RAMAN SCATTERING STUDY OF A TWO-DIMENSIONAL $S = 1$ QUANTUM SPIN SYSTEM Ni$_5$(TeO$_3$)$_4$Cl$_2$

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The transition metal tellurium oxychloride, Ni$_5$(TeO$_3$)$_4$Cl$_2$, has been investigated by the Raman scattering method at temperatures of 15–300 K. Sixty two phonon modes (of the total 69 Raman-active phonon modes allowed for the monoclinic C_{2h}^6 structure) are identified in the spectra, and their behavior is analyzed. Several distinct features are observed in Raman spectra at low temperatures: (i) three low-frequency bands (22.3, 29.4, and 49.0 cm^{-1} at $T = 15$ K) with a temperature behavior characteristic of the one-magnon scattering and (ii) a band at 56.3 cm^{-1} with a pronounced temperature dependence. The origin of the low-temperature bands is discussed.

1. Introduction

A great deal of interest in magnetism has been recently been devoted to theoretical and experimental investiga-

Fig. 1. Ni ion configuration in a single layer of the Ni$_5$(TeO$_3$)$_4$Cl$_2$ crystal. Thick line frames Ni ions in a single unit cell

tions of low-dimensional spin systems [1–3]. This interest has been stimulated by theoretical predictions of a rich phase diagram and novel magnetic properties which originate from the interplay of the geometric frustration and quantum fluctuations in low dimensions. In general, the behavior of frustrated systems is difficult to predict; the frustration can lead to a microscopic degeneracy and qualitatively to new states of matter. Magnetic systems offer good examples in the form of spin lattices, where all interactions between spins cannot be simultaneously satisfied. It is frequently assumed that the spin lattice of a magnetic system containing a transition metal is the same as the geometric arrangement of its metal ions. For complex magnetic systems, such intuitive approach is often incorrect, because the spin exchange interaction strength is not determined by the distance between two spin sites but by the overlap between their magnetic orbitals. The crystal structure, namely positions of nonmagnetic neighboring ions can affect the spin exchange interaction and hence the topology of the spin lattice.

Recently, the investigation of the ternary phase diagram NiO-NiCl$_2$-TeO$_2$ has led to the synthesis of new transition-metal tellurium oxohalogenides with the general chemical formula Ni$_5$(TeO$_3$)$_4$X$_2$ (X = Br, Cl) [4]. These compounds have clearly a pronounced layered structure. The nickel ions have a $3d^8$ electronic configuration, with spin $S = 1$, forming a quasi-two-dimensional magnetic structure. Each layer is made of groups of five strongly distorted Ni-octahedra into a [Ni$_5$O$_{17}$X$_2$] "claw unit" with some unusually short Ni^{2+}– Ni^{2+} distances (Fig. 1). These units are then linked via the corner sharing to next-nearest neighbors. The magnetic properties should therefore be dictated by the
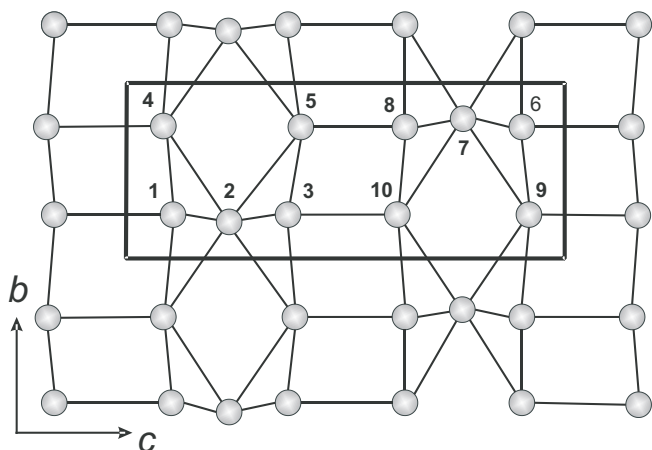
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strong magnetic interaction within each "claw unit". Because the Ni^{2+} ($S = 1$) moments in a unit are arranged in an interesting double triangular topology, the frustration may play a significant role [5].

In the previous investigations, considerable efforts have been put into the basic experimental studies of $Ni_5(TeO_3)_4Cl_2$ [4, 6, 7]. The magnetic susceptibility of $Ni_5(TeO_3)_4Cl_2$ shows a Curie–Weiss behavior with negative Curie–Weiss temperature $\Theta = -50$ K [4] (powder) and $\Theta = -49$ K [7] and $\Theta = -60$ K [8] (single crystals). The negative sign of the Curie–Weiss temperature indicates antiferromagnetic correlations between the spin moments of nickel ions. The powder sample undergoes a transition into the antiferromagnetic ordered state at $T_N = 23$ K [4]. In single crystals, the magnetic transitions were observed at temperatures of 28.5 K [8] and 21 K [7]. Magnetization measurements indicate that there is no ferromagnetic moment in the ordered state [7]. The direction of the easy axis was found orthogonal to the bc-plane. The anisotropic character of the magnetic susceptibility was found in [7, 8] as well. In one aspect, the result in [8] is striking: in the susceptibility measurement taken along the b-axis, there is no trace of any anomaly related to the magnetic ordering. The latter observation is incompatible with the standard Nèel-type ordering pattern and indicates a complex magnetic structure (as well as magnetism in general) of $Ni_5(TeO_3)_4Cl_2$.

In high-field electron-spin resonance investigations of $Ni_5(TeO_3)_4Cl_2$ single crystal, ten spin-resonance modes with characteristic magnetic-field dependences were discovered [6]. Two of them are degenerate in the zero field, and three appear only in high magnetic fields. The two-dimensional model discussed by Mihaly et al. [6] reproduces only a part of the observed excitations, and further investigations including neutron and Raman scattering are necessary for a complete exploration of the magnetic structure in this compound.

Here, we report the first Raman scattering study of a nickel-tellurium-oxychloride $Ni_5(TeO_3)_4Cl_2$ single crystal in the temperature range above and below T_N. Raman spectroscopy can probe simultaneously excitations arising from spin and lattice degrees of freedom and, thus, can shed light on the low-temperature magnetic ground state, magnetic anisotropy, and a role of the geometric frustration.

2. Experiment

The Raman spectra were measured on an oriented single-crystal sample of dimensions $3 \times 4 \times 0.2$ mm^3 with the

b and c axis which are parallel to the edges of the slab. The 632.8-nm line of a He–Ne (~ 30 mW) laser was used in the experiments to reduce the beam-induced heating of the orange colored $Ni_5(TeO_3)_4Cl_2$ sample, as well as to enhance the scattered light intensity. The scattered light was analyzed with a double Jobin Yvon U1000 monochromator and detected with a cooled photomultiplier RCA 31034 and a photon counting system. The right-angle scattering geometry was used. The laboratory coordinates X and Z were chosen to be parallel to the c and b axes of the crystal, respectively, while Y is perpendicular to cb plane.

The temperature interval of 5–300 K was covered using an optical cryostat. The sample was kept in the exchange gas atmosphere. The sample temperature was monitored by a copper-constantan thermocouple, but taking the local heating of the sample due to the laser irradiation into consideration, the proper temperature was estimated from the Stokes/anti-Stokes intensity ratios.

3. Results and Discussion

The crystal $Ni_5(TeO_3)_4Cl_2$ is monoclinic, of space group $C2/c$ (C_{2h}^6), $Z = 4$ with the following unit cell dimensions: $a = 19.5674$ Å, $b = 5.2457$ Å, $c = 16.3084$ Å, and $\beta = 125.29°$ [4]. The primitive unit cell contains two formula units. Since the crystal is inversion-symmetric, the irreducible representations are symmetric (g) or antisymmetric (u). A normal mode decomposition of the space group gives

$$\Gamma_{vib} = 34A_g + 35B_g + 34A_u + 35B_u.$$

Of the total 138 Γ-point phonon modes, 66 are infrared-active, and 69 are Raman-active. According to group theory, A_g and B_g modes are allowed for XX, YY, ZZ, XY, YX and XZ, YZ, ZX, ZY scattering configurations, respectively [9].

In Fig. 2,a, the low-temperature (15 K) polarized Raman spectra of $Ni_5(TeO_3)_4Cl_2$ in the frequency region of 3–260 cm^{-1} are shown. Narrow and well-distinguished phonon peaks with different intensities are observed. Spectra are well polarized with the leakage of forbidden modes not exceeding 5% intensity of the allowed ones. The above-mentioned characteristics of the system surely allow identifying the number and the symmetry of all phonon modes. Figures 2,b and 2,c show Raman spectra in the frequency regions 260–550 and 550–900 cm^{-1}, respectively. It is necessary to note that the phonon peaks in Figs. 2,b and 2,c have a larger
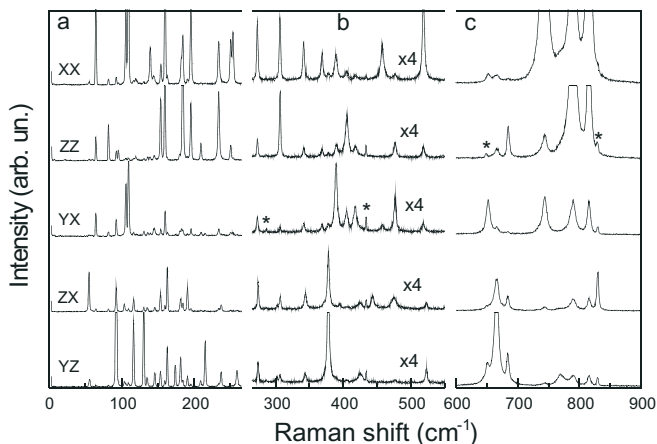
Fig. 2. Raman spectra of the $Ni_5(TeO_3)_4Cl_2$ single crystal in various scattering configurations ($T = 15$ K). Spectral resolution is 1.8, 1.8, and 3.0 cm^{-1} in (a), (b), and (c), respectively. The asterisks in all Raman spectra denote laser plasma lines

Fig. 3. (a) Low-frequency polarized Raman spectra of $Ni_5(TeO_3)_4Cl_2$ ($T = 15$ K). (b) Raman spectra at 15 and 25 K (below and above T_N) in the ZZ polarization configuration. The arrows indicate bands which appear in the antiferromagnetic phase. Spectral resolution is 1.8 cm^{-1}

intensity and linewidth in the higher frequency region. Large differences in the intensities of the Raman tensor components XX, ZZ, and YX of most A_g modes are observed. This simply reflects the high optical anisotropy of the material.

Precise measurements allowed us to observe weak and broad Raman spectra at low temperatures in the low-frequency region of 20–50 cm^{-1} (Fig. 3,(a)). These lines are seen in the XX and ZZ scattering geometries.

We will focus now on the temperature dependence of the Raman line intensities, frequencies, and linewidths extracted by fitting the corresponding spectra. Three lines with frequencies of 22.3, 29.4, and 49.0 cm^{-1} fade away with increasing temperature and are not seen in the spectra at $T = 25$ K (Fig. 3,(b)), while lines with frequencies > 50 cm^{-1} (except the line at 55.1 cm^{-1}, and this frequency region will be discussed later) show no anomalies with temperature and can be identified as phonons. The experimental Raman peak frequencies (in the unit of wave numbers) and the symmetries of all modes are presented in Table 1. Of the 69 phonon modes maximally expected for the monoclinic C_{2h}^6 structure, 62 ($32A_g + 30B_g$) phonon modes were clearly discovered in Raman experiments.

With decreasing temperature up to 15 K, no extra phonon modes appear in Raman spectra, by indicating that $Ni_5(TeO_3)_4Cl_2$ has no structural transformation in this temperature region.

Following the earlier assignments [10,11], the modes in the highest-frequency well-separated region of Raman spectra (> 650 cm^{-1}) can be attributed to the stretching
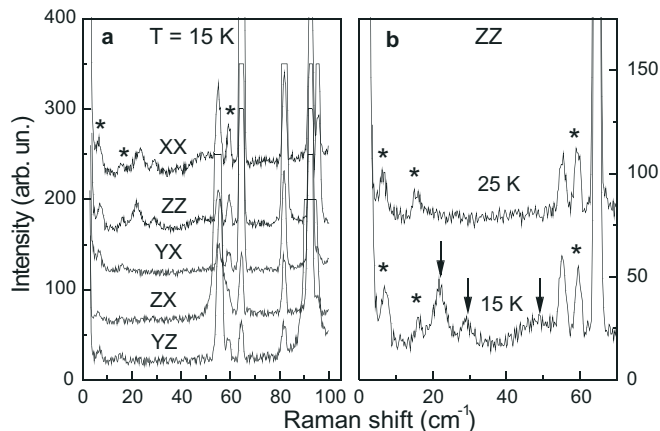
modes of Te–O bonds. For an isolated TeO_3^{2-} group, there are the symmetric and antisymmetric stretchings of the Te-O bonds ($\nu_1(A_1)$ and $\nu_3(E)$ with frequencies of 758 and 703 cm^{-1}, respectively) [10]. In our experiments, we have observed ten ($5A_g + 5B_g$) out of the twelve ($6A_g + 6B_g$) Te-O stretching modes predicted for the monoclinic C_{2h}^6 structure of the crystal $Ni_5(TeO_3)_4Cl_2$.

In the frequency region 250–550 cm^{-1}, the symmetric and antisymmetric bending modes of O–Te–O bonds ($\nu_2(A_1)$ and $\nu_4(E)$) are expected. Ni–O and Ni–Cl bonds vibrations are expected in this frequency region as well [10, 12]. Phonons with energies < 250 cm^{-1} can be attributed as translational and vibration modes [11]. Assignments of vibration modes in the different spectral regions are not strict, since the motion of nickel and fluorine ions is partially coupled with vibration and bending modes of TeO_3^{2-} units.

In Fig. 3,b, we show the low-frequency part of the Raman spectra of $Ni_5(TeO_3)_4Cl_2$ at two temperatures, namely above and below T_N [4, 7]. As clearly seen, three weak and broad lines are observed at 15 K. The disappearance of these lines just above T_N is typical of one-magnon excitations. The one-magnon mode is Raman active by virtue of spin-orbit couplings. The pronounced one-magnon excitations suggest the strong magnetic anisotropy, consistent with electron-spin resonance results [6]. At the same time, the observation of one-magnon excitations only in diagonal components of the Raman tensor is somewhat unusual. A complicate spin lattice might be responsible for that.

Electron-spin resonance investigations [6] revealed that the nature of magnetism in the studied compound is quite complex and cannot be interpreted at present in all details. There are some reasons for such a complexity: (i) nonequivalent crystallographic positions of Ni^{2+} ions in distorted octahedral coordinations, (ii) essentially different distances between magnetic ions, which leads to a difference of exchange interactions, and (iii) significant magnetic anisotropy. While the exchange-interaction model used to describe $Ni_5(TeO_3)_4Cl_2$ [6] correctly explains some properties of the low-energy magnetic excitations, the authors noted the importance of further investigations for the complete description of this compound.

$Ni_5(TeO_3)_4Cl_2$ has a layered structure with $Ni_5Te_4O_{12}$ sheets and chlorine in the space between sheets. Magnetic Ni^{2+} ions have three different crystallographic positions and are located inside of NiO_6 and NiO_5Cl octahedra. Five Ni-octahedra form a structural unit with a "claw" shape (see Fig. 1). Each

"claw" unit is linked via eight corners to its four nearest neighbors. The magnetic unit cell of $Ni_5(TeO_3)_4Cl_2$ has twenty Ni^{2+} ions (ten Ni^{2+} ions on each of the two NiO sheets). Since the coupling between sheets is expected to be weak, it is reasonable to consider the antiferromagnetic structure of $Ni_5(TeO_3)_4Cl_2$ with ten magnetic sublattices formed by Ni^{2+} ions in a single layer.

In Table 2, we present the energies of magnetic excitations from Raman scattering investigations together with the data from [6,7]. The frequencies of magnetic excitations agree with the corresponding modes of resonance investigations [6] (see Table 2). In our Raman experiment, we did not observe two lines with the lowest energies identified earlier as antiferromagnetic resonance modes [7, 13–15]. Perhaps, a low intensity or insufficiently low temperatures of our Raman experiment did not allow us to observe them. We note that antiferromagnetic resonance modes in the isostructural compound $Ni_5(TeO_3)_4Br_2$ were observed only at temperatures $T < \frac{1}{2}T_N$ [13–15],

T a b l e 1. Frequencies (in cm^{-1}), scattering configurations, and symmetry of the phonon Raman lines in the $Ni_5(TeO_3)_4Cl_2$ crystal at 15 K. Error in the determination of frequencies is equal to $\pm0.2 - \pm0.4$ cm^{-1} depending on the intensity and width of phonon lines

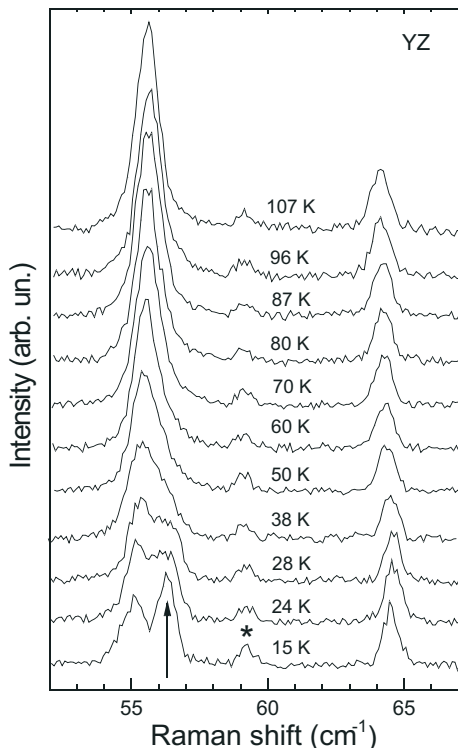| Frequency (cm^{-1})	Symmetry	Experimental scattering geometry	Frequency (cm^{-1})	Symmetry	Experimental scattering geometry	Free TeO$_3$ Unit [10] (cm^{-1})
55.1	B_g	ZX	253.4	A_g	XX	
64.5	A_g	XX	259.0	B_g	YZ	
81.8	A_g	ZZ	272.8	A_g	XX	
92.5	B_g	YZ	273.8	B_g	ZX,YZ	
95.4	A_g	ZZ	301.8	B_g	ZX	
103.8	B_g	ZX	306.3	A_g	ZZ,XX	$\nu_4(E)$
105.8	A_g	ZZ,XX	341.5	A_g	XX	326
109.4	A_g	XX,YX	343.8	B_g	YZ	
116.5	B_g	YZ	368.5	A_g	XX	
119.6	A_g	XX	377.9	B_g	YZ	$\nu_2(A_1)$
130.5	B_g	YZ	389.3	A_g	XX,YX	364
134.8	B_g	YZ	395.0	B_g	ZX	
139.2	A_g	XX	405.0	A_g	ZZ	
144.5	A_g	XX,YX	417.9	A_g	YX	
145.6	B_g	YZ	425.0	B_g	ZX,YZ	
153.5	B_g	ZX,YZ	443.7	B_g	ZX	
153.8	A_g	ZZ	457.9	A_g	XX	
159.7	A_g	ZZ,XX	474.6	B_g	ZX	
162.9	B_g	ZX,YZ	476.8	A_g	YX	
174.0	B_g	YZ	518.8	A_g	XX	
181.4	B_g	YZ	523.2	B_g	YZ	
182.5	A_g	XX	651.1	B_g	YZ	
184.4	A_g	ZZ	652.3	A_g	YX	
190.7	B_g	ZX	666.0	B_g	YZ	$\nu_3(E)$
195.4	A_g	ZZ,XX	684.2	B_g	YZ	703
209.0	B_g	YZ	684.9	A_g	ZZ	
209.4	A_g	ZZ	743.9	A_g	XX	
215.1	B_g	YZ	770.1	B_g	YZ	
233.7	A_g	ZZ	789.9	A_g	ZZ,XX	$\nu_1(A_1)$
237.1	B_g	YZ	815.6	A_g	ZZ,XX	758
250.3	A_g	XX	829.9	B_g	ZX	

Fig. 4. Temperature dependent Raman spectra in the frequency region 52–67 cm^{-1} in the YZ polarization. Spectral resolution is 0.6 cm^{-1}. The arrow indicates a Raman line with unexpected temperature behavior

and that is why strong spin fluctuations were suggested in the temperature region $\frac{1}{2} T_{\text{N}} < T < T_{\text{N}}$.

A wide band at ~ 49 cm^{-1} came into the frequency region of a twofold degenerate mode at 46 cm^{-1} [6] which splits into two modes only in finite magnetic fields. Perhaps, this wide band splits in the Raman experiment at lower temperatures or in a magnetic field.

T a b l e   2. Comparison of Raman data (at 15 K) with frequencies of spin resonance modes (at 2.5 K) [6]. Asterisks denote the modes which are visible only at high fields, and their zero-field frequencies were determined in [6] by extrapolation from a finite field to zero

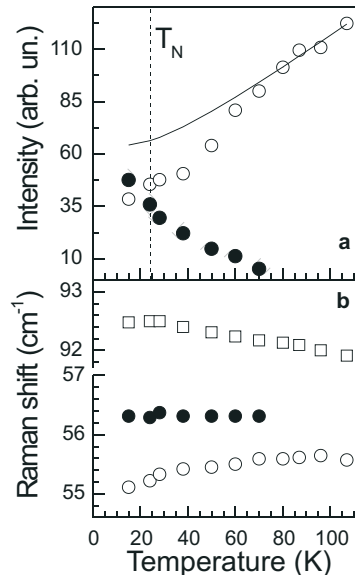| Raman data at $T = 15$ K	[6] at $T = 2.5$ K	[7]
	13.5	11.0
	17.3	13.2
22.3±0.5 (XX, ZZ)	24.4	
	25.5*	
29.4±0.5 (XX, ZZ)	29*	
	32.2	
49.0±1.0 (XX, ZZ)	46 (2)	
56.3±0.1 (YZ)	56	
	63*	
	68.5 (2)	

Fig. 5. Plot of the integrated intensities of the lines at around 55 and 56 cm^{-1} (*a*) and peak positions of the respective line and a phonon line at 92.5 cm^{-1} versus temperature (*b*). The solid curve shows the expected temperature dependence for a harmonic oscillator with a frequency of 55.1 cm^{-1}

At last, we will turn to the discussion of an intrigue feature with unexpected temperature behavior which is present in the Raman spectra at low temperatures (Fig. 4). The frequency of the 56.3-cm^{-1} mode observed at $T = 15$ K in the Raman spectra coincides with that of a spin-resonance mode at 56 cm^{-1} [6]. Its peak position is practically temperature independent. The notable thing is that this line vanishes around 70 K ($\approx 2.8\,T_{\text{N}}$), well above T_{N}. A remarkable observation is that the 56.3-cm^{-1} mode is coupled with the 55.1-cm^{-1} B_{g} phonon mode. As clearly seen from Fig. 5, the 55.1-cm^{-1} mode softens nonlinearly with decreasing temperature in contrast with all other phonon modes. Also the 55.1- and 56.3-cm^{-1} modes show different behaviors in their intensities (see Figs. 4 and 5). The 56.3-cm^{-1} mode increases in intensity with decreasing temperature, while the 55.1-cm^{-1} mode decreases in intensity for temperatures below $T \approx 70$ K with deviations from the expected Bose–Einstein behavior.

The nature of the 56.3-cm^{-1} magnetic mode is not clear. An interpretation in terms of one-magnon excitations does not agree with its temperature behavior, namely its persistence to temperatures far above T_{N}. On the other hand, the interpretation of this mode as two-magnon excitations is unconvincing due to its linewidth which is narrow and comparable to the linewidth

of phonon modes. Moreover, it was shown that the frequency position of the 56-cm^{-1} mode has a strong dependence on an applied magnetic field [6], which is not characteristic of two-magnon excitations [16]. The above-presented arguments allow us to speculate that this peak is related to a crystal field excitation of Ni^{2+} ions in the [Ni$_5$O$_{17}$X$_2$] "claw" unit in the paramagnetic state. The degenerated ground state ^{3}F of the free ion Ni^{2+} splits into discrete levels under the combined effect of the spin-orbit and crystal field interactions, and the electronic transitions between split levels of the ground state are allowed in the Raman scattering. In Ni$_5$(TeO$_3$)$_4$Cl$_2$, the crystal field splitting scheme can be different for different Ni^{2+} ions, depending strongly on the crystallographic ion coordination and the crystal field strength.

We hope that our further investigations, namely the Raman scattering studies at lower temperatures and in an applied magnetic field, will help one to clear up some of the very interesting features of the peculiar compound Ni$_5$(TeO$_3$)$_4$Cl$_2$ which are still under debates.

4. Conclusions

The Raman spectra of a single crystal Ni$_5$(TeO$_3$)$_4$Cl$_2$ have been measured and analyzed. In different scattering geometries, we observed 62 phonon modes out of the 69 ones predicted by a group-theoretic analysis for the monoclinic C^6_{2h} lattice symmetry. The temperature behavior of the phonon modes testifies to the absence of a structural phase transition in the temperature range 15–300 K. At low temperatures, a number of additional weak peaks appear in the low-energy Raman spectra. Three of them with frequencies of 22.3, 29.4, and 49.0 cm^{-1} vanish at around T_N with rising temperature. This is a typical behavior for the one-magnon scattering. The line at 56.3 cm^{-1} exhibits the anomalous temperature dependence; with increasing temperature, it disappears at around 2.8 T_N. Moreover, this line displays a strong interaction with the phonon mode at 55.1 cm^{-1}. Further, Raman investigations will be carried out to complete the exploration of the Ni$_5$(TeO$_3$)$_4$Cl$_2$ compound.

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РАМАНОВЕ РОЗСІЯННЯ СВІТЛА В ДВОВИМІРНІЙ $S = 1$ КВАНТОВІЙ СПІНОВІЙ СИСТЕМІ Ni$_5$(TeO$_3$)$_4$Cl$_2$

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Р е з ю м е

Телуровий оксохлорид перехідного металу, Ni$_5$(TeO$_3$)$_4$Cl$_2$, було досліджено методом спектроскопії раманового розсіяння світла в інтервалі температур 15–300 K. Шістдесят дві фононні моди (із загальної кількості 69 раман-активних фононних мод, що дозволені для моноклинної C^6_{2h}-структури) були ідентифіковані в спектрах та їх поведінка проаналізована. Декілька додаткових особливостей було виявлено при низьких температурах: а) три низькочастотні полоси (22,3, 29,4 и 49,0 см$^{-1}$ при $T = 15$ K) з температурною поведінкою, що характерна для одномагнонного розсіяння, та б) полоса з частотою 56,3 см$^{-1}$ та незвичайною температурною поведінкою. Обговорена можлива природа низькотемпературних полос в раманових спектрах.