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Features of the crystal structure and long-range magnetic order in honeycomb layered $\text{K}_2\text{Ni}_2\text{TeO}_6$

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Abstract

Layered honeycomb oxides $\text{A}_2\text{Ni}_2\text{TeO}_6$ are emerging as promising candidates for advanced spintronic devices and potassium-ion energy storage systems due to their unique quasi-two-dimensional magnetic and transport properties. In this work, we present a neutron powder diffraction study of the crystal and magnetic structure of $\text{K}_2\text{Ni}_2\text{TeO}_6$ over the temperature range 4–300 K. The sample crystallizes in the hexagonal space group $P6_3/mcm$ featuring alternating magnetic and non-magnetic layers. Below the Néel temperature ($T_N \approx 22.8$ K) the material exhibits a complex, incommensurate amplitude-modulated magnetic structure with a propagation vector $\mathbf{k} = (1/2 - \delta; \delta; 1/3 + \delta)$ with a relatively small incommensurability $\delta = 0.03$. Within the honeycomb layers, Ni^{2+} ions form a hexagonal honeycomb lattice centered on Te^{6+} ions. Crucially, the large interlayer spacing in $\text{K}_2\text{Ni}_2\text{TeO}_6$ significantly suppresses the interlayer exchange interaction compared to its lithium analog $\text{Li}_2\text{Ni}_2\text{TeO}_6$, stabilizing a quasi-two-dimensional magnetic ground state. These findings provide critical insights into the magneto-structural coupling in frustrated honeycomb lattices and highlight the potential of $\text{K}_2\text{Ni}_2\text{TeO}_6$ for applications in 2D magnetism, quantum materials, and high-voltage electrochemical energy storage.

Keywords: quasi-two-dimensional magnetism, layered honeycomb oxides, magnetic structure, neutron powder diffraction, spintronic material

INTRODUCTION

The sample $\text{K}_2\text{Ni}_2\text{TeO}_6$ belongs to a large class of quasi-two-dimensional oxides that has attracted extensive attention in recent years because of their diverse and non-trivial magnetic and transport properties, with potential applications in advanced electronics, spintronics, and energy storage technologies [1, 2]. From a fundamental perspective, quasi-two-dimensional oxides initially attracted the attention of researchers due to their ability to exhibit two-dimensional magnetism and high ionic conductivity, which are critical for next-generation solid-state batteries and electronic devices [3, 4].

Interest in such materials increased further for honeycomb-shaped crystal or magnetic structures following the discovery of graphene [5] and Kitaev magnetism [6]. Recently, compounds with high-spin ions $3d^7$ Co^{2+} with $S = 1/2$, and then $3d^7$ Fe^{+} and Ni^{3+} with $S = 1$ and even Cr^{3+} compounds with $S = 3/2$ were announced as candidates for Kitaev spin liquids [7-13].

$\text{A}_2\text{Ni}_2\text{TeO}_6$ layered oxides of the with Ni^{2+} and $S=1$ stand somewhat apart. They are not classified as materials with $3d^7$ ions, but they have the same honeycomb structure of the magnetic layer and, for the sodium composition, exhibit a zigzag spin structure in the ordered state, like most magnets that are candidates for Kitaev materials. Among the $\text{A}_2\text{Ni}_2\text{TeO}_6$ family, perhaps only $\text{Na}_2\text{Ni}_2\text{TeO}_6$ has been studied in sufficient detail so far. [14-18].

When studying the magnetism of layered quasi-two-dimensional compounds, there is undoubted interest in researching the interlayer exchange interaction, significant, albeit small in magnitude, which will lead to going beyond the framework of the J_1 – J_2 – J_3 model currently most commonly used for honeycomb compositions, and which takes into account only the interactions between the first (J_1), second (J_2) and third (J_3) neighbor magnetic atoms in the layer [19, 20].

We have already published the first results of a neutron diffraction study of the lithium composition, $\text{Li}_2\text{Ni}_2\text{TeO}_6$, containing the smallest alkali ion with the minimal distances between magnetic layers, where interlayer interaction is expected [21, 22]. In this work, we turn to the potassium compound, $\text{K}_2\text{Ni}_2\text{TeO}_6$, which has larger interlayer distances between magnetic layers than the related compounds $\text{Li}_2\text{Ni}_2\text{TeO}_6$ and $\text{Na}_2\text{Ni}_2\text{TeO}_6$.

In recent years, the compound $\text{K}_2\text{Ni}_2\text{TeO}_6$ has been investigated in several studies focusing on its crystal structure, as well as its electrochemical and magnetic properties [23–28]. Both experimental and computational methods have been employed in these works. Experimental techniques have included X-ray diffraction [23, 24], measurements of static and dynamic magnetic properties [24, 26] and studies of K^{+} ion dynamics and bulk magnetism using muon spin rotation and relaxation ($\mu^+\text{SR}$) [24]. Regarding electrochemical properties, key characteristics such as defect formation energies,

electronic structure, ionic diffusion coefficients, average open-circuit voltage, transition metal migration, intermediate high-voltage phases, and related parameters have been examined [28].

Theoretical calculations have been carried out using various implementations of density functional theory (DFT), including spin-polarized DFT+U methods [27] and DFT-based energy-mapping analyses [26]. For our study, it is crucial to note that the type and characteristics of the spin ordering in the ground state of $\text{K}_2\text{Ni}_2\text{TeO}_6$ have not yet been determined experimentally by neutron diffraction. The zigzag-type magnetic structures proposed in several prior works were either inferred by analogy with other honeycomb compounds or derived from specific DFT calculations [25, 26]. According to these works, the honeycomb layers in $\text{K}_2\text{Ni}_2\text{TeO}_6$ adopt a zigzag magnetic order, wherein ferromagnetic zigzag chains are coupled to each other antiferromagnetic owing to strongly antiferromagnetic third-neighbor exchange interactions, while the first-neighbor spin exchanges are ferromagnetic. Moreover, it has been suggested that adjacent zigzag honeycomb layers exhibit a preference for ferromagnetic interlayer coupling.

This work reports a neutron powder diffraction (NPD) study of the layered oxide to determine, refine, and describe its crystal structure and spin ordering, and to specify the structural parameters over the temperature range $T = 4 - 300$ K and the magnetic structure in the ordered state at $T = 4 - 30$ K.

2. Experiment

The $\text{K}_2\text{Ni}_2\text{TeO}_6$ sample investigated in the present study was synthesized by the solid-state ion-exchange reaction in a molten salt medium, as detailed in reference [26]. NPD data were collected on the SPODI diffractometer at the Heinz Maier-Leibnitz Zentrum (MLZ) [27].

Measurements were conducted in Debye–Scherrer transmission geometry high-resolution instrumental configuration, employing a vertically focusing Ge(331) monochromator (take-off angle $2\theta_m = 155^\circ$) to select a monochromatic neutron beam with wavelength $\lambda = 2.5362$ Å. The effective angular resolution of the diffractometer, defined as the full width at half maximum (FWHM) of the instrumental profile function, was $\Delta(2\theta) \approx 0.05^\circ$ at the minimum of the resolution function under the employed step-scanning protocol, achieved via sequential repositioning of the 80-channel ^3He position-sensitive detector array with fixed 10' Soller collimators.

Diffraction patterns were recorded over an angular range of $2\theta = 0-100^\circ$ with a step increment of $\Delta(2\theta) = 0.05^\circ$, ensuring sufficient counting statistics for reliable extraction of both nuclear and magnetic Bragg contributions. Measurements were performed at $T = 300$ K to refine the crystallographic parameters in the paramagnetic state, and subsequently at temperatures spanning T

= 4–30 K encompassing the region below and in the immediate vicinity of the Néel temperature (T_N = 22.8 K) to systematically track the evolution of long-range magnetic order.

Rietveld full-profile refinement of the acquired neutron diffraction patterns was performed using the FullProf software suite [30]. Visualization of the crystallographic and magnetic structure models of the investigated compound was carried out with the VESTA program [31].

3. Results and discussion

3.1. Crystal structure

In previously published studies [23, 25, 26], the crystal structure of $K_2Ni_2TeO_6$ was investigated using X-ray diffraction techniques. In the present work, we performed neutron diffraction experiments in two temperature ranges of particular interest: at $T = 300$ K, to refine the crystallographic parameters and obtain a complete description of the diffraction pattern including a few low-intensity reflections not reported in the aforementioned studies and $T = 4 - 30$ K, to examine the paramagnetic phase near T_N and to develop a model of long-range magnetic order in the ground state.

The clear advantage of neutron diffraction in this study lies not only in the high-precision determination of crystallographic parameters particularly the accurate positioning of light atoms such as oxygen and potassium against the background of the relatively heavy tellurium, thereby unambiguously defining the crystal structure. Second, it provides the capability to probe the magnetic structure, including the type of magnetic ordering and the spin configuration of nickel ions in the potassium tellurate.

The results of the Rietveld refinement of the powder diffraction data collected at $T = 300$ K are presented in Figure 1.

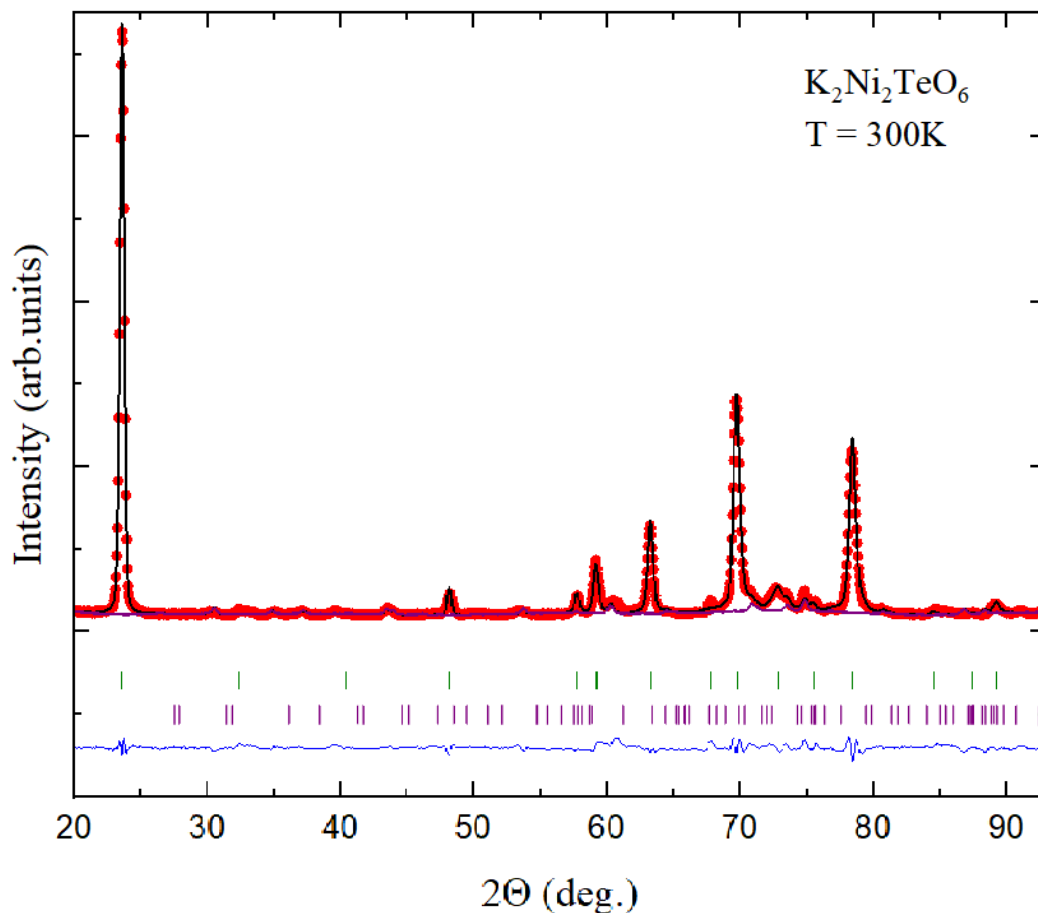


Fig. 1 Rietveld refinement results of neutron powder diffraction (NPD). Red circles represent the experimental data; the solid black line shows the determined diffraction profile; the blue line indicates the difference between experiment and calculation, vertically shifted downward for clarity; green vertical ticks denote Bragg peak positions: the upper row corresponds to the main phase — $K_2Ni_2TeO_6$ — and the lower row to the minor impurity phase — K_2CO_3 (purple profile). No Bragg neutron scattering is observed at scattering angles below 20° .

The studied sample crystallizes in the hexagonal space group $P6_3/mcm$, which belongs to the P2 structural type, where "P" denotes prismatic coordination of the alkali metal ion and "2" refers to stacking repeat period. This space group implies that all atoms except potassium occupy one crystallographic site. Consequently, there is no significant variation is observed in the metal–oxygen (M – O) bond distances (Tables 1 and 2). The occupancy of the K3 site is close to zero; therefore, this site was excluded from the calculations of bond lengths and bond angles.

An impurity phase of potassium carbonate K_2CO_3 was detected in the amount of 6.9 wt.% (Space group: $P2_1/c$; $a=5.6005$; $b=9.7458$; $c=6.9278 \text{ \AA}$; $\alpha=\gamma=90^\circ$; $\beta=99.4^\circ$)

Table 1 - Crystallographic data for $\text{K}_2\text{Ni}_2\text{TeO}_6$ (from neutron powder diffraction at $T=300$ K) space group $P6_3/mcm$ $a = b = 5.25118(1)$ Å, $c = 12.4292(8)$ Å; $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$; $V = 296.82(2)$ Å³. Agreement factors are $R_p = 5.33\%$; $R_{wp} = 7.25\%$; $R_{exp} = 3.30\%$; $\chi^2 = 4.77$

Atom	Site	x/a	y/b	z/c	Occupancy
K1	6g	0.42662(4)	0.00000	0.25000	0.112
K2	4c	0.66667	0.33333	0.25000	0.014
K3	2a	0.00000	0.00000	0.25000	0.006
Ni	4d	0.66667	0.33333	0.00000	0.1667
O	12k	0.69288(8)	0.69288(8)	0.58285(2)	0.5000
Te	2b	0.00000	0.00000	0.00000	0.0833

Table 2 - Selected interatomic distances and bond angles for $\text{K}_2\text{Ni}_2\text{TeO}_6$ at $T = 300\text{K}$

	Bond distances (Å)			Bond angles (deg.)
		Sum of radii [32]		
Ni - O	2.091(3)	2.09	Ni – O - Ni	92.47(2)
Ni - Ni First neighbors	3.032(3)	-	O – Ni - O	98.43(3)
Ni - Ni Second neighbors	5.253(4)	-	Ni – Ni - Ni	119.98(1)
Ni - Ni Third neighbors	6.061(4)	-		
Ni - Ni Interlayer	6.215(5)	-		
Te - O	1.966(4)	1.96		
K1 - O	2.791(3)	2.78		
K2 - O	2.787(4)	2.78		

The crystal structure of $K_2Ni_2TeO_6$ consists of alternating layers stacked along the c axis: magnetic layers formed by edge-sharing TeO_6 and NiO_6 octahedra, and non-magnetic layers consisting of KO_6 prisms (see Fig .2).

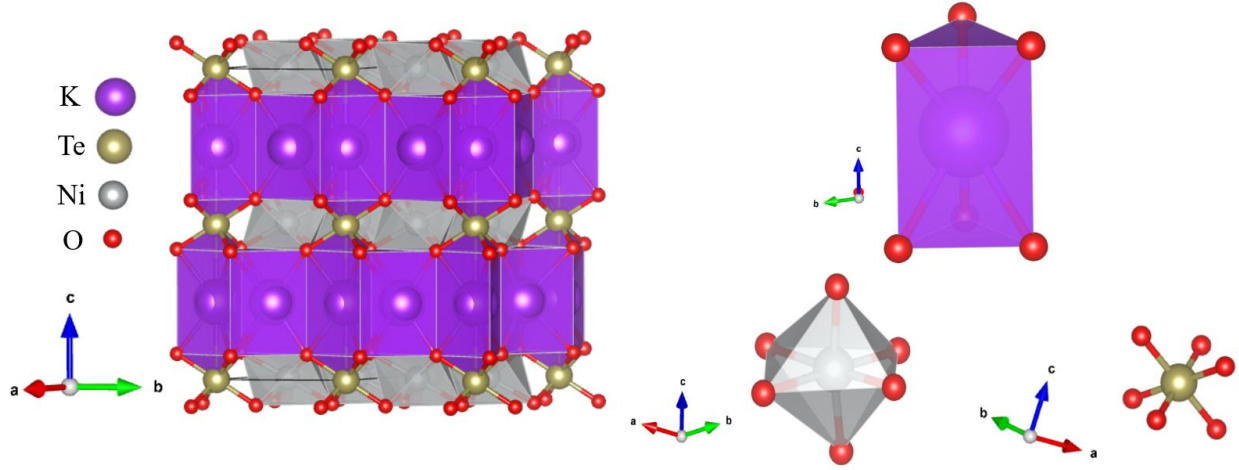


Fig. 2 Crystal structure of $K_2Ni_2TeO_6$. Oxygen octahedra centered by Ni atoms are colored according to the nickel ion color; oxygen prisms centered by K atoms are colored according to the potassium ion color; oxygen octahedra centered by Te atoms are left uncolored.

The architecture of the magnetic layers is of particular interest: it forms a rigid, honeycomb-like hexagonal network where each tellurium atom, located at the center of an oxygen octahedron, is surrounded by six nickel atoms (also residing at the centers of oxygen octahedra) (Fig.3). These structural feature may underlie the nontrivial physical properties observed in this system, noted in the Introduction.

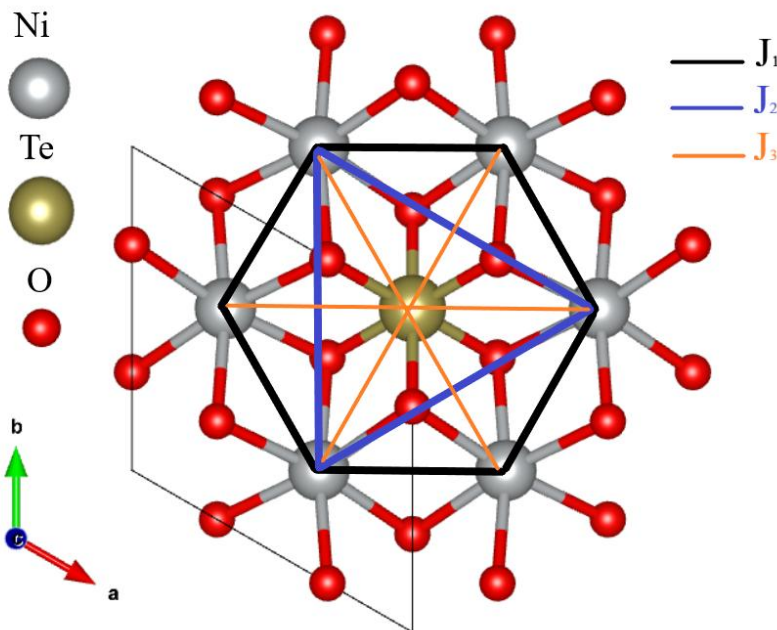


Fig. 3 Crystal structure of the magnetic layer. J_1 , J_2 , and J_3 denote the exchange couplings between first-, second-, and third-nearest-neighbor Ni^{2+} ions, respectively (drawn directly between the Ni ions conditionally). The parallelogram illustrates the projection of the unit cell on the ab -plane. The line thicknesses of the exchange couplings J_1 , J_2 , and J_3 are varied solely for visual clarity and do not represent the relative magnitudes or contributions of the corresponding exchange interactions.

Each nickel atom is in a high-spin state ($S = 1$), consistent with earlier X-ray absorption spectroscopy (XAS) studies at the Ni K -edge (~ 8.34 keV) on $\text{K}_2\text{Ni}_2\text{TeO}_6$ samples [25]. Studies confirmed the divalent Ni^{2+} state through comparison with the reference compound NiO. Furthermore, electron paramagnetic resonance (EPR) data in the paramagnetic phase reveal a single broad Lorentzian line, characteristic of Ni^{2+} ions in octahedral coordination [26] as well. The high-spin Ni^{2+} state corresponds to a $3d^8$ electronic configuration (formally $3d^8 4s^0$ in the solid state), with two unpaired electrons occupying the $d(x^2-y^2)$ and dz^2 orbitals, enabling covalent bonding with the 2p orbitals of oxygen anions. Notably, in $\text{K}_2\text{Ni}_2\text{TeO}_6$, the interlayer spacing between magnetic is significantly larger than the intralayer Ni – Ni distance corresponding to the J_3 exchange path, usually the strongest in such systems (Fig. 3). This structural feature implies that, while the crystal structure is three-dimensional, the magnetic behavior is expected to be quasi-two-dimensional, as the intralayer exchange interactions (J_1 , J_2 , J_3) are likely to dominate the formation of long-range magnetic order compared to the much weaker interlayer coupling (J_z). Additionally, the arrangement of potassium ions within the non-magnetic layers exhibits a distinctive feature. As noted above, the alkali metal occupies three distinct Wyckoff positions within the unit cell: $2a$, $4c$, and $6g$ (Fig. 4).

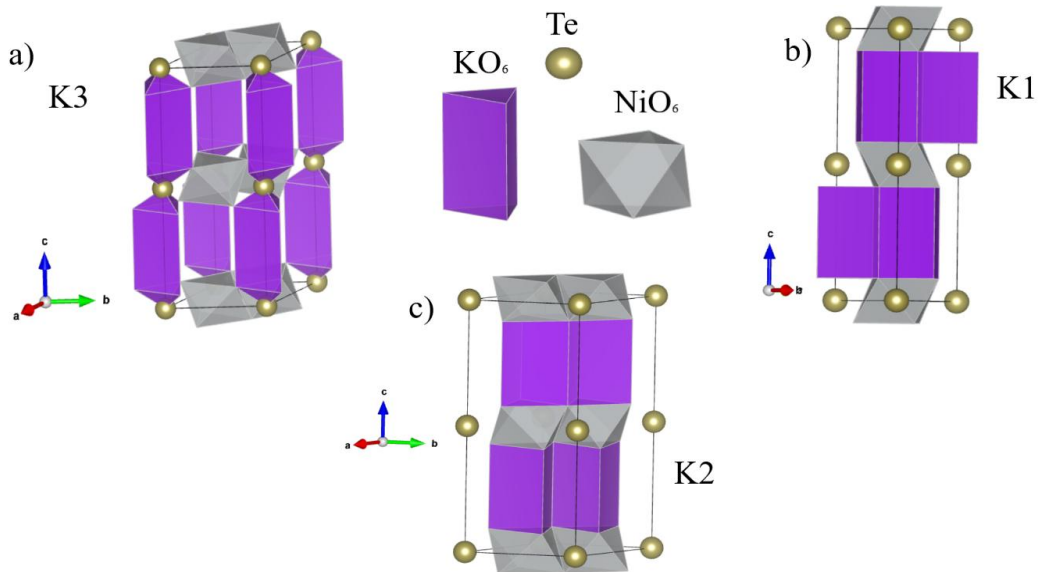


Fig. 4 Possible arrangements of oxygen prisms with central potassium ions in the non-magnetic layers: (a) K3 ions at the $2a$ ($0\ 0\ \frac{1}{4}$) site; (b) K2 ions at the $4c$ ($\frac{2}{3}\ \frac{1}{3}\ \frac{1}{4}$) site; (c) K1 ions

at the 6g ($x = 0.125$) site. Oxygen ions reside at the prism vertices and are omitted for clarity. Alkali metal ions are located at the prism centers but are not shown as well in the figure for visual simplicity.

The oxygen triangular prism formed with the K3 ion shares faces exclusively with TeO_6 octahedra. In contrast, the K1 prism shares faces solely with NiO_6 octahedra, while the K2 prism shares faces with both TeO_6 and NiO_6 octahedra. Occupancy factors for all three potassium sites, calculated based on experimental data, are listed in Table 1. In our previous study of the related compound $\text{Na}_2\text{Ni}_2\text{TeO}_6$, we proposed that the occupancy of the analogous, energetically unfavorable Na3 site, which is (sandwiched between two TeO_6 octahedra) is effectively zero, which would suppress interlayer exchange interactions [16]. The authors of reference [17] reached the same conclusion. A similar situation is observed here: excluding the least-occupied K3 sites does not disrupt the continuity of cation migration pathways between the K1 and K2 sites, which are connected via relatively wider migration channels.

The overall potassium deficiency is likely attributable to the presence of a K_2CO_3 impurity phase (6.9 wt.%). The synthesis of the investigated compound was carried out at a temperature of $T = 700\text{ }^\circ\text{C}$, whereas the melting and decomposition temperatures of potassium carbonate are $891\text{ }^\circ\text{C}$ and $1200\text{ }^\circ\text{C}$, respectively; therefore, under these conditions, the completeness of the chemical reaction cannot be unequivocally assured [23]. The reduction in the number of possible exchange interactions between magnetic layers further supports the hypothesis that the establishment of three-dimensional (3D) long-range magnetic order in this compound is inherently hindered.

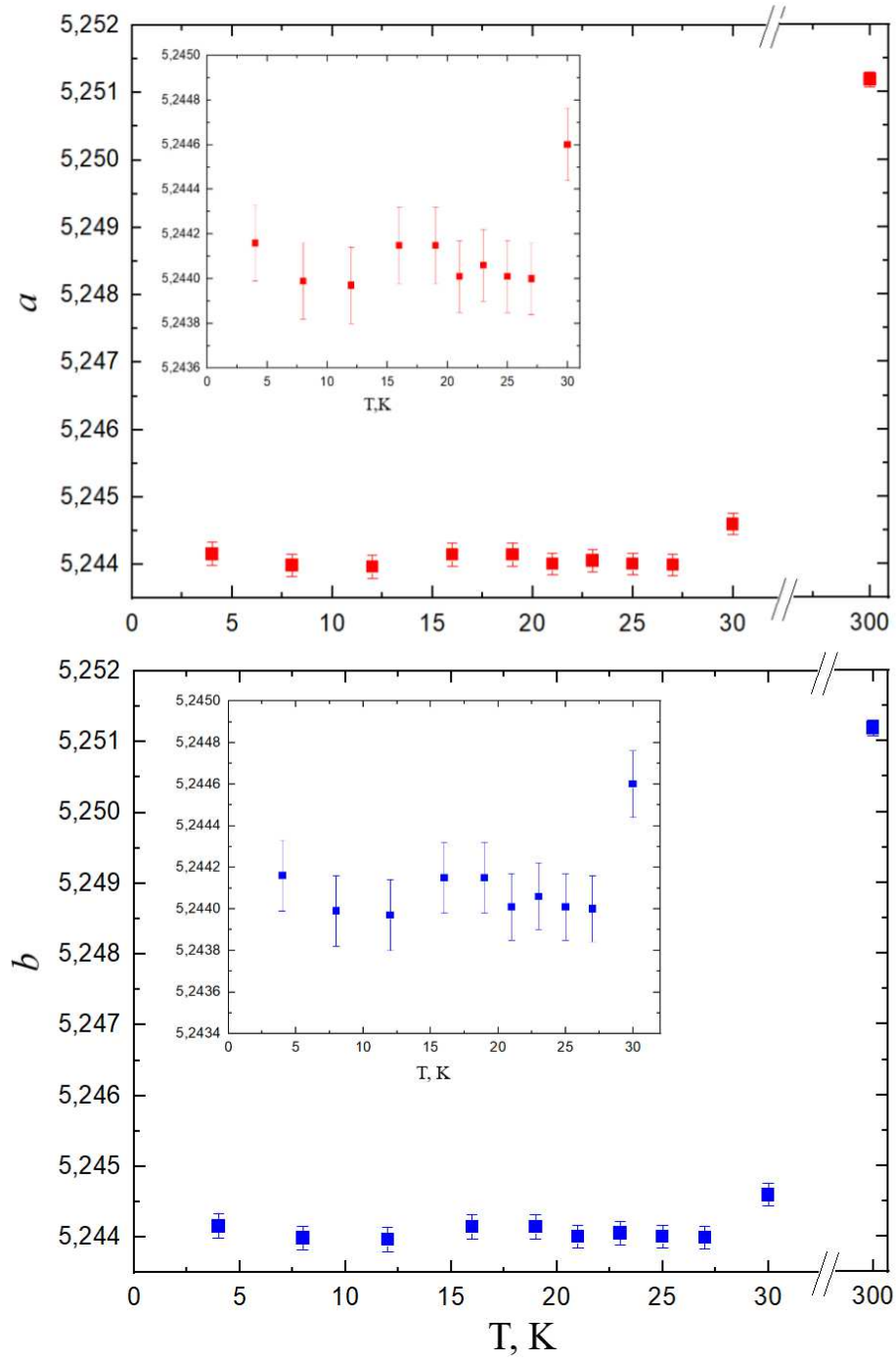


Fig. 5 Temperature dependence of the in-plane lattice parameters a and b of the crystallographic unit cell over the temperature range $T = 4 - 300$ K. Insets in each panel provide an enlarged view of the parameter evolution within the narrow temperature interval $T = 4 - 30$ K, corresponding to the long range magnetic ordered state.

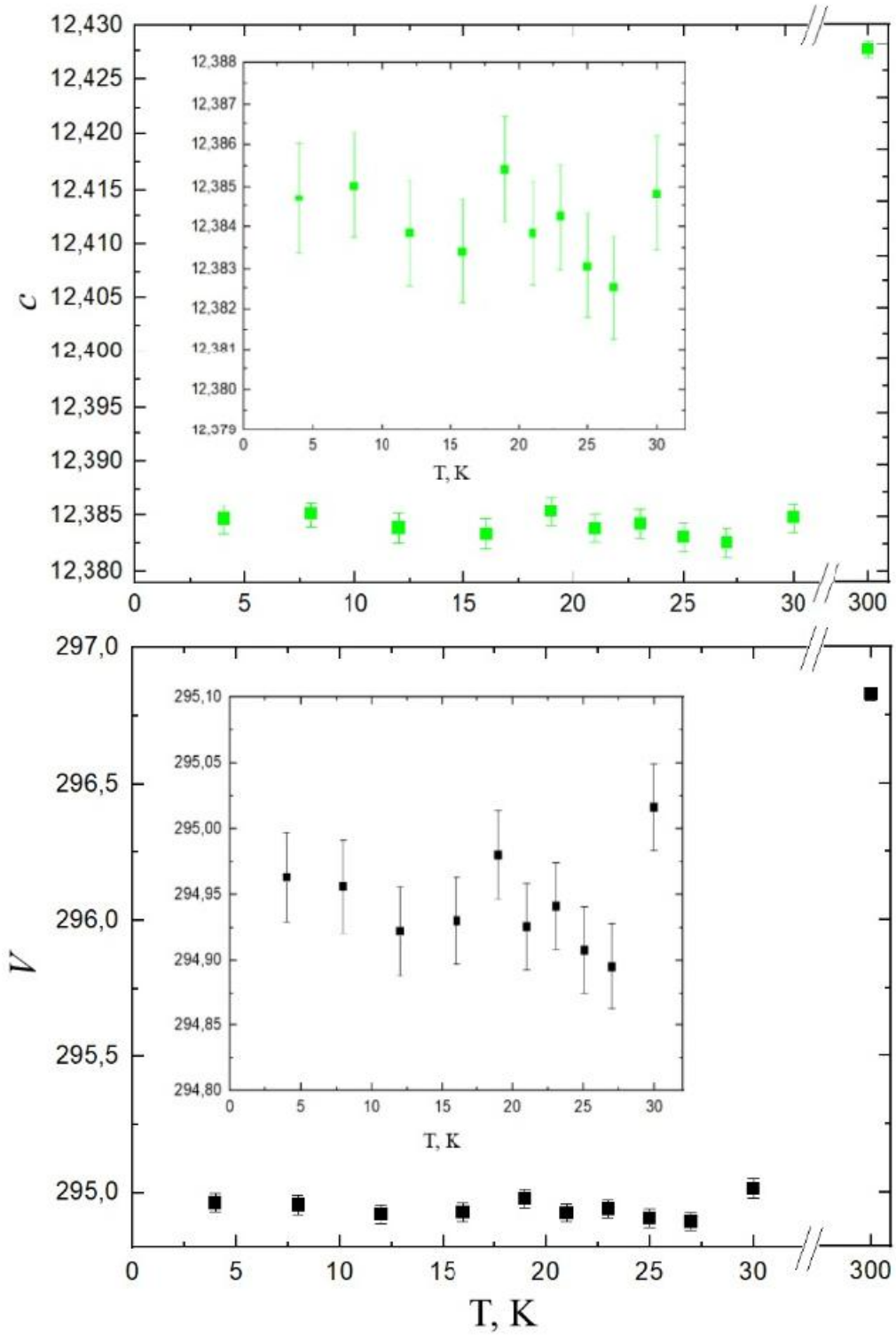


Fig. 6 Temperature dependence of the out-of-plane lattice parameter c and unit cell volume V over the entire investigated temperature range ($T = 4 - 300$ K). Insets in each panel show an enlarged view of the parameter evolution within the narrow temperature interval $T = 4 - 30$ K.

The temperature dependence of the unit cell parameters was determined from experimental data. Upon cooling in the paramagnetic state, a systematic reduction of all lattice parameters is observed, followed by their stabilization in the magnetic ordered state (Figs. 5 and 6). No evidence of structural phase transitions was detected.

Analysis of the temperature dependence of the lattice parameters a , b , c , and V (Figs. 5 and 6) reveals a systematic behavior in the vicinity of $T_N \approx 25$ K. Within experimental uncertainty, the parameters a , b , c , and V exhibit a correlated evolution throughout the entire investigated temperature range. Collectively, these observations provide direct experimental evidence of magnetostructural coupling in the studied compound, $\text{K}_2\text{Ni}_2\text{TeO}_6$. Thus, magnetic ordering exerts a direct influence on the crystal lattice, manifesting as a coherent rearrangement of the structural parameters (within experimental error) upon crossing the Néel temperature

Using the lattice parameters, interatomic distances, and bond angles (Tables 1 and 2), bond valence sums for each ion in the unit cell were calculated with the Bond_Str program (FullProf suite). The obtained values are: $\text{Ni}^{2+} — 1.92(3)$; $\text{O}^{2-} — 1.97(2)$; $\text{Te}^{6+} — 6.02(2)$; $\text{K}^+ — 1.01(2)$.

3.2. Magnetic structure

To investigate the features of magnetic ordering in $\text{K}_2\text{Ni}_2\text{TeO}_6$, low-temperature NPD studies were performed below the Néel temperature (T_N) and in the paramagnetic state just above T_N to taking into account the contribution of nuclear neutron scattering. The temperature-dependent evolution of the neutron diffraction data, collected on the SPODI diffractometer over the range of 4 – 300 K, is presented in Fig. 7.

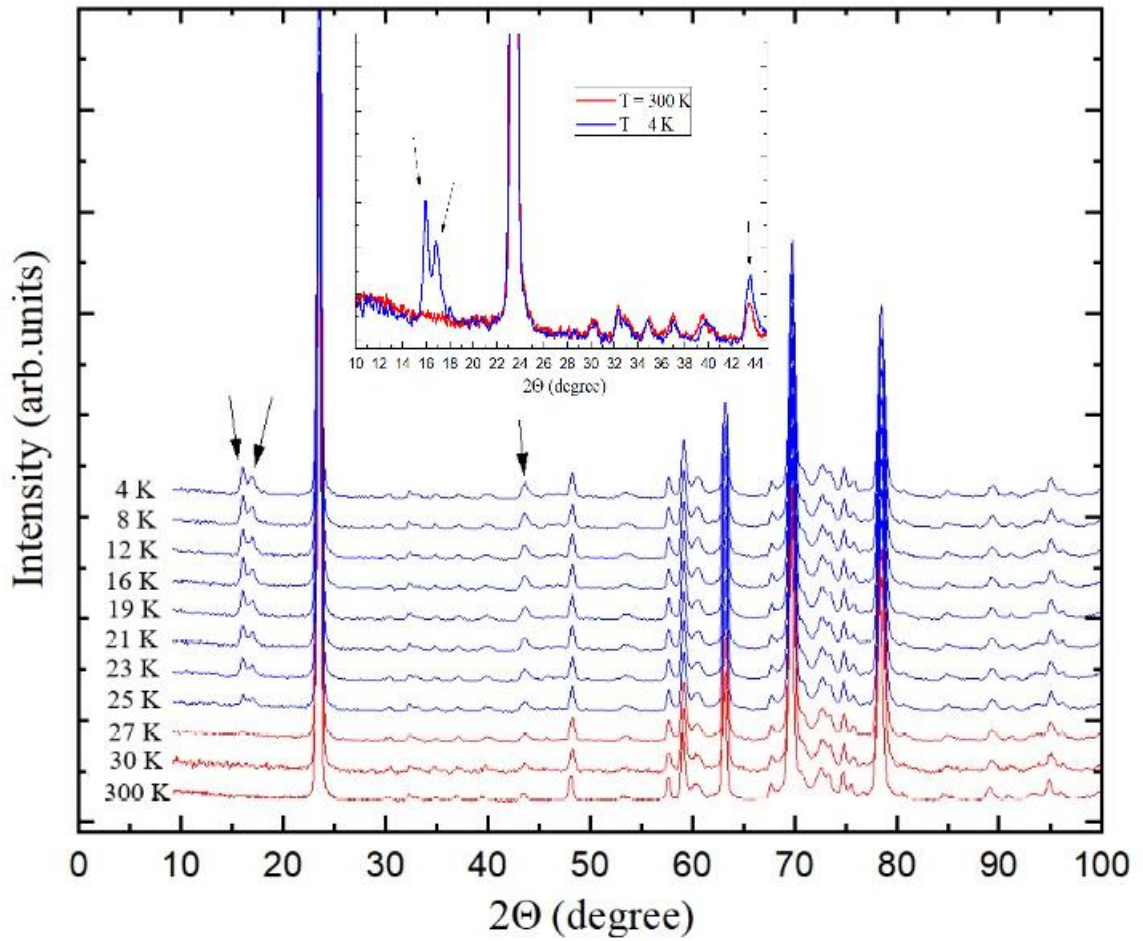


Fig. 7 Temperature dependence of neutron scattering intensity in the range $T = 4 - 300$ K, illustrating the emergence and evolution of magnetic neutron scattering. Arrows indicate the most intense magnetic Bragg peaks. Neutron diffraction patterns recorded in the paramagnetic state are highlighted in red, whereas those representing the superposition of nuclear and magnetic scattering (evidencing the establishment of long-range magnetic order) are shown in blue. Inset: Magnified view of the magnetic contribution to the diffraction pattern ($T = 300$ K, 4 K).

Neutron diffraction patterns collected below 27 K reveal the appearance of additional magnetic Bragg peaks, confirming the onset of long-range magnetic order. Three of the most prominent magnetic reflections are clearly discernible in the low-angle region ($2\Theta = 16^\circ$, 16.9° and 43.6°). Notably, the emergence of magnetic peaks at angles lower than the first nuclear reflection ($hkl = 002$, $2\Theta = 23.63^\circ$) provides unambiguous evidence for antiferromagnetic ordering, which is consistent with prior bulk magnetization measurements [24, 26]. As shown in the inset of Fig. 7 (comparing data at $T = 300$ K and 4 K), the contribution of magnetic scattering to the diffraction pattern is unambiguously evident. Analysis of the most intense magnetic reflections using the k-search tool (FullProf suite) led to incommensurate magnetic propagation vector

$\mathbf{k} = (0.47(1) \ 0.03(2) \ 0.37(4))$. The modest incommensurability is observed along all three crystallographic directions; allowing the vector to be expressed in the general form: $\mathbf{k} = (1/2 - \delta; \delta; 1/3 + \delta)$ with $\delta = 0.03(1)$. This implies that the magnetic unit cell is approximately doubled along the a -axis, unchanged along b , and tripled along c , relative to the crystallographic unit cell.

We have additionally performed a comparative Profile Matching refinement analysis for three magnetic propagation vectors: $(1/2, 0, 1/3)$ (Fig. 8b), $(1/2, 0, 1/2)$ (Fig. 8c), and the model proposed in this work, characterized by an incommensurability parameter $\delta = 0.03(1)$ (Fig. 8a). As illustrated, the magnetic propagation vector incorporating the incommensurability parameter yields the best refinement convergence. Neglecting this parameter significantly deteriorates the fitting quality, preventing an accurate description of magnetic reflections in the low-angle region. The vector $(1/2, 0, 1/2)$ was adopted based on the analysis reported in reference [17]. The difference between the magnetic propagation vectors $\mathbf{k} = (1/2, 0, 1/3)$ for $\text{K}_2\text{Ni}_2\text{TeO}_6$ and $\mathbf{k} = (1/2, 0, 1/2)$ for $\text{Na}_2\text{Ni}_2\text{TeO}_6$ reflects a reconstruction of the magnetic periodicity along the crystallographic c -axis, driven by the substitution of the alkali cation. The larger ionic radius of K^+ relative to Na^+ induces an expansion of the crystal lattice, resulting in an increased interlayer spacing and a modification of the super-superexchange pathway geometry. In the sodium compound, the more compact structure enhances interlayer super-superexchange interactions, thereby stabilizing an antiferromagnetic configuration with a doubled periodicity along the c -axis. In the potassium system, the weakening of interlayer exchange is proposed to promote magnetic frustration within the layered sublattice. The presumed competition between ferro- and antiferromagnetic interactions along the c -direction is minimized in the configuration with a tripled magnetic unit cell, realized by the propagation vector component $k_z = 1/3$. Thus, the transition from the magnetic propagation vector $(1/2, 0, 1/2)$ to $(1/2, 0, 1/3)$ demonstrates the high sensitivity of the magnetic ground state in layered nickel tellurates to variations in distances between magnetic layers.

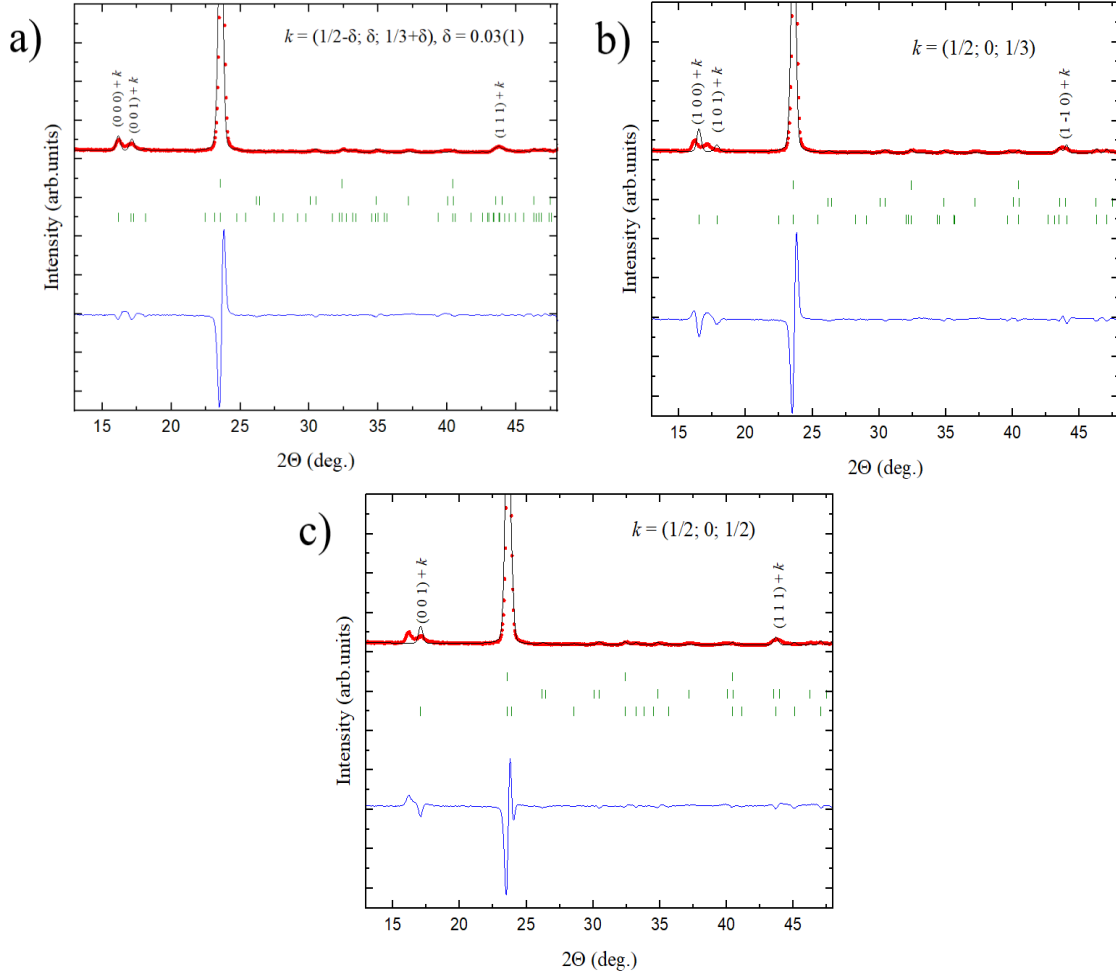


Fig. 8 Profile Matching refinement for three propagation vectors: (a) $\mathbf{k} = (1/2 - \delta, \delta, 1/3 + \delta)$ with $\delta = 0.03(1)$ ($R_p = 13.1\%$; $R_{wp} = 21.4\%$; $R_{exp} = 3.53\%$; $\chi^2 = 36.6$); (b) $\mathbf{k} = (1/2, 0, 1/3)$ ($R_p = 17.3\%$; $R_{wp} = 24.6\%$; $R_{exp} = 3.46\%$; $\chi^2 = 50.7$); (c) $\mathbf{k} = (1/2, 0, 1/2)$ ($R_p = 17.0\%$; $R_{wp} = 23.6\%$; $R_{exp} = 3.46\%$; $\chi^2 = 46.7$).

Using the BASIreps program (FullProf software suite) and the basis-vector approach of irreducible representations, a magnetic structure model was proposed based on the experimental diffraction pattern recorded at the lowest experimental temperature $T = 4$ K. The treatment utilized the positions of magnetic Bragg reflections, structural information specifically the space group, symmetry operators, and the atomic coordinates of the magnetic ion obtained from the Rietveld refinement of neutron diffraction data at the same temperature, along with the determined magnetic propagation vector $\mathbf{k}$. Based on this analysis, the irreducible representation compatible with the observed magnetic structure was identified as:

$$\Gamma_{mag} = 3\Gamma_1^1$$

In our case, the irreducible representation corresponds to a linear combination of three one-dimensional reducible representations, which constitute the real part of the magnetic moments Fourier transform Ψ . For each Ni atom occupying the same Wyckoff position, the basis functions are given by: $\Psi_1 = (100)$; $\Psi_2 = (010)$; $\Psi_3 = (001)$. These functions characterize the translational symmetry of the magnetic moment along the crystallographic axes: (100) along the x-direction, (010) along the y-direction, and (001) along the z-direction. The coefficients of these basis vectors were refined via Rietveld analysis using the FullProf software suite to determine both the orientation and magnitude of the Ni^{2+} magnetic moments. The results of this processing for the low-temperature NPD data are presented in Fig. 9.

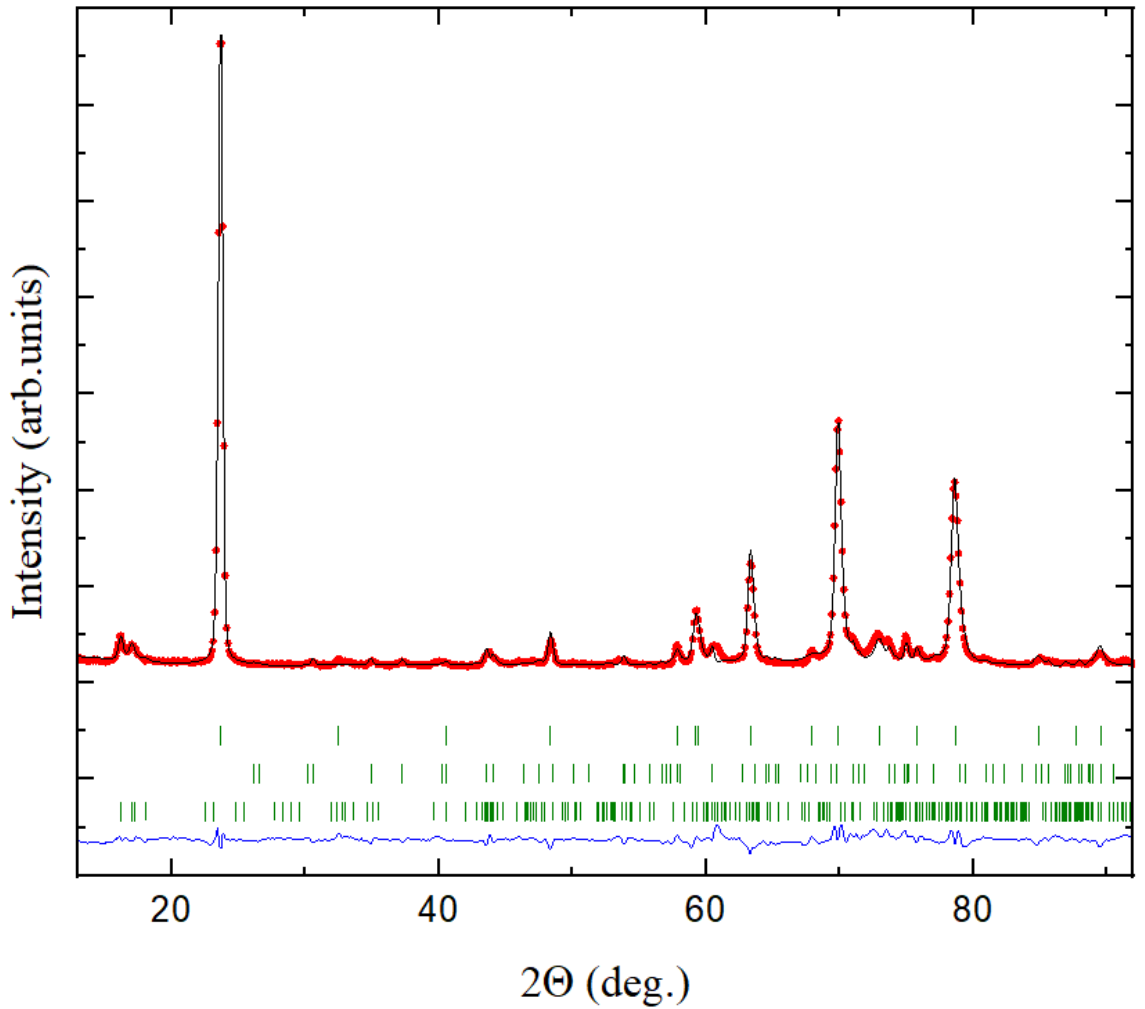


Fig. 9 Rietveld refinement of neutron powder diffraction data for $\text{K}_2\text{Ni}_2\text{TeO}_6$ at $T = 4$ K. Red circles denote the experimental data points; the black solid curve represents the calculated diffraction profile; the blue curve indicates the difference between experiment and the refined model; green vertical ticks mark the Bragg peak positions of individual phases: the top row corresponds to the main crystallographic phase ($P6_3/mcm$), the middle row to the secondary potassium carbonate

impurity phase, and the bottom row to the magnetic scattering contribution from the main phase. Agreement factors are $R_p = 7.20\%$; $R_{wp} = 9.84\%$; $R_{exp} = 3.39\%$; $\chi^2 = 8.43$; $R_M = 10.7\%$

A full-profile analysis of NPD collected at $T = 4$ K enabled the creation of the magnetic structure model of $K_2Ni_2TeO_6$. The magnetic unit cell of this compound contains two magnetic sublattices consisting of Ni ions occupying the $4d$ Wyckoff site described by the fractional coordinates: $(1/3; 2/3; 0)$; $(2/3; 1/3; 0)$ and $(1/3; 2/3; 1/2)$; $(2/3; 1/3; 1/2)$, given that the lattice parameters a and b of the crystallographic unit cell are equal, the x and y coordinates are symmetry-equivalent.

The three-dimensional magnetic structure of $K_2Ni_2TeO_6$ is rather complex. Overall, the magnetic order is amplitude-modulated, with the amplitude-modulated spiral propagating along the c -axis (Fig.10), which corresponds to the stacking layers direction. Within the honeycomb sublattice formed by Ni^{2+} ions, the spin arrangement adopts a "zigzag" pattern: three adjacent magnetic moments are aligned in one direction, while the other three point in the opposite direction (Fig. 10a). When considering the entire ab magnetic plane, the Ni spins exhibit a zig-zag ferro-magnetic chain-order. (Fig. 10b). Each such ferromagnetic double zig-zag ferro-magnetic chain-order is antiferromagnetic coupled to its neighboring ferromagnetic chains.

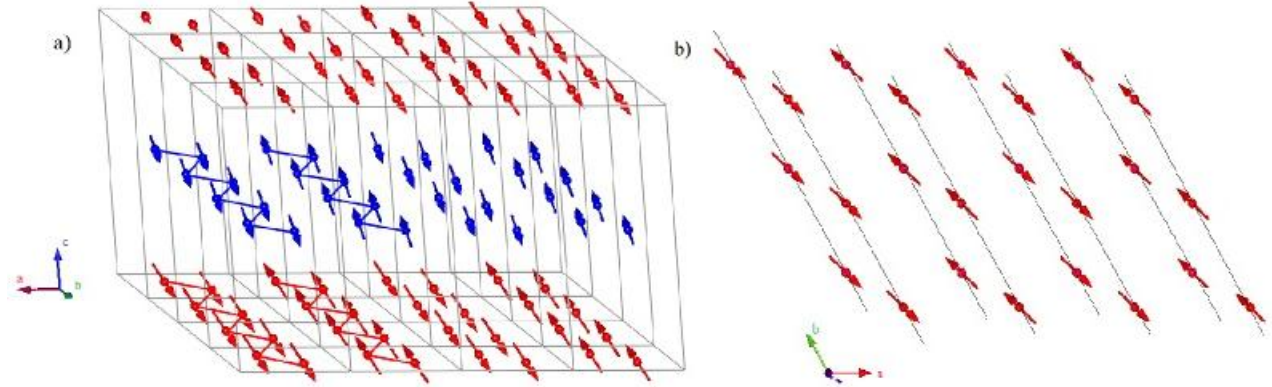


Fig. 10 Magnetic structure of $K_2Ni_2TeO_6$ at $T = 4$ K. (a) Illustration of the zigzag-type magnetic ordering within the honeycomb-like arrangement of Ni^{2+} ions; b) zig-zag ferromagnetic chain-order spin arrangement of nickel ions, manifested as two adjacent one-dimensional chains — projection onto the magnetic ab plane (only one layer, comprising “red” Ni^{2+} ions, is shown).

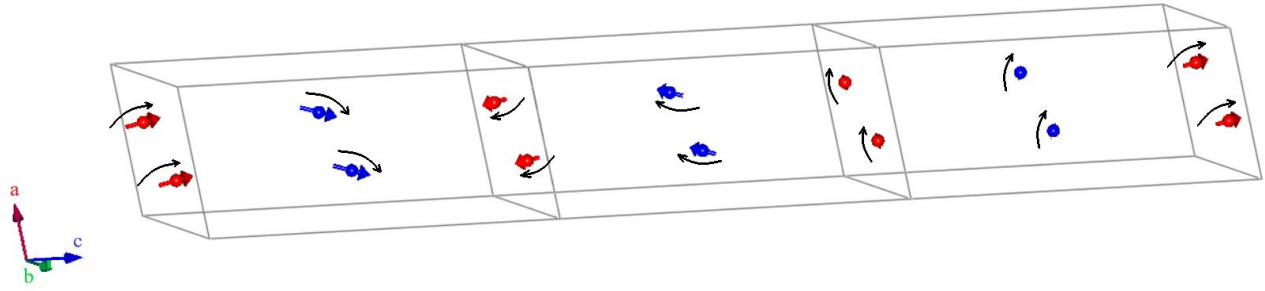


Fig. 11 Propagation of the amplitude-modulated spin spiral, accompanied by modulation of the magnitude of the Ni^{2+} magnetic moments, along the layer-stacking c -axis.

Figure 11 illustrates the propagation of the amplitude-modulated spin spiral along the crystallographic c -axis, which coincides with the stacking direction of the honeycomb layers in $\text{K}_2\text{Ni}_2\text{TeO}_6$. The magnetic moments of Ni^{2+} ions rotate progressively from one layer to the next, forming a long-period amplitude-modulated spiral modulation characterized by the incommensurate propagation vector $\mathbf{k} = (1/2 - \delta; \delta; 1/3 + \delta)$ with $\delta \approx 0.03$. This amplitude-modulated arrangement is accompanied by a subtle modulation of the magnetic moment magnitudes across the two crystallographically distinct Ni sublattices, with refined values of $M(1) = 2.31(4) \mu_B/\text{Ni}^{2+}$ and $M(2) = 2.12(4) \mu_B/\text{Ni}^{2+}$ at $T = 4$ K. The dots in the schematic represent individual Ni^{2+} magnetic moments, whose orientations remain parallel within each ab -plane but undergo a systematic rotation upon translation along the c -direction.

The amplitude-modulated spiral spin structure developing along the c -axis direction is presumably related to the non-zero component of the propagation vector $k_z = 1/3 + \delta$

Within the framework of representational analysis and low-dimensional magnetism in general, the magnetic moment of the i -th atom in the system is related to the magnetic moment of the "zeroth" atom via the phase factor $\exp(ik \cdot \mathbf{R})$ where $\mathbf{k}$ is the magnetic propagation vector and $\mathbf{R}$ is the translation vector of the crystal lattice. Upon Fourier transformation, the magnetic moment is expressed as a linear combination of the refined coefficients and the basis vectors generated by the BASIREPS program:

$$\mathbf{M} = \text{BASR} \cdot \cos(2\pi \mathbf{k} \cdot \mathbf{R}) + \text{BASI} \cdot \sin(2\pi \mathbf{k} \cdot \mathbf{R})$$

where BASR is the real part (cosine component) and BASI is the imaginary part (sine component) of the Fourier transform.

In our refinement, the basis vectors are strictly defined as:

$$\text{BASR} = (1 \ 0 \ 0) \ (0 \ 1 \ 0) \ (0 \ 0 \ 1)$$

$$\text{BASI} = (0 \ 0 \ 0) \ (0 \ 0 \ 0) \ (0 \ 0 \ 0)$$

The real part (BASR) allows the Ni^{2+} magnetic moments to adopt an arbitrary orientation in three-dimensional space, as their direction is determined by the linear combination of the refined coefficients along the crystallographic axes.

A critically important result for the incommensurate magnetic structure is that the imaginary part (BASI) is strictly equal to zero.

A non-zero imaginary part (with a non-zero real part) would induce a cycloidal rotation of the magnetic moment (a true amplitude-modulated spiral). However, since $\text{BASI} = 0$, the second term of the equation vanishes.

Consequently, the magnetic structure represents not a cycloidal spiral, but an amplitude-modulated spiral. The magnitude of the magnetic moment is modulated strictly according to the cosine law, oscillating from a maximum to zero and back. This specific amplitude-modulated ground state is not accidental; it is fundamentally dictated by the structural features of the $\text{K}_2\text{N}_2\text{TeO}_6$ crystal lattice and the presence of magnetic frustration:

i) there is a strong competition of exchange interactions within the honeycomb layer. The nearest-neighbor interaction (J_1) is strongly ferromagnetic, and third-neighbor interaction (J_3) is strongly antiferromagnetic. The system minimizes its energy by splitting into two distinct magnetic sublattices.

ii) along the crystallographic c -axis, there is a weak super-superexchange interaction mediated by alkali metal ions. A feature of this structure is the potassium ion deficiency, in particular, the practically zero occupancy of the $2a$ (K3) Wyckoff site.

This potassium deficiency absence disrupts the geometry and dynamics of the interlayer exchange interactions. Since the system cannot simultaneously satisfy all competing in-plane (J_1, J_3) and interlayer exchange interactions, it resolves this frustration by adopting an incommensurate amplitude-modulated structure.

The refined total magnetic moments for the Ni^{2+} ions are $M(1) = 2.31(4) \mu_B/\text{Ni}^{2+}$ ($m_x = 0.678$ $m_y = -1.621$ $m_z = 1.491$) for one magnetic sublattice and $M(2) = 2.12(4) \mu_B/\text{Ni}^{2+}$ ($m_x = -0.063$ $m_y = -1.872$ $m_z = 1.067$) for the other. These values are consistent with the expected magnetic moment for the high-spin state ($S = 1$), which is $2.83 \mu_B/\text{Ni}^{2+}$, as well as with the effective magnetic moment $2.24 \mu_B/\text{Ni}^{2+}$ derived from bulk magnetic measurements reported in Ref. [23].

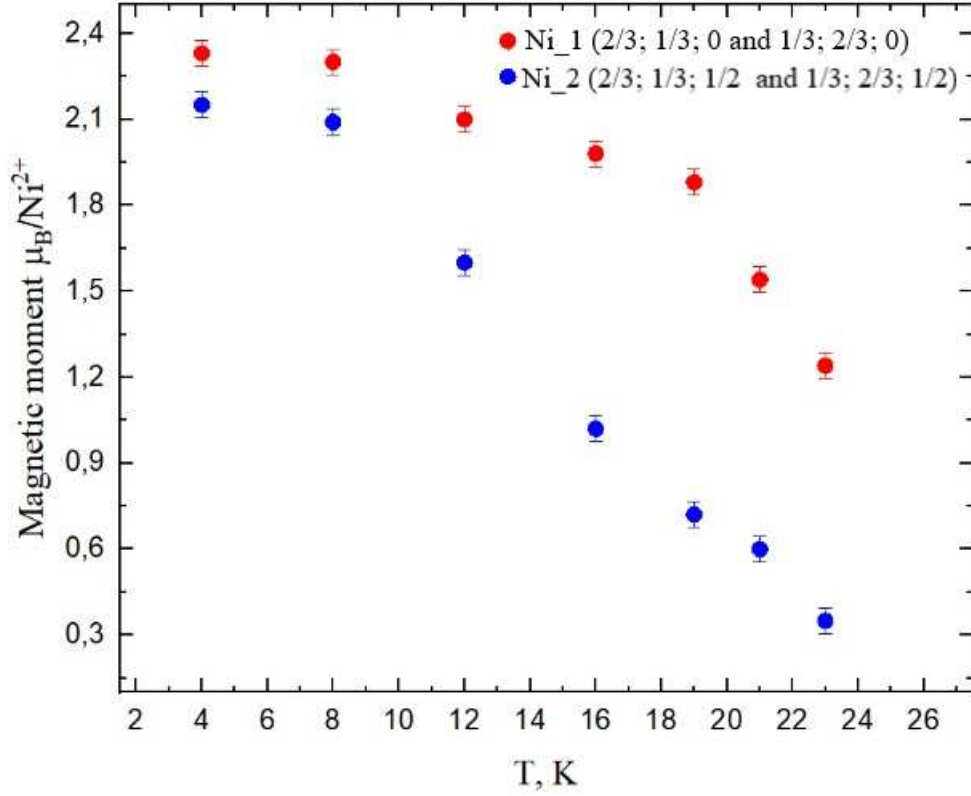


Fig. 12 Magnetic moment as a function of temperature.

A study was conducted on the temperature dependence of the magnetic moment for both sites of nickel ions, characterized by a regular decrease up to the $T_N = 22.8$ K [23].

Quadratic approximations of the temperature dependence magnetic moment were obtained for two pairs atoms within the magnetic sublattice:

$$M_1(T) = -0.0081T^2 + 0.1591T + 2.2131;$$

$$M_2(T) = -0.0016T^2 - 0.0588T + 2.5038;$$

The difference in the constant term of the quadratic functions corresponds to a deviation in the zero-temperature magnetic moments that lies within the experimental uncertainty.

Both moments extrapolated to $T \rightarrow 0$ K fall below the theoretical spin-only value of $2.828 \mu_B/\text{Ni}^{2+}$. For sublattice 1 (red), the initial positive slope ($dM/dT > 0$ at low T) combined with a negative quadratic coefficient gives rise to a maximum in the moment at approximately 9.8 K; a similar non-monotonic behavior is observed for sublattice 2 (blue) with a maximum at 12.8 K. The distinct curvatures of the two $M(T)$ dependencies reflect different energy scales of spin-lattice coupling for the two sublattices, which can be attributed to differences in the magnetic ordering within each sublattice.

Based on the obtained spin-ordering model, we propose that the exchange coupling within the magnetic layers are mediated by two mechanisms: superexchange between: $\text{Ni}^{2+} - \text{O}^{2-} - \text{Ni}^{2+}$ and super-superexchange through the nonmagnetic ion Te^{6+} : $\text{Ni}^{2+} - \text{O}^{2-} - \text{Te}^{6+} - \text{O}^{2-} - \text{Ni}^{2+}$.

We propose that both exchange mechanisms originate from the overlap between the Ni^{2+} orbitals $d(x^2-y^2)$ and dz^2 —the oxygen $2p$ orbitals. This is due to the direct spatial orientation of the e_g orbitals toward the oxygen ligands in an octahedral coordination, in contrast to the t_{2g} orbitals ($d(xy); d(xz); d(yz)$), whose lobes are oriented between the ligands and are therefore farther from the oxygen centers within the octahedron. In the super-superexchange pathway, the nonmagnetic Te^{6+} ion acts as an additional bridge, facilitating electron exchange through the overlap of $2p$ (O^{2-}) and $5p$ (Te^{6+}), orbitals, thereby forming a covalent $\text{O}^{2-} - \text{Te}^{6+} - \text{O}^{2-}$ linkage that mediates the magnetic interaction.

The ferromagnetic nature of the nearest-neighbor interaction J_1 in the Ni^{2+} magnetic sublattice is governed by the geometry of the $\text{Ni}-\text{O}-\text{Ni}$ bridge, which features a bond angle of $\sim 92.5^\circ$. According to the Goodenough–Kanamori rules, at angles close to 90° , orthogonal overlap between the e_g orbitals of Ni^{2+} ions ($3d^8$, high-spin $S = 1$) and the oxygen $2p$ ligand orbitals dominates, stabilizing parallel spin alignment and forming ferromagnetic zigzag chains. In contrast, the antiferromagnetic third-neighbor interaction J_3 is mediated via a longer super-superexchange pathway involving the nonmagnetic Te^{6+} cation ($\text{Ni}-\text{O}-\text{Te}-\text{O}-\text{Ni}$). In this configuration, the covalent $\text{O}^{2-}-\text{Te}^{6+}-\text{O}^{2-}$ linkage facilitates efficient antiferromagnetic charge transfer, stabilizing the antiparallel arrangement of adjacent ferromagnetic zigzags. Consequently, the zigzag magnetic order in $\text{K}_2\text{Ni}_2\text{TeO}_6$ emerges from the competition between the strong intrachain ferromagnetic exchange J_1 and the longer-range antiferromagnetic exchange J_3 .

A key feature of this magnetic structure is the isolation of the layers containing magnetic ions from one another. As noted above, both intra-layer and inter-layer $\text{Ni} - \text{Ni}$ distances have been discussed. Based on the presented calculations, it is reasonable to conclude that the inter-layer exchange interaction (J_z) can be neglected within the framework of the proposed model due to the dominant contribution of the intra-layer exchange interaction (J_1 ; J_2 and J_3). This assumption may account for the absence of observable interlayer magnetic interactions. This contrasts with another member of this family $\text{Li}_2\text{Ni}_2\text{TeO}_6$ as reported in Ref. [23], which was dedicated to the investigation of its crystal and magnetic structures derived from the $\text{K}_2\text{Ni}_2\text{TeO}_6$. In that study, it was found that spin ordering in $\text{Li}_2\text{Ni}_2\text{TeO}_6$ is characterized by the formation of two pairwise-ordered magnetic sublattices with interaction along c -axis establishing a three-dimensional magnetic order without the formation of zigzag-like structures.

This behavior arises from interlayer interactions of magnetic moments, which are facilitated by the relatively short interlayer distances along the c -axis.

It should be noted that the ion-exchange reaction $\text{K}_2\text{Ni}_2\text{TeO}_6 \rightarrow \text{Li}_2\text{Ni}_2\text{TeO}_6$ leads a structure with the orthorhombic space group $Cmca$, accompanied by a distinct reduction in symmetry. The symmetry lowering occurs because the small Li^+ ion, cannot adopt the prismatic coordination environment with oxygen ions. Consequently, a significant difference emerges in the interatomic distances in $\text{Li}_2\text{Ni}_2\text{TeO}_6$: the interlayer separation is 5.289(5) Å, whereas the distance between third-neighbor Ni^{2+} ions within the magnetic layers is substantially longer at 5.94(4) Å. This proximity of magnetic layers enhances the interlayer exchange interaction (J_z), thereby promoting three-dimensional (3D) magnetic ordering (Table 3).

A clear structural similarity exists between the two samples, $\text{K}_2\text{Ni}_2\text{TeO}_6$ and $\text{Li}_2\text{Ni}_2\text{TeO}_6$, despite their differing space-group symmetry. In both the crystal structure features alternating magnetic and non-magnetic layers stacked along the crystallographic c -axis, with the magnetic layers exhibiting an identical honeycomb-like arrangement in the ab -plane. The electronic configuration of the Ni^{2+} ion ($S = 1$), combined with the analogous crystallographic architecture, leads to comparable mechanisms governing the formation of magnetic exchange couplings. The e_g orbitals of the high-spin magnetic Ni^{2+} ion facilitate both superexchange and super-superexchange pathways, which underpin the establishment of long-range magnetic order.

Table 3 – Comparison of crystal structure parameters for $\text{K}_2\text{Ni}_2\text{TeO}_6$ (space group $P6_3/mcm$) and $\text{Li}_2\text{Ni}_2\text{TeO}_6$ (space group $Cmca$).

Parameter, Å	Sample	
	$\text{Li}_2\text{Ni}_2\text{TeO}_6$	$\text{K}_2\text{Ni}_2\text{TeO}_6$
a	5.0007(1)	5.25118(1)
b	8.7891(1)	5.25118(1)
c	5.1621(3)	12.4292(4)
V	214.65(2)	296.82(2)
Ni - Ni (First neighbors)	2.97(3)	3.031(3)
Ni - Ni (Second neighbors)	5.14(3)	5.251(4)
Ni - Ni (Third neighbors)	5.94(4)	6.063(4)
Ni - Ni (Interlayer)	5.298(5)	6.214(5)

However, a significant structural difference arises from the distances between the magnetic layers, which is dictated by the ionic radii of the interlayer cations: $r_{K^+}=1.51 \text{ \AA}$ (prismatic coordination), $r_{Li^+} = 0.90 \text{ \AA}$ (tetrahedral coordination) [31].

Conclusion

In summary, the layered tellurate $\text{K}_2\text{Ni}_2\text{TeO}_6$ was successfully synthesized, and its structural and magnetic structure were investigated using neutron powder diffraction. The compound crystallizes in the hexagonal space group $P6_3/mcm$, with no structural phase transitions observed between 4 and 300 K. The magnetic structure, refined at 4 K, reveals an incommensurate, amplitude-modulated spin spiral propagating along the c-axis. Within the Ni^{2+} honeycomb sublattice, a zigzag spin configuration emerges, characterized by a zig-zag ferro-magnetic chain-order in the ab -plane. An important finding of this work is the significant suppression of the interlayer exchange interaction (J_z) due to the large interlayer spacing and specific potassium ion distribution, which stabilizes a distinct quasi-two-dimensional magnetic ground state compared to the more compact $\text{Li}_2\text{Ni}_2\text{TeO}_6$. This result, which appears obvious at first glance, is not so apparent due to differences in the crystallographic structures of the compounds being compared.

From a technological perspective, the robust in-plane magnetic order, combined with the large interlayer spacing and potassium ion mobility, makes $\text{K}_2\text{Ni}_2\text{TeO}_6$ a highly promising candidate for advanced applications. Specifically, these structural features are highly desirable for high-voltage cathode materials in potassium-ion batteries. Furthermore, the frustrated zigzag magnetic order and the suppression of 3D coupling position $\text{K}_2\text{Ni}_2\text{TeO}_6$ as an excellent model system for exploring 2D Kitaev-like physics, spintronics, and topological magnetic devices. This work not only resolves the magnetic ground state of $\text{K}_2\text{Ni}_2\text{TeO}_6$ but also paves the way for the rational design of layered oxides for next-generation electronic and energy storage technologies.

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Author contributions

N.S. Fokin: investigation, experimental data mathematical processing. A. E. Susloparova: methodology, investigation, experimental data mathematical processing. A.I. Kurbakov: methodology, investigation, writing—original draft, and project administration.

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Conflict of interest

The authors declare that they have no conflicts of interest

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