // *Journal of Applied Crystallography*. — 1975. — Vol. 8. — P. 233–239.
11. Sawada A., Asahi T. NQR Detection of Local Magnetic Fields in Diamagnetic Crystals // *Solid State Nuclear Magnetic Resonance*. — 1999. — Vol. 15. — P. 1–14.
12. Ruziev, U. M. (2025). Enhancing Solid–Liquid Separation In Nitric Acid Leaching Of Low-Grade Alumina Ores.
13. Abdisamiyevich, S. A., Xudaynazar o‘g‘li, E. U., Mamarasulovich, R. U., & Ilyosjon o‘g‘li, X. I. (2025). ROASTING OF ALUMINA-CONTAINING MATERIAL IN A ROTARY KILN. *GREAT BRITAIN-SCIENTIFIC REVIEW OF THE PROBLEMS AND PROSPECTS OF MODERN SCIENCE AND EDUCATION*, 1(1), 22-28.
14. Ray S.K., Choudhury R.N.P. Electric Field Gradient Studies in Bi-Based Compounds Using NQR Technique // *Journal of Physics and Chemistry of Solids*. — 2005. — Vol. 66, No. 3. — P. 449–455.