



Magnetic properties of Fe₂P-type Tb₆FeTe₂, Tb₆CoTe₂, Tb₆NiTe₂ and Er₆FeTe₂ compounds

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ABSTRACT

The magnetic ordering of the Fe₂P-type Tb₆FeTe₂, Tb₆CoTe₂, Tb₆NiTe₂ and Er₆FeTe₂ phases (space group *P6₂m*) has been investigated through magnetization measurement and neutron powder diffraction. Tb₆FeTe₂, Tb₆CoTe₂ and Tb₆NiTe₂ demonstrate high-temperature ferromagnetic and low-temperature spin reorientation transitions, whereas Er₆FeTe₂ shows antiferromagnetic transition, only.

The Tb₆FeTe₂ and Tb₆NiTe₂ phases show same high-temperature collinear ferromagnetic structure, whereas Tb₆FeTe₂ is the commensurate non-collinear ferromagnet and Tb₆NiTe₂ is the canted ferromagnetic cone with $\mathbf{K}_1 = [0, 0, \pm 3/10]$ and $\mathbf{K}_2 = [\pm 2/9, \pm 2/9, 0]$ wave vectors at 2 K. The magnetic structure of Er₆FeTe₂ is a flat spiral with $\mathbf{K}_1 = [0, 0, \pm 1/10]$ at 2 K. The magnetic entropy change for Tb₆NiTe₂ is $\Delta S_m = -4.86$ J/kg K at 229 K for the field change $\Delta\mu_0 H = 0-5$ T.

In addition, novel Fe₂P-type Gd₆FeTe₂, Zr₆FeTe₂, Hf₆FeTe₂, Dy₆NiTe₂, Zr₆NiTe₂ and Hf₆NiTe₂ phases have been obtained.

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1. Introduction

The *R*₆*TX*₂ phases (*R* = Gd–Tm, *T* = Mn, Fe, Co, Ni, Ru and *X* = Sb, Bi, Te) are known to adopt a Fe₂P-type structure (space group *P6₂m*, no. 189) [1–4]. In the Fe₂P-type structure, the *R* atoms occupy the 3*g* site (*X*_{R1}, 0, 1/2) and 3(*f*) site (*X*_{R2}, 0, 0), transition metal atoms occupy the special 1*b* position (0, 0, 1/2), and antimony (bismuth, tellurium) atoms occupy the special 2*c* site (1/3, 2/3, 0) (Fig. 1a). In general, the rare-earth Fe₂P-type compounds demonstrate two ferromagnetic transitions: into a high-temperature collinear ferromagnetic state (Tb₆FeBi₂, Tb₆CoTe₂, Ho₆FeSb₂, Ho₆FeBi₂, Ho₆MnBi₂ and Ho₆CoTe₂) and into a low-temperature non-collinear ferromagnetic state (Tb₆FeBi₂, Ho₆FeSb₂, Ho₆FeBi₂, Ho₆MnBi₂ and Ho₆CoTe₂) [5–7]. Ho₆CoBi₂ shows a high-temperature collinear ferromagnetic ordering, too, but the low-temperature ferromagnetic one has a wave vector $\mathbf{K} = [0, 0, \pm 1/5]$ [7], and Ho₆FeTe₂ has a high-temperature antiferromagnetic ordering and low-temperature ferromagnetic one [8]. No local moment was detected on the transition metal site. Both the nature of the transition metal and the distortion of the unit cell strongly influence the magnetic ordering temperature and the magnetic structure in these compounds. The Mn-containing phases

show the highest magnetic ordering temperatures among the whole series.

Magnetocaloric properties have been investigated for Tb₆FeSb₂, Tb₆FeBi₂ [9] and Gd₆CoTe₂ [8]. The Tb₆FeSb₂ has a magnetic entropy change $\Delta S_m = -2.24$ J/kg K at *T*_C = 256 K for the field change $\Delta H = 0-2$ T, Tb₆FeBi₂ shows $\Delta S_m = -2.56$ J/kg K at *T*_C = 246 K for $\Delta H = 0-2$ T [8], whereas Gd₆CoTe₂ demonstrates $\Delta S_m = -4.5$ J/kg K at *T*_C = 220 K and $\Delta S_m = -6.5$ J/kg K at *T*_{CN} = 180 K for $\Delta H = 0-5$ T.

To understand the effect of transition metal and *p*-element atoms on the magnetic properties of novel *R*₆*TX*₂ phases has been investigated through the combination of magnetization measurement and neutron powder diffraction.

2. Experimental details

The phases under discussion were prepared by arc-melting in an electric arc furnace under an argon atmosphere using a non-consumable tungsten electrode and a water-cooled copper tray. Pieces of tellurium, zirconium, hafnium (purity 99.99 wt%), gadolinium, terbium, dysprosium, erbium, iron and nickel (99.9 wt% purity for all of the elements) were used as the starting components. Titanium was used as a getter during arc-melting. The arc-melted samples were annealed at 1070 K for 200 h in an argon atmosphere and quenched in ice-cold water.

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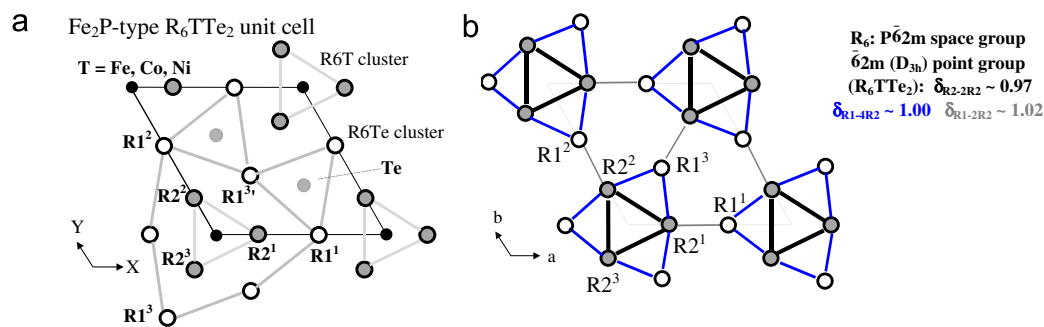


Fig. 1. (a) Unit cell of Fe₂P-type R₆TTe₂ and (b) the P $\bar{6}2m$ s rare-earth sublattice with the R₂–2R₂, R₁–4R₂ and R₁–2R₂ shortest bonds indicated.

Table 1
Crystallographic data and magnetic properties of the Fe₂P-type R₆FeTe₂ and Tb₆CoTe₂ phases (space group P $\bar{6}2m$, no. 189, atomic sites: R1 3(g) [X_{R1},0,1/2], R2 3(f) [X_{R2},0,0], T 1(b) [0,0,1/2], Te 2(c) [1/3,2/3,0]).

Compound	Unit cell data 300 K	Atomic positions at 300 K	R _F (%)	T _{CN} (K) (H=0.05 T)	M _{sat} /R (μ _B)	μ ₀ H _c (T)	ΔS _m (J/kg K)	T _N ND (K)	Magnetic structure ^c
Sc ₆ FeTe ₂ ^a	a=0.77570 nm c=0.38808 nm								
Y ₆ FeTe ₂ ^a	a=0.82065 nm c=0.39984 nm								
Gd ₆ FeTe ₂ ^b	a=0.83446(6) nm c=0.40345(2) nm	X _{Gd1} =0.5939(4) X _{Gd2} =0.2417(4)	6.1						
Tb ₆ FeTe ₂ ^b	a=0.82753(6) nm c=0.40175(2) nm	X _{Tb1} =0.5945(5) X _{Tb2} =0.2400(5)	5.1	T _C =160 K T _N =36 K				T _C ND =160 K T _{CN} ND =36 K	•F _C : M ^{K0} _{(Tb1, Tb2)C} (P31m), K ₀ =[0,0,0] (M _{Tb1} =6.2μ _B , M _{Tb2} =9.0μ _B at 50 K) •F _C –AF _{ab} –F _{ab} : M ^{K0} _{(Tb1, Tb2)C} (P31m), M ^{K0} _{(Tb1,Tb2)ab} (Pm2) (M _{Tb1} =9.0μ _B , M _{Tb2} =9.0μ _B at 2 K)
Tb ₆ CoTe ₂ [6]	a=0.83087(4) nm c=0.39627(2) nm	X _{Tb1} =0.5975(3) X _{Tb2} =0.2382(3)	3.8	T _C =174 K T _{CN1} =52 K T _{CN2} =27 K		~2 At 5 K		T _C ND =174 K T _{CN} ND =52 K	•F _C : M ^{K0} _{(Tb1, Tb2)C} (P31m), K ₀ =[0,0,0] (M _{Tb1} =5.7μ _B , M _{Tb2} =9.0μ _B at 58 K) •F _C –AF _{ab} –F _{ab} : M ^{K0} _{(Tb1, Tb2)C} (P31m), M ^{K0} _{(Tb1,Tb2)ab} (Pm2) (M _{Tb1} =8.1μ _B , M _{Tb2} =9.0μ _B at 2 K)
Dy ₆ FeTe ₂ [17]	a=0.8236(1) nm c=0.40102(4) nm	X _{Dy1} =0.589(1) X _{Dy2} =0.241(1)	4.3	T _C =135 K T _{CN} =86 K T _m =20 K	8.7 (2 K, 9 T)		–12.5 (9 T) ~0 (9 T)		
Ho ₆ FeTe ₂ ^b [8]	a=0.81894(4) nm c=0.39939(2) nm	X _{Ho1} =0.5997(5) X _{Ho2} =0.2386(5)	5.4					T _N ND =24 K T _C ND =8 K	•AF _{ab} : M ^{K1} _{(Ho1,Ho2)ab} (flat spiral) K ₁ =[0,0,±1/9] (M _{Ho1} =6.5μ _B , M _{Ho2} =8.0μ _B at 10 K) •F _C –AF _{ab} : M ^{K0} _{(Ho1,Ho2)C} (P31m) K ₀ =[0,0,0], M ^{K1} _{(Ho1,Ho2)ab} (flat spiral) K ₁ =[0,0,±1/9] (M _{Ho1} =9.1μ _B , M _{Ho2} =9.6μ _B at 2 K)
Er ₆ FeTe ₂	a=0.81565(8) nm c=0.39827(8) nm	X _{Er1} =0.5967(5) X _{Er2} =0.2407(8)	6.2					T _N ND =18 K	•AF _{ab} : M ^{K1} _{(Er1,Er2)ab} (flat spiral) K ₁ =[0,0,±1/10] (M _{Er1} =5.6μ _B , M _{Er2} =7.5μ _B at 2 K)
Tm ₆ FeTe ₂ ^a	a=0.81038 nm c=0.39715 nm								
Lu ₆ FeTe ₂ ^a	a=0.80524 nm c=0.39581 nm								
Zr ₆ FeTe ₂ ^b	a=0.77176(3) nm c=0.36346(2) nm	X _{Zr1} =0.5919(5) X _{Zr2} =0.2438(5)	7.2						
Hf ₆ FeTe ₂ ^b	a=0.76378(6) nm c=0.35419(4) nm	X _{Hf1} =0.5959(5) X _{Hf2} =0.2442(5)	7.6						

^a Tentative from the atomic radii rule.
^b The crystallographic data used with permission of—© JCPDS—International Centre for Diffraction Data.
^c F—ferromagnetic component; AF—antiferromagnetic component. The magnetic component is directed along the c-axis (F_C) or lies in the ab plane (F_{ab}, AF_{ab}).

The quality of the samples before the neutron diffraction study was evaluated using X-ray diffraction and electron microprobe analysis. The X-ray data were obtained on a diffractometer DRON-3.0 (CuKα radiation, 2θ=5–120°, step 0.02°, 10 s/step). The lattice constants were derived using the Rietan-program [10] in the isotropic approximation (Tables 1 and 2).

A “Camebax” microanalyser was employed to perform microprobe X-ray spectral analyses of the samples. The quantitative

microprobe analysis of the Fe₂P-type samples gave 66±1,...,2 at% of rare earth, 11±1 at% of iron and 33±1,...,2 at% of tellurium.
The neutron diffraction studies were carried out on the powder D1B diffractometer [11] (Institute Laue-Langevin, Grenoble, France) from 184 to 2 K for Tb₆FeTe₂, from 28 down to 2 K for Er₆FeTe₂ and from 300 down to 2 K for Tb₆NiTe₂ (temperature step 2–5 K). The neutron diffraction data were refined using the FULLPROF98-program [12].

Table 2

Crystallographic data and magnetic properties of the Fe₂P-type R₆NiTe₂ phases (space group $P\bar{6}2m$, no. 189, atomic sites: R1 3(g) [$X_{R1}, 0, 1/2$], R2 3(f) [$X_{R2}, 0, 0$], Ni 1(b) [$0, 0, 1/2$], Te 2(c) [$1/3, 2/3, 0$]).

Compound	Unit cell data 300 K	Atomic positions at 300 K	R_F (%)	T_{CN} (K) ($H=0.01$ T)	$\mu_0 H_C$ (T)	ΔS_m^c (J/kg K)	T_{CN}^{ND} (K)	Magnetic structure ^{b,d}
Gd ₆ NiTe ₂ [1]	$a=0.8412$ nm $c=0.39577$ nm	$X_{Gd1}=0.6035$ $X_{Gd2}=0.2356$						
Tb ₆ NiTe ₂ ^a	$a=0.83464(6)$ nm $c=0.39300(2)$ nm	$X_{Tb1}=0.5932(5)$ $X_{Tb2}=0.2368(5)$	6.4	$T_C=228$ K $T_N=52$ K $T_{CN}=36$ K	~ 1.5 at 5 K	-4.86	$T_C=228$ K $T_N=55$ K $T_{CN}=44$ K	F_C : $M_{(Tb1, Tb2)C}^{K0}$ (P31m) ($M_{Tb1}^{K0}=6.5\mu_B$, $M_{Tb2}^{K0}=6.5\mu_B$ at 100 K) F_C–AF_{ab} : $M_{(Tb1, Tb2)C}^{K0}$ (P31m), $M_{(Tb1, Tb2)ab}^{K1}$ (flat spiral) ($M_{Tb1}^{K0}=7.0\mu_B$, $M_{Tb2}^{K0}=8.9\mu_B$, $M_{Tb1,2}^{K1}=1.24\mu_B$ at 50 K) F_C–AF_{abC}–F_{ab} : $M_{(Tb1, Tb2)C}^{K0}$ (P31m), $M_{(Tb1, Tb2)ab}^{K0}$ (Pm2), $M_{(Tb1, Tb2)ab}^{K1, K2}$ (flat spiral) ($M_{Tb1}^{K0}=8.9\mu_B$, $M_{Tb2}^{K0}=8.9\mu_B$, $M_{Tb1,2}^{K1, K2}=1.74\mu_B$ at 2 K)
Dy ₆ NiTe ₂ ^a	$a=0.83021(3)$ nm $c=0.39128(2)$ nm	$X_{Dy1}=0.5946(3)$ $X_{Dy2}=0.2409(3)$	4.8					
Zr ₆ NiTe ₂ ^a	$a=0.76691(3)$ nm $c=0.36953(2)$ nm	$X_{Zr1}=0.5912(4)$ $X_{Zr2}=0.2404(4)$	5.0					
Hf ₆ NiTe ₂ ^a	$a=0.75888(4)$ nm $c=0.35927(2)$ nm	$X_{Hf1}=0.5955(5)$ $X_{Hf2}=0.2414(4)$	6.7					

^a The crystallographic data used with permission of—© JCPDS—International Centre for Diffraction Data.

^b **F**—ferromagnetic component; **AF**—antiferromagnetic component. The magnetic component is directed either along the *c*-axis (**F_C**), lies in the *ab* plane (**F_{ab}**, **AF_{ab}**) or has some direction in the space (**AF_{abc}**).

^c at 229 K, for the 0–5 T field change.

^d The wave vectors are $K_0=[0,0,0]$, $K_1=[0,0,\pm 3/10]$ and $K_2=[\pm 2/9,\pm 2/9,0]$.

Table 3

Interatomic distances in Tb₆FeTe₂ and Tb₆NiTe₂ and their ratio to the sum of the corresponding atomic radii $\delta=D/(R_{atomic1}+R_{atomic2})$: (a) Tb₆FeTe₂ and (b) Tb₆NiTe₂.

Atom1–Atom2	<i>D</i> (nm)	δ	Coordination number	Atom1–Atom2	<i>D</i> (nm)	δ	Coordination number
Tb1–4Te	0.32177	1.00	13	Tb1–4Te	0.32049	1.00	13
–1Fe	0.33556	1.11		–1Ni	0.33953	1.12	
–4Tb2	0.35462	1.00		–4Tb2	0.35475	1.00	
–2Tb2	0.35554	1.00		–2Tb2	0.35651	1.00	
–2Tb1	0.40175	1.13		–2Tb1	0.39300	1.10	
Tb2–2Fe	0.28248	0.94	14	Tb2–2Ni	0.27870	0.92	14
–2Te	0.32150	1.00		–2Te	0.32605	1.02	
–2Tb2	0.34400	0.97		–2Tb2	0.34233	0.96	
–4Tb1	0.35462	1.00		–4Tb1	0.35475	1.00	
–2Tb1	0.35554	1.00		–2Tb1	0.35651	1.00	
–2Tb2	0.40175	1.13		–2Tb2	0.39300	1.13	
Fe–6Tb2	0.28248	0.94	11	Ni–6Tb2	0.27870	0.92	11
–3Tb1	0.33556	1.11		–3Tb1	0.33953	1.12	
–2Fe	0.40175	1.62		–2Ni	0.39300	1.58	
Te–3Tb2	0.32150	1.00	11	Te–6Tb1	0.32049	1.00	11
–6Tb1	0.32177	1.00		–3Tb2	0.32605	1.02	
–2Te	0.40175	1.40		–2Te	0.39300	1.37	

The dc magnetization was measured on a commercial SQUID magnetometer (Quantum Design) in the 2–300 K temperature range and in the applied field up to 5 T.

3. Results and discussion

3.1. Crystal structure

The structure of the Fe₂P-type R₆Te₂ phases projected onto the *ab* plane is shown in Fig. 1a. The Fe₂P-type lattice contains the transition metal and Te sublattices with the $6/mmm$ (D_{6h}) point group and the rare-earth sublattice with the $\bar{6}2m$ (D_{3h}) point group ($P\bar{6}2m$ space group). The rare-earth atoms occupy the following positions: R1¹ ($X_{R1}, 0, 1/2$), R1² ($0, X_{R1}, 1/2$), R1³ ($-X_{R1}, -X_{R1}, 1/2$); R2¹ ($X_{R2}, 0, 0$), R2² ($0, X_{R2}, 0$) and R2³ ($-X_{R2}, -X_{R2}, 0$). The shortest R1–Te,

R2–Te, R1–R2 interatomic distances are close to the sum of metallic radii of pure elements, whereas the R2–T and R2–R2 interatomic distances are less than the sum of metallic radii [13]. The large “transition metal–transition metal” distances preclude the magnetic ordering within the transition metal sublattice. The interatomic distances of Tb₆FeTe₂ and Tb₆NiTe₂ are shown in Table 3. The rare-earth atoms form semi-isolated clusters with the $\bar{6}2m$ (D_{3h}) point group as shown in Fig. 1b.

The *a*, *c* cell parameters and the volume of the unit cell, *V*, of the Fe₂P-type phases increase with the size of *R* atoms, whereas the *c/a* ratio shows the opposite trend for the R₆Te₂ phases (Fig. 2). The dependencies between the lattice parameters and atomic radii for rare-earth compounds are somewhat different from those for the zirconium and hafnium compounds which is most likely due to the different valent states of the rare earths (3+) and zirconium/hafnium (4+), like in Fe₂P-type phases with Sb and Bi [1–3].

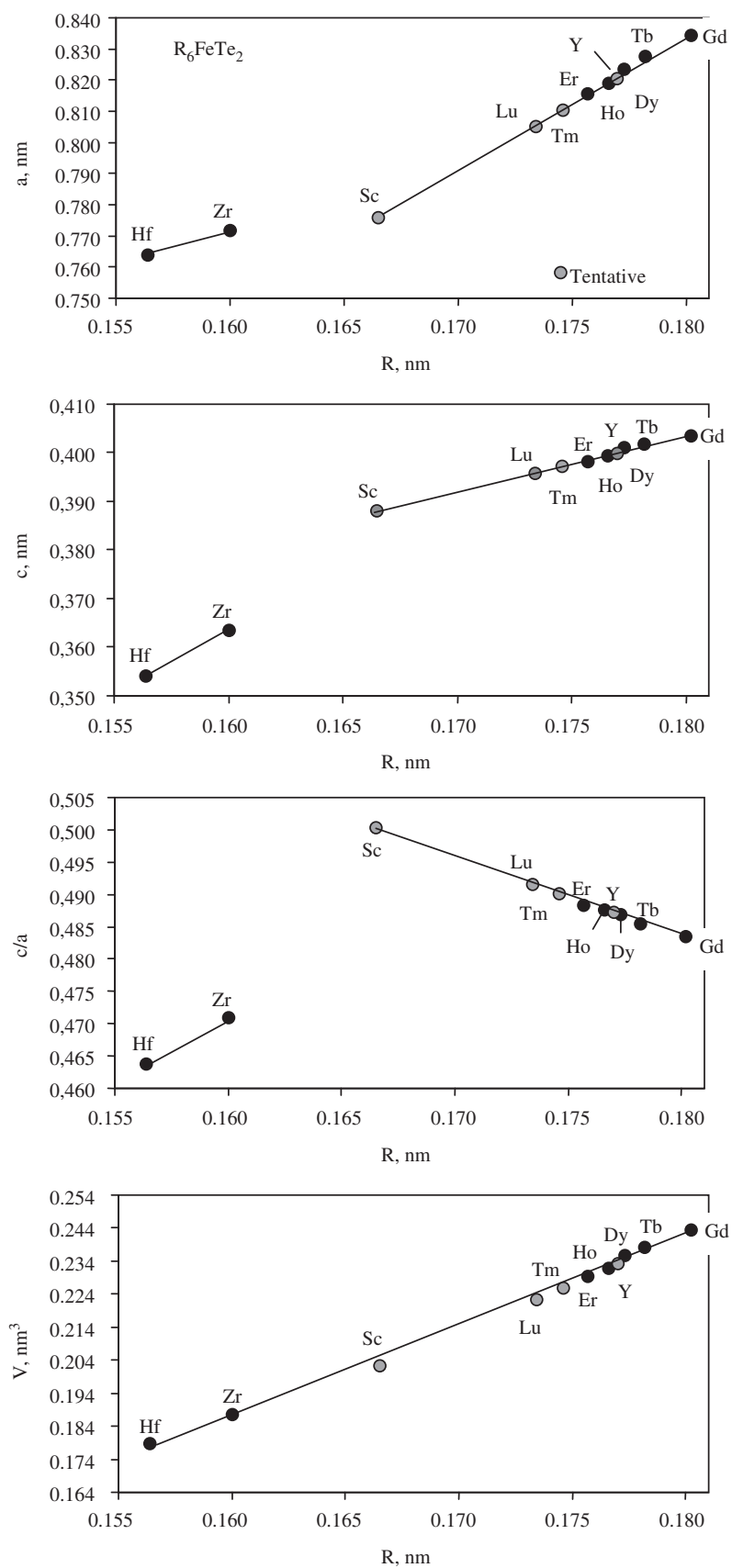


Fig. 2. Cell parameters vs. atomic radii, R , of rare earths, zirconium and hafnium for the $R_6\text{FeTe}_2$ phases. The gray symbols correspond to the lattice parameters of hypothetical compounds not studied here but whose lattice parameters are deduced from the general trend of the lanthanide contraction. The error bars are smaller than the corresponding symbols.

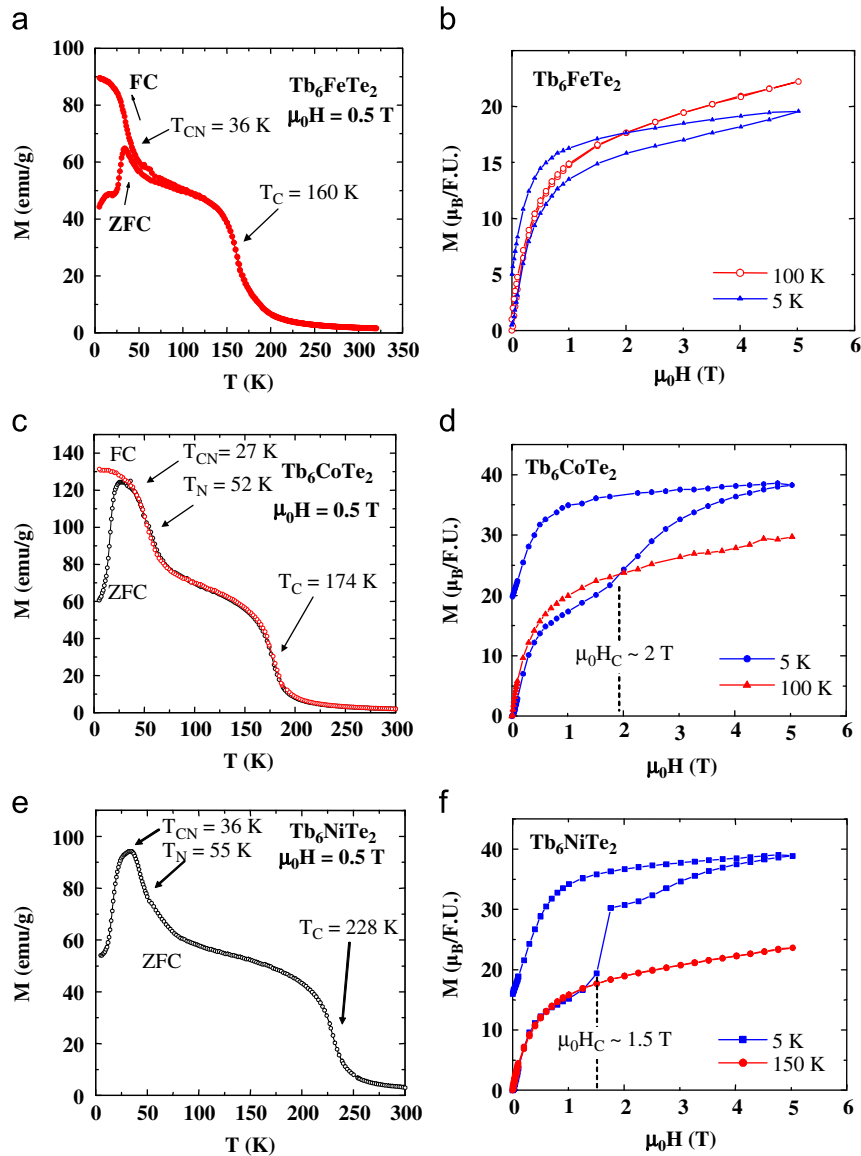


Fig. 3. Magnetization vs. temperature for Tb_6FeTe_2 (a), Tb_6CoTe_2 (c) and Tb_6NiTe_2 (e) and vs. magnetic field for Tb_6FeTe_2 (b), Tb_6CoTe_2 (d) and Tb_6NiTe_2 (f).

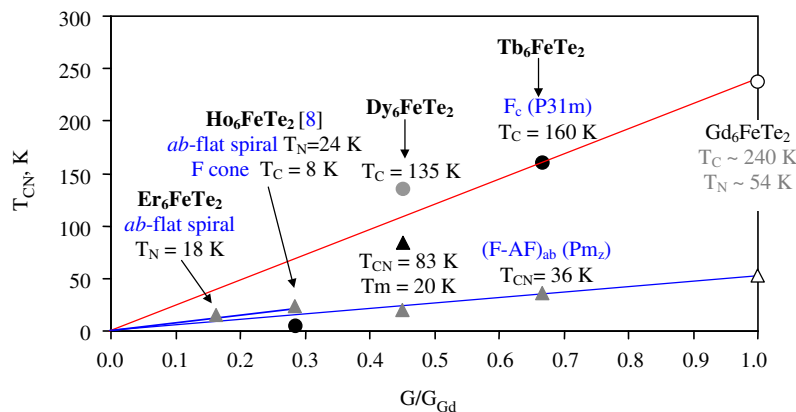


Fig. 4. Magnetic transition temperatures vs. de Gennes factor for R_6FeTe_2 with different magnetic structures (circles represent Curie temperatures, triangles Neel or mixed AF-F transition temperatures). The magnetic transition temperatures for Gd_6FeTe_2 are tentative and derived from de Gennes rule. Details of the Tb_6FeTe_2 and Er_6FeTe_2 magnetic structures are presented in the **Magnetic structure** section.

The Fe_2P -type Sc_6FeTe_2 , Y_6FeTe_2 , Tm_6FeTe_2 and Lu_6FeTe_2 phases are hypothetical from the chemical properties and crystal structure of Sc, Y, Lu and Tm pure metals [13] and from comparison with series of Sb- and Bi-containing Fe_2P -type rare earth phases [1–3].

The a and c parameters for the hypothetical Sc_6FeTe_2 , Y_6FeTe_2 , Tm_6FeTe_2 and Lu_6FeTe_2 phases with the same structure were extracted from the extrapolation of the corresponding linear fits (Table 1 and Fig. 2). Changes in the lattice parameters of $R_6\text{NiTe}_2$ as a function of the R atomic radii is similar to those observed for $R_6\text{FeTe}_2$, and they can be rationalized in terms of the lanthanide contraction.

3.2. Magnetization

Magnetization measurements indicate two or three magnetic transitions for Tb_6FeTe_2 , Tb_6CoTe_2 and Tb_6NiTe_2 (Fig. 3 and Tables 1 and 2). The high-temperature magnetic transitions are of a ferromagnetic type, and the low-temperature ones may correspond to the reorientation of magnetic moments and appearance of

antiferromagnetic components in the ferromagnetic system. The 5 K magnetization vs. field data reveal metamagnetic transition in the ferromagnetic state for Tb_6CoTe_2 at $\mu_0 H_C \sim 2$ T and for Tb_6NiTe_2 at $\mu_0 H_C \sim 1.5$ T. The saturation magnetization of Tb_6FeTe_2 at 5 K is lower than that at 100 K, and this is analogous to the Tb_6CoTe_2 behavior below 2 T (Fig. 3). Most likely, the critical field value for Tb_6FeTe_2 is larger than 5 T.

Temperatures of the ferromagnetic transitions in $R_6\text{FeTe}_2$ do not follow the de Gennes rule, while those of the low temperature transitions obey this rule (Fig. 4). Therefore, the high-temperature magnetic structures of Tb_6FeTe_2 , Dy_6FeTe_2 and Ho_6FeTe_2 could be different, whereas the low-temperature magnetic structures of Tb_6FeTe_2 , Ho_6FeTe_2 and Er_6FeTe_2 could be similar.

3.3. Magnetocaloric effect

The magnetocaloric effect for Tb_6NiTe_2 was evaluated from the magnetization vs. field (M vs. H) data measured around the Curie temperatures with 7 K increments. The magnetic field changed

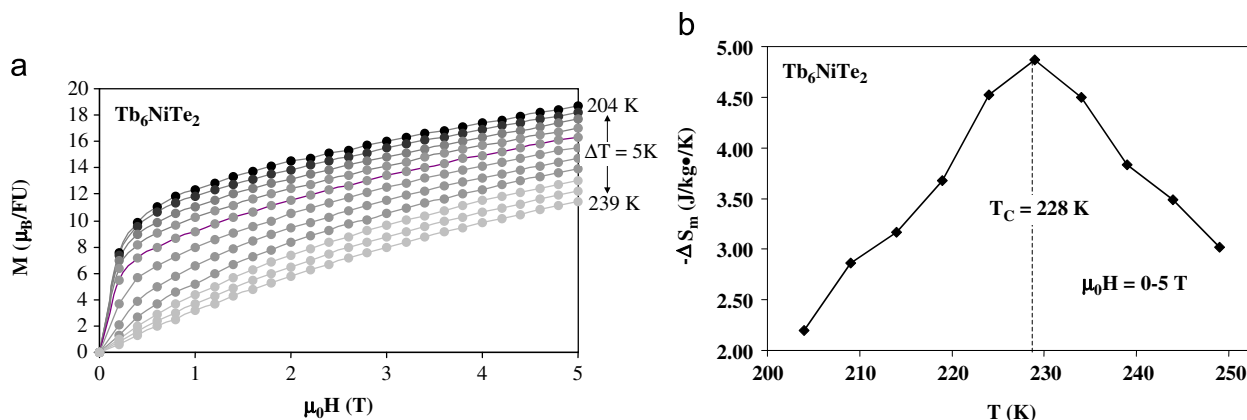


Fig. 5. (a) Magnetization vs. magnetic field and (b) isothermal entropy change, ΔS_m , of Tb_6NiTe_2 as function of temperature.

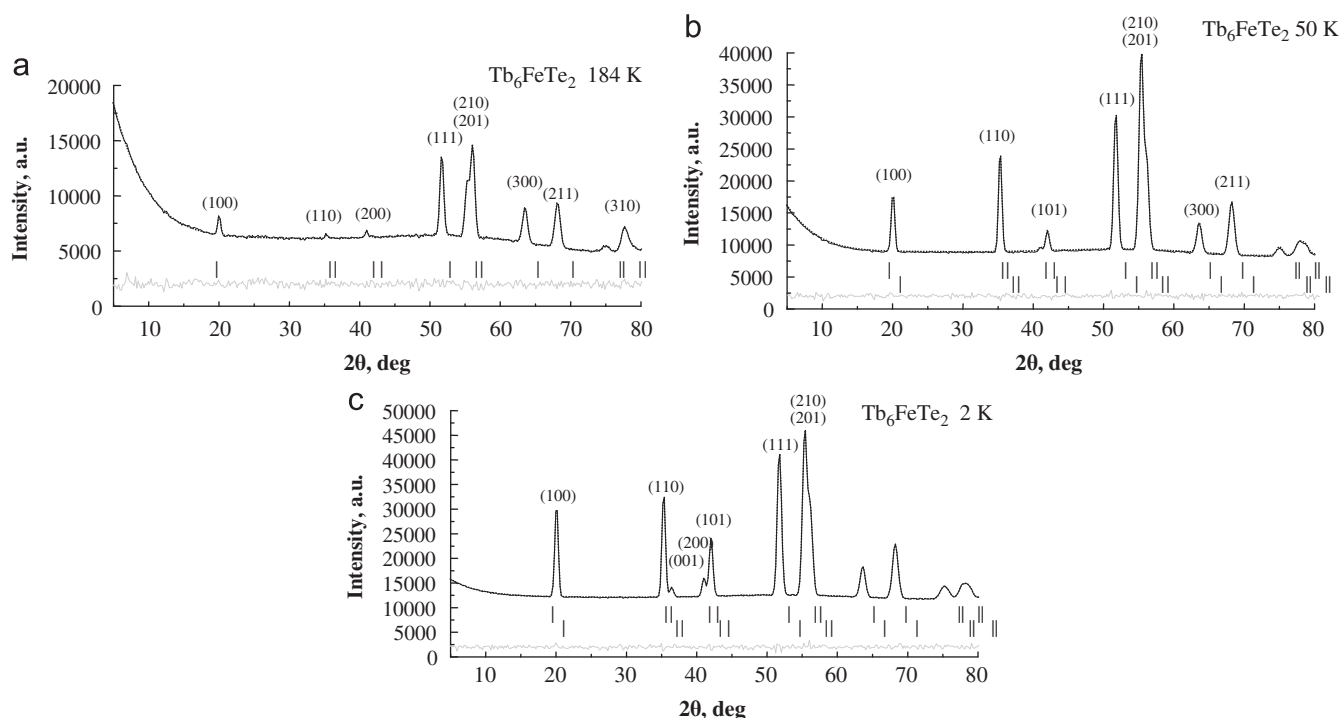


Fig. 6. Neutron diffraction patterns of Tb_6FeTe_2 at (a) 184 K (paramagnetic state), (b) 50 K (collinear ferromagnetic) and (c) 2 K (non-collinear ferromagnetic) ($\lambda = 0.254$ nm).

from 0 to 5 T in 0.2 T steps. MCE in terms of the isothermal entropy change, ΔS_m , was calculated from the magnetization data (Fig. 5a) through the Maxwell equation [14]: $\left(\frac{\partial S(T,H)}{\partial H}\right)_T = \left(\frac{\partial M(T,H)}{\partial T}\right)_H$. Through the integration of the partial derivative of magnetization, M , with respect to temperature, T , over a change in the magnetic field, H , an expression for ΔS is obtained as $\Delta S(T)_{\Delta H} = \int_{H_1}^{H_2} \left(\frac{\partial M(T,H)}{\partial T}\right)_{H,P} dH$. In practice a numerical integration is performed using the following

formula: $\Delta S(T)_{\Delta H} = \sum_i \frac{M_{i+1} - M_i}{T_{i+1} - T_i} \Delta H$, where ΔH is a change in magnetic field and M_i and M_{i+1} are the values of magnetization at temperatures T_i and T_{i+1} , respectively.

The magnetocaloric effect for Tb_6NiTe_2 in terms of the isothermal entropy change, $-\Delta S_m$, has the maximum value of 4.86 J/kg K at 229 K for the 0–5 T field change (Fig. 5b). The maximum $|\Delta S_m|$ value is close to the values observed for isostructural Tb_6FeSb_2 , Tb_6FeBi_2 [9] and Gd_6CoTe_2 [8] and corresponds to the

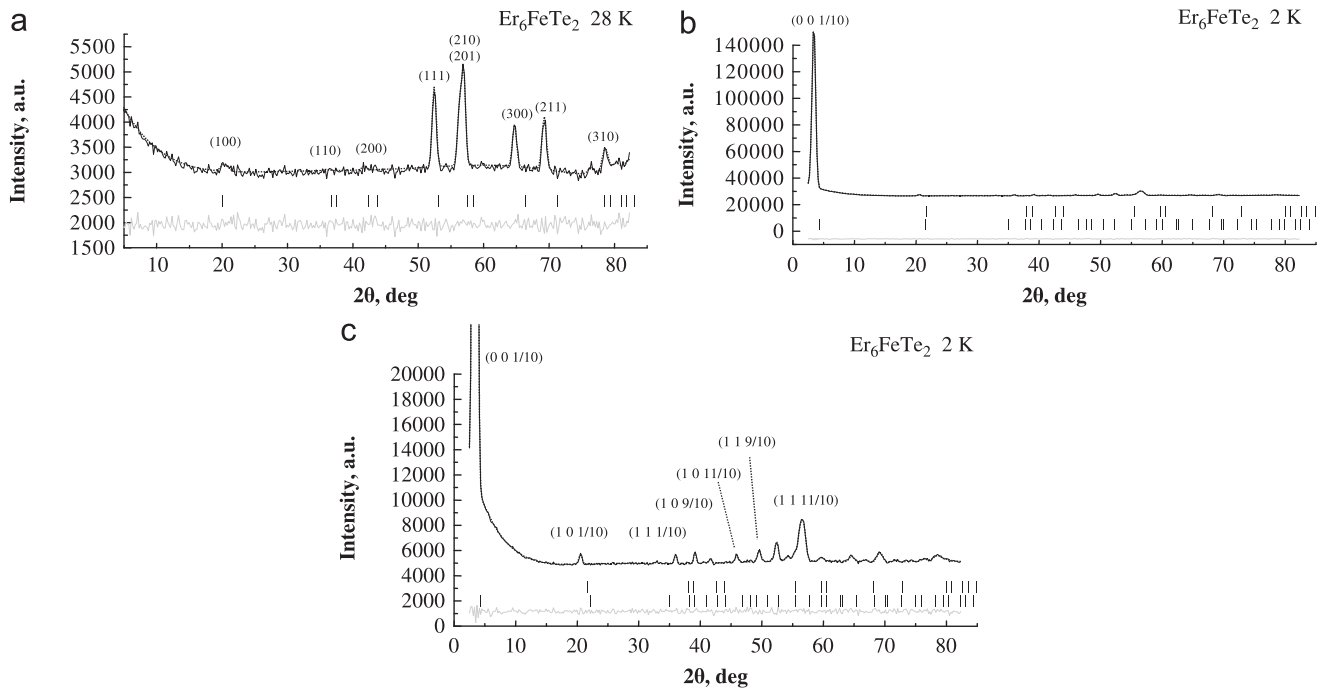


Fig. 7. Neutron diffraction pattern of Er_6FeTe_2 at (a) 28 K (paramagnetic state) and (b, c) 2 K (flat spiral) ($\lambda = 0.254$ nm). Fig. 2b gives the general view of the neutron diffraction pattern at 2 K.

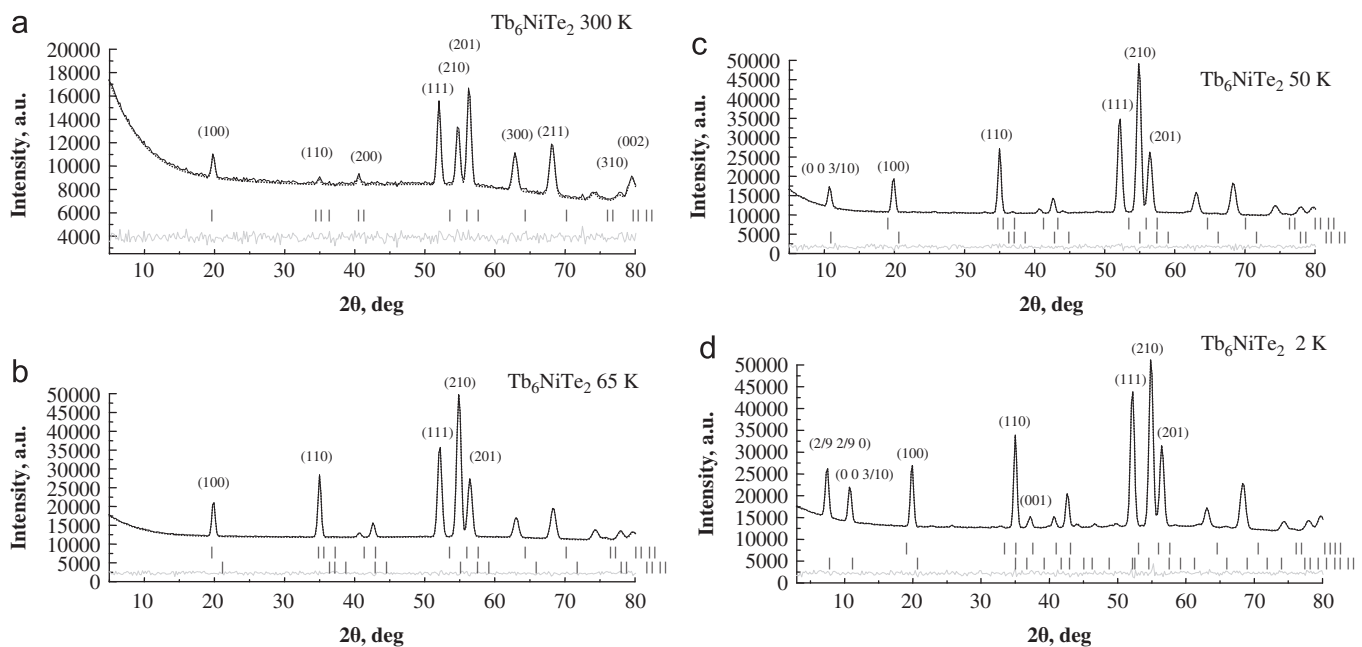


Fig. 8. Neutron diffraction pattern of Tb_6NiTe_2 at (a) 300 K (paramagnetic state), (b) 65 K (collinear ferromagnetic), (c) 50 K (ferromagnetic cone) and (d) 2 K (canted ferromagnetic cone) ($\lambda = 0.254$ nm).

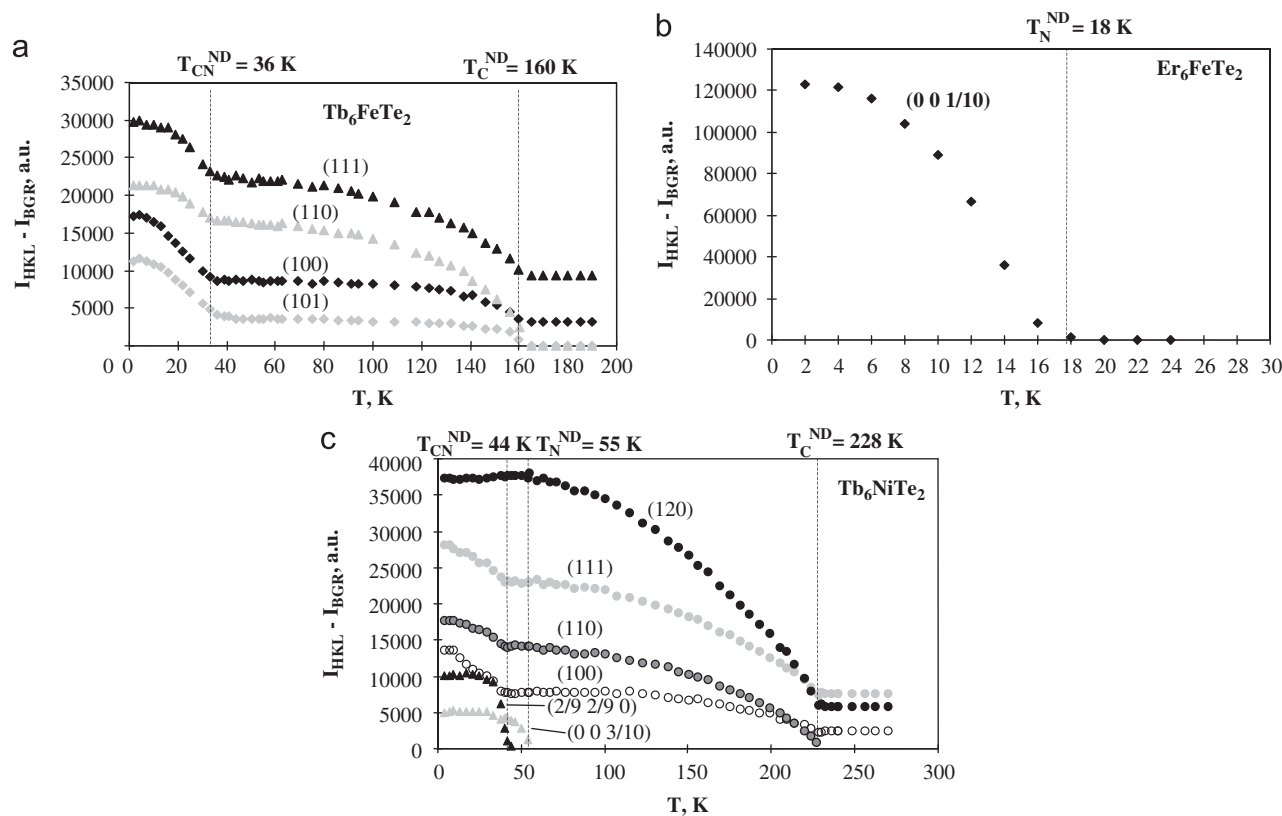


Fig. 9. Thermal variation of intensity of magnetic reflections in (a) Tb₆FeTe₂, (b) Er₆FeTe₂ and (c) Tb₆NiTe₂.

Table 4
Symmetry operations for the general and special sites of the $\bar{6}2m$ (D_{3h}) point group [15].

N	x/a	y/b	z/c	Symmetry operation of general site
1	X	Y	Z	1
2	−Y	X−Y	Z	3 ₁
3	−X+Y	−X	Z	3 ₂
4	X	Y	−Z	m _Z
5	−Y	X−Y	−Z	3 ₁ m _Z
6	−X+Y	−X	−Z	3 ₂ m _Z
7	Y	X	−Z	2 _{XX}
8	X−Y	−Y	−Z	3 ₁ 2 _{XX} =2 _{XX} 3 ₂ =2 _X
9	−X	−X+Y	−Z	3 ₂ 2 _{XX} =2 _{XX} 3 ₁ =2 _Y
10	Y	X	Z	m _{XX}
11	X−Y	−Y	Z	3 ₁ m _{XX} =m _Y
12	−X	−X+Y	Z	3 ₂ m _{XX} =m _X
N	x/a	y/b	z/c	Symmetry operation of special site [X _{R1} ,0,1/2] and [X _{R2} ,0,0]
R1 ¹	X _{R1}	0	1/2	{1,m _Z ,2 _X ,m _Y }
R2 ¹	X _{R2}	0	0	
R1 ²	0	X _{R1}	1/2	{3 ₁ ,3 ₁ m _Z ,2 _{XX} ,m _{XX} }={1,m _Z ,2 _X ,m _Y }3 ₁
R2 ²	0	X _{R2}	0	
R1 ³	−X _{R1}	−X _{R1}	1/2	{3 ₂ ,3 ₂ m _Z ,2 _Y ,m _X }={1,m _Z ,2 _X ,m _Y }3 ₂
R2 ³	−X _{R2}	−X _{R2}	0	

collinear ferromagnetic ordering of rare-earth magnetic moments along the c-axis [5].

3.4. Neutron diffraction study

3.4.1. Magnetic transitions

Figs. 6–8 show the neutron power diffraction patterns recorded at different temperatures in a zero magnetic field for Tb₆FeTe₂,

Er₆FeTe₂ and Tb₆NiTe₂. No incommensurate magnetic reflections were detected for Tb₆FeTe₂, both commensurate magnetic reflections with $\mathbf{K}_0=[0,0,0]$ and incommensurate ones with $\mathbf{K}_1=[0,0,\pm 3/10]$ and $\mathbf{K}_2=[\pm 2/9,\pm 2/9,0]$ were observed for Tb₆NiTe₂ and only incommensurate $\mathbf{K}_1=[0,0,\pm 1/10]$ reflections were detected for Er₆FeTe₂. Thermal variations in the intensities of the magnetic reflections indicate magnetic transitions at 160 K and 36 K for Tb₆FeTe₂, at 18 K for Er₆FeTe₂ and at 228, 55 and 44 K for Tb₆NiTe₂ (Fig. 9).

3.4.2. Magnetic structure

The symmetry operations of the $\bar{6}2m$ (D_{3H}) point group are given in Table 4 [15]. This point group includes $D_3 = \{C_3, 2_{XX}C_3\}$, $C_{3v} = \{C_3, m_{XX}C_3\}$ and $C_{3H} = \{C_3, m_ZC_3\}$ subgroups of index 2, C_{2v} (D_{1H}) = $\{1, m_Z, 2_X, m_Y\}$, $\{1, m_Z, 2_{XX}, m_X\}$, $\{1, m_Z, 2_Y, m_{XX}\}$ subgroups of index 3, $C_3 = \{1, 3_1, 3_2\}$ subgroups of index 4 and $C_{1v} = \{1, m_Z\}$, $\{1, m_X\}$, $\{1, m_Y\}$, $\{1, m_{XX}\}$, $D_1 = \{1, 2_X\}$, $\{1, 2_{XX}\}$, $\{1, 2_Y\}$ subgroups of index 6 [15]. The possible magnetic point groups for the $\bar{6}2m$ (D_{3H}) point group are the above-mentioned "colorless" and "black-white" (Shubnikov) $\{D_3, m_ZD_31'\}$, $\{C_{3v}, m_ZC_{3v}1'\}$, $\{C_{3H}, 2_{XX}C_{3H}1'\}$, $\{C_{1v}, 2_XC_{1v}1'\}$, $\{D_1, m_ZD_11'\}$ point groups. Magnetic symmetries for special directions of the rare-earth magnetic moments on special sites $[X_{R1}, 0, 1/2]$ and $[X_{R2}, 0, 0]$ are given in Fig. 10.

The magnetic structures of the Fe₂P-type phases were determined in terms of the symmetry of the above-mentioned magnetic point groups. The evolution of the magnetic order during cooling can be clearly identified from the development of magnetic reflections for

Tb₆FeTe₂, Er₆FeTe₂ and Tb₆NiTe₂ (Figs. 6–8). Magnetic structures and temperatures of the magnetic transitions were determined from the refinements of neutron powder diffraction data. The crystallographic and magnetic parameters for Tb₆FeTe₂, Tb₆NiTe₂ and Er₆FeTe₂ are shown in Tables 5–7. Refined values of the rare-earth magnetic moments have to be compared to the theoretical values of the Tb and Er ions ($M_{Tb^{3+}} = 9 \mu_B$ and $M_{Er^{3+}} = 9 \mu_B$) in the trivalent state [16].

3.5. Tb₆FeTe₂

Below 160 K, Tb₆FeTe₂ has a collinear magnetic structure with the C_{3v} (**3 m**) magnetic point group (**P31m** magnetic space group) for the Tb sublattice (the Tb magnetic moments are ferromagnetically ordered along the *c*-axis): $\{M_{Tb1}^{(0)}, M_{Tb2}^{(0)}\}$ (**P31m**) (Fig. 10 (I) and Fig. 11a). The magnetic moments of Tb1 and Tb2 have

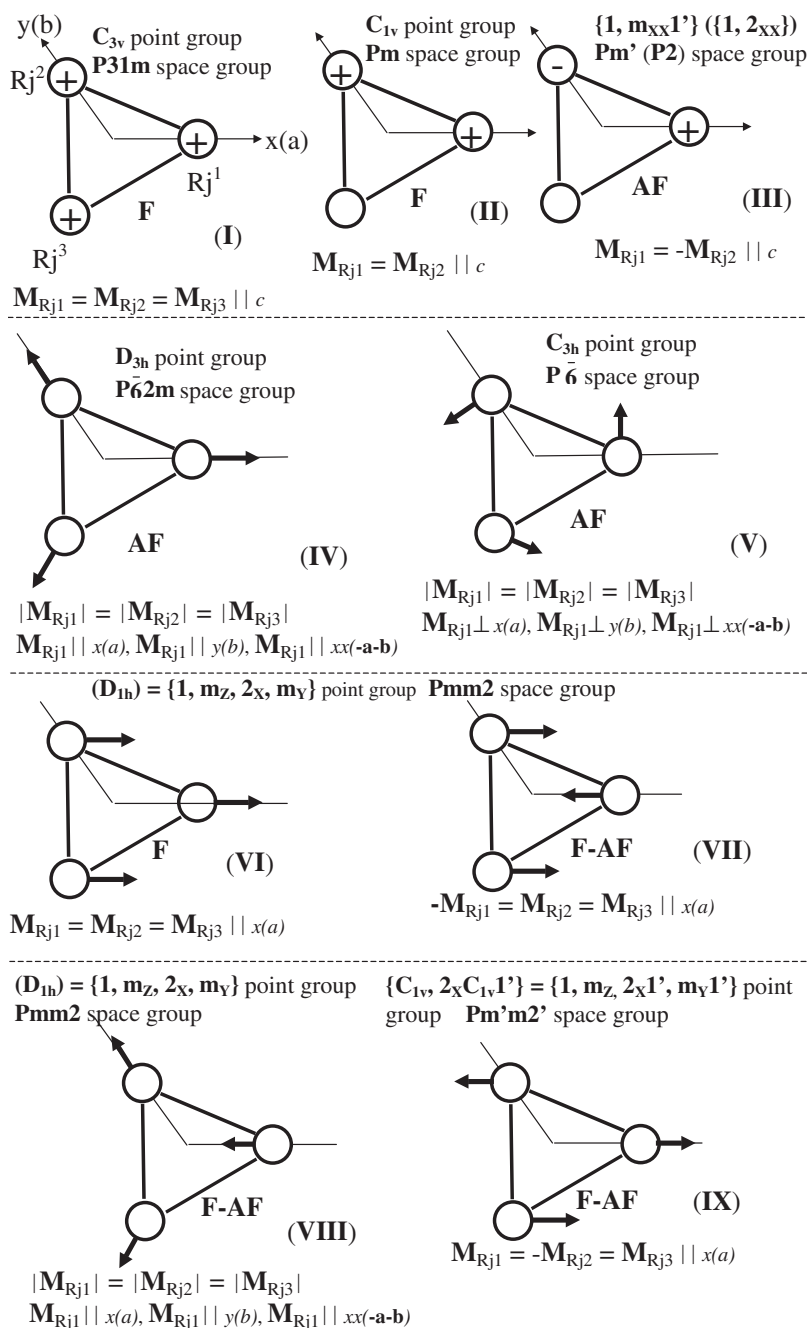


Fig. 10. Magnetic symmetries of the special $[X_{R1}, 0, 1/2]$ and $[X_{R2}, 0, 0]$ sites of the $\bar{6}2m$ (D_{3H}) point group ($P\bar{6}2m$ space group).

Table 5
Crystallographic and magnetic parameters of the Fe₂P-type Tb₆FeTe₂ phase.

T_{CN}	T_{CN}^{ND}	Type	T^a	Unit cell data	R_F	Atom	M_j^{K0}	φ_j^{K0}	θ_j^{K0}	R_F^m
		Paramagnetic	300 ^b	$a=0.82753(6)$ nm $c=0.40175(2)$ nm $X_{Tb1}=0.5945(5)$ $X_{Tb2}=0.2400(5)$	5.1					
		Paramagnetic	193	$a=0.82655(5)$ nm $c=0.40148(3)$ nm $X_{Tb1}=0.5966(7)$ $X_{Tb2}=0.2394(6)$	8.5					
160	160	F_C:M_{(Tb1, Tb2)C}^{K0} (P31m)}	50	$a=0.82534(5)$ nm $c=0.40084(3)$ nm $X_{Tb1}=0.5975(6)$ $X_{Tb2}=0.2400(4)$	5.6	Tb1 ¹ Tb1 ² Tb1 ³ Tb2 ¹ Tb2 ² Tb2 ³	6.2(1) 6.2(1) 6.2(1) 9.0(1) 9.0(1) 9.0(1)	0 0 0 0 0 0	0 0 0 0 0 0	5.2
36	36	F_C–AF_{ab}–F_{ab}:M_{(Tb1,Tb2)ab}^{K0} (Pm₂) M_{(Tb1, Tb2)C}^{K0} (P31m)}}	2	$a=0.82519(5)$ nm $c=0.40069(3)$ nm $X_{Tb1}=0.5976(7)$ $X_{Tb2}=0.2395(3)$	3.6	Tb1 ¹ Tb1 ² Tb1 ³ Tb2 ¹ Tb2 ² Tb2 ³	9.0(2) 9.0(2) 9.0(2) 9.0(2) 9.0(2) 9.0(2)	–42(2) 42(2) 42(2) 42(2) –42(2) –42(2)	52(1) 52(1) 52(1) 15(1) 15(1) 15(1)	5.6

T_{CN} (K) and T_{CN}^{ND} (K) are the magnetic transition temperatures from magnetic measurements and neutron diffraction studies. **F** a ferromagnetic component, **AF** an antiferromagnetic component. X_{Tb1} and X_{Tb2} are the atomic position parameters. M_j^{K0} (μ_B) is the magnetic moment of the corresponding atom with wave vectors $\mathbf{K}_0=[0,0,0]$; φ_j^{K0} and θ_j^{K0} are the angles (deg) of the corresponding magnetic moment with the a and c axes. Reliability factors R_F (crystal structure) and R_F^m (magnetic structure) are given in percent (%).

^a Temperature for which the crystallographic and magnetic parameters are reported for a given magnetic state.
^b X-ray data.

Table 6
Crystallographic and magnetic parameters of the Fe₂P-type Tb₆NiTe₂ phase.

T_{CN}	T_{CN}^{ND}	Type of magnetic ordering	T^a	Unit cell data	R_F	Atom	M_j^{K0}	φ_j^{K0}	θ_j^{K0}	$M_j^{K1, K2}$	Wave vector	R_F^m
		Paramagnetic	300 ^b	$a=0.83464(6)$ nm $c=0.39300(2)$ nm $X_{Tb1}=0.5932(5)$ $X_{Tb2}=0.2368(5)$	6.4							
		Paramagnetic	300	$a=0.8343(2)$ nm $c=0.3933(1)$ nm $X_{Tb1}=0.597(1)$ $X_{Tb2}=0.234(1)$	5.2							
	228	F_C: M_{(Tb1, Tb2)C}^{K0} (P31m)}	100	$a=0.8326(1)$ nm $c=0.39261(7)$ nm $X_{Tb1}=0.596(1)$ $X_{Tb2}=0.236(1)$	2.7	Tb1 ¹ Tb1 ² Tb1 ³ Tb2 ¹ Tb2 ² Tb2 ³	6.5(2) 6.5(2) 6.5(2) 8.7(2) 8.7(2) 8.7(2)	0 0 0 0 0 0	0 0 0 0 0 0			2.4
52	55	F_C–AF_{ab}: M_{(Tb1, Tb2)C}^{K0} (P31m)}	50	$a=0.8326(1)$ nm $c=0.39250(6)$ nm $X_{Tb1}=0.596(1)$ $X_{Tb2}=0.235(1)$	3.6	Tb1 ¹ Tb1 ² Tb1 ³ Tb2 ¹ Tb2 ² Tb2 ³	7.0(2) 7.0(2) 7.0(2) 8.9(2) 8.9(2) 8.9(2)	0 0 0 0 0 0	0 0 0 0 0 0	1.24(3) 1.24(3) 1.24(3) 1.24(3) 1.24(3) 1.24(3)	K₁	5.2
		M_{(Tb1, Tb2)ab}^{K1} (flat spiral)}				Tb2 ¹ Tb2 ² Tb2 ³	8.9(2) 8.9(2) 8.9(2)	0 0 0	0 0 0	1.24(3) 1.24(3) 1.24(3)		
33	44	F_C–AF_{abc}–F_{ab}:M_{(Tb1,Tb2)ab}^{K0} (Pm₂)}	2	$a=0.83272(9)$ nm $c=0.39259(6)$ nm $X_{Tb1}=0.597(1)$ $X_{Tb2}=0.235(1)$	2.6	Tb1 ¹ Tb1 ² Tb1 ³ Tb2 ¹ Tb2 ² Tb2 ³	8.9(2) 8.9(2) 8.9(2) 8.9(2) 8.9(2) 8.9(2)	–36(2) 36(2) 36(2) 36(2) –36(2) –36(2)	45(2) 45(1) 45(2) 11(2) 11(2) 11(1)	1.74(3) 1.74(3) 1.74(3) 1.74(3) 1.74(3) 1.74(3)	K₁, K₂	3.8
		•M_{(Tb1, Tb2)C}^{K0} (P31m)}				Tb2 ¹ Tb2 ² Tb2 ³	8.9(2) 8.9(2) 8.9(2)	36(2) –36(2) –36(2)	11(2) 11(2) 11(1)	1.74(3) 1.74(3) 1.74(3)		
		•M_{(Tb1, Tb2)ab}^{K1, K2} (flat spiral)}										

T_{CN} (K) and T_{CN}^{ND} (K) are the magnetic transition temperatures from magnetic measurements and neutron diffraction studies. **F** a ferromagnetic component, **AF** an antiferromagnetic component. X_{Tb1} and X_{Tb2} , are the atomic position parameters. M_j^{K0} , $M_j^{K1, K2}$ (μ_B) are the magnetic moments of the corresponding atom with wave vectors $\mathbf{K}_0=[0,0,0]$, $\mathbf{K}_1=[0,0,\pm 3/10]$ and $\mathbf{K}_2=[\pm 2/9,\pm 2/9,0]$. φ_j^{K0} and θ_j^{K0} are the angle (deg) of corresponding magnetic moments with the a and c axes. The cone axis of the flat spirals with \mathbf{K}_1 and \mathbf{K}_2 coincides with the magnetic moment directions of the corresponding atom, the cone angles $\beta_j^{K1}=\beta_j^{K2}=90$ deg. Reliability factors R_F (crystal structure) and R_F^m (magnetic structure) are given in percent (%).

^a Temperature for which the crystallographic and magnetic parameters are reported for a given magnetic state.
^b X-ray data.

significantly different values (Table 5). Below 36 K, the reflections indicate ferromagnetic and antiferromagnetic orderings in the ab plane (Fig. 6c). The (VII), (VIII) and (IX) variants of the magnetic symmetry (Fig. 10) would agree with such behavior. Variant (VII) has a good agreement with experimental data (**D_{1H}**=**{1, m_z, 2_x, m_y}** point group, **Pmm2** space group) (Fig. 11b), but the best fit is achieved for a “canted” ferromagnetic ordering with the **C_{1v}**=**{1, m_z}** magnetic point group (**Pm₂** magnetic space group) shown in

Table 7Crystallographic and magnetic parameters of the Fe₂P-type Er₆FeTe₂ phase.

T_N^D	Type	T^a	Unit cell data	R_F	Atom	M_j	R_F^b
	Paramagnetic	300 ^b	$a=0.81565(8)$ nm $c=0.39827(8)$ nm $X_{Er1}=0.5967(5)$ $X_{Er2}=0.2407(8)$	6.2			
	Paramagnetic	28	$a=0.8154(6)$ nm $c=0.3977(5)$ nm $X_{Er1}=0.599(4)$ $X_{Er2}=0.239(4)$	7.8			
18	AF_{ab}: {M_{Er1}, M_{Er2}}^{K1} (flat spiral)	2	$a=0.8147(4)$ nm $c=0.3975(4)$ nm $X_{Er1}=0.596(4)$ $X_{Er2}=0.236(4)$	6.7	Er1 ¹ Er1 ² Er1 ³ Er2 ¹ Er2 ² Er2 ³	5.6(2) 5.6(2) 5.6(2) 7.5(2) 7.5(2) 7.5(2)	3.0

T_N^D (K) is the magnetic transition temperature from the neutron diffraction studies. **AF** an antiferromagnetic component. X_{Er1} and X_{Er2} , are the atomic position parameters. M_j (μ_B) is the magnetic moment of the corresponding atom with wave vectors $\mathbf{K}_1=[0,0,\pm 1/10]$ (magnetic phase is zero for all atoms, cone angle is 90°, cone axis coincides with the c-axis). Reliability factors R_F (crystal structure) and R_F^b (magnetic structure) are given in percent (%).

^a Temperature for which the crystallographic and magnetic parameters are reported for a given magnetic state.

^b X-ray data.

Fig. 11c). Thus, below 36 K the Tb₆FeTe₂ magnetic structure becomes a non-collinear ferromagnet due to the presence of magnetic point group $\mathbf{C}_{1v}=\{\mathbf{1}, \mathbf{m}_z\}$ with the *ab* components: $\{\mathbf{M}_{(Tb1, Tb2)ab}^{K0}\} (\mathbf{P1})=\{\mathbf{M}_{(Tb1, Tb2)C}^{K0}\} (\mathbf{P31m})+\{\mathbf{M}_{(Tb1, Tb2)ab}^{K0}\} (\mathbf{Pm}_z)$. Models with other magnetic point groups had no satisfactory agreement with the experimental data. The magnetic structure projected onto the *ab* plane consists of collinear, ferromagnetically ordered domains (Fig. 11c).

The symmetry of the high-temperature magnetic ordering (**P31m**) closes the symmetry of the rare-earth sublattice ($P\bar{6}2m$ space group), whereas the low-temperature magnetic ordering leads to a decrease in the magnetic symmetry down to **P1**.

The thermal variations of the terbium magnetic moments are shown in Fig. 12a. Details of the Tb₆FeTe₂ magnetic structure are given in Table 5.

3.6. Tb₆NiTe₂

Below 228 K, Tb₆NiTe₂ has a collinear magnetic structure with the \mathbf{C}_{3v} (**3 m**) magnetic point group (**P31m** magnetic space group) for the Tb sublattice (the Tb magnetic moments are ferromagnetically ordered along the c-axis) (Fig. 10 (I) and Fig. 11a): $\{\mathbf{M}_{(Tb1, Tb2)C}^{K0}\} (\mathbf{P31m})$, like in Tb₆FeTe₂ and Tb₆CoTe₂ [6]. The magnetic moments of Tb1 and Tb2 have strongly different values (Table 6).

Below 55 K the magnetic structure of Tb₆NiTe₂ is a ferromagnetic cone. The terbium magnetic components with a $\mathbf{K}_0=[0,0,0]$ wave vector are ferromagnetically coupled and directed along the c-axis ($\{\mathbf{M}_{(Tb1, Tb2)C}^{K0}\} (\mathbf{P31m})$), whereas the terbium magnetic component with a $\mathbf{K}_1=[0,0,\pm 3/10]$ wave vector (flat spiral: cone angle 90°, magnetic phase is zero for all atoms) are arranged in the *ab* plane (Fig. 11d).

Below 44 K the commensurate part of Tb₆NiTe₂ magnetic structure becomes a non-collinear ferromagnet due to the presence of magnetic point group $\mathbf{C}_{1v}=\{\mathbf{1}, \mathbf{m}_z\}$ for the *ab* components: $\{\mathbf{M}_{(Tb1, Tb2)ab}^{K0}\} (\mathbf{P1})=\{\mathbf{M}_{(Tb1, Tb2)C}^{K0}\} (\mathbf{P31m})+\{\mathbf{M}_{(Tb1, Tb2)ab}^{K0}\} (\mathbf{Pm}_z)$, like in Tb₆FeTe₂ and Tb₆CoTe₂ [6] (Fig. 11c), whereas the incommensurate part of the Tb₆NiTe₂ magnetic structure is a set of flat spirals with the $\mathbf{K}_1=[0,0,\pm 3/10]$ and $\mathbf{K}_2=[\pm 2/9,\pm 2/9,0]$ wave vectors (cone angle 90°, magnetic phase is zero for all atoms, cone axes coincide with the directions of the commensurate magnetic moments of the corresponding atoms). The magnetic structure consists of canted ferromagnetic cones (Fig. 11e). The thermal

variations of the terbium magnetic moments are shown in Fig. 12b. Details of the Tb₆NiTe₂ magnetic structure are given in Table 6.

The following decrease in symmetry is observed for the terbium sublattice: $P\bar{6}2m$ (paramagnetic state) \rightarrow **P31m** (high-temperature magnetic ordering) \rightarrow **P1** (low-temperature magnetic ordering).

3.7. Er₆FeTe₂

Below 18 K Er₆FeTe₂ is a pure antiferromagnet and its magnetic structure is a flat spiral with wave vector $\mathbf{K}_1=[0,0,\pm 1/10]$ (the cone axis coincides with the c-axis, cone angle is 90°, magnetic phase is zero for all atoms) (Fig. 11d). The magnetic structure consists of ferromagnetically ordered (in the *ab* plane) Er magnetic moments that rotate along the c-axis, and it is similar to the high-temperature magnetic structure of Ho₆FeTe₂ [8]. The thermal variations of the erbium magnetic moments are shown in Fig. 12c. The magnetic moments of Er1 and Er2 have different values. Details of the Er₆FeTe₂ magnetic structure are given in Table 7. The symmetry of the erbium sublattice decreases from $P\bar{6}2m$ (paramagnetic state) to **P1** (antiferromagnetic ordering).

The Tb₆FeTe₂, Tb₆CoTe₂ [6] and Tb₆NiTe₂ have the same high-temperature and commensurate low-temperature magnetic structures. In general, the magnetic moments of the R2 site are bigger than those of the R1 site: $M_{R2} > M_{R1}$. Due to specific features of the low-temperature magnetic structure the Ho₆FeTe₂ and Tb₆FeTe₂ compounds show metamagnetic transition in mixed magnetic state, similar to the Tb₆CoTe₂ and Tb₆NiTe₂ systems (Figs. 3 and 11).

The symmetry of the rare-earth sublattice in pure rare-earth metals ($P6_3/mmc$, **D_{6H}** point group) is close to that in Fe₂P-type phases ($P\bar{6}2m$, **D_{3H}** point group). For this reason, the magnetic structure of the corresponding Fe₂P-type phases correlates with the magnetic structure of the corresponding pure rare earths: Tb₆FeTe₂, Tb₆CoTe₂ and Tb₆NiTe₂ have the magnetic structures similar to those of pure Tb [16], Ho₆FeTe₂ [6] and Er₆FeTe₂ have the magnetic structures similar to those of Ho and Er [16].

The structural and magnetic role of the transition metals (Fe, Co, Ni) in the Fe₂P-type phases is not quite clear. Their atomic radii are unlikely to determine the distortion of the rare-earth sublattices as the R2–T distances are smaller than the sum of metallic radii (Table 3), however the cell parameters do correlate with the size of the transition metals: $a_{R6NiTe2} > a_{R6CoTe2} > a_{R6FeTe2}$ and $c_{R6NiTe2} < c_{R6CoTe2} < c_{R6FeTe2}$ (Tables 1 and 2). Also the high-temperature magnetic orderings reveal dependence on the

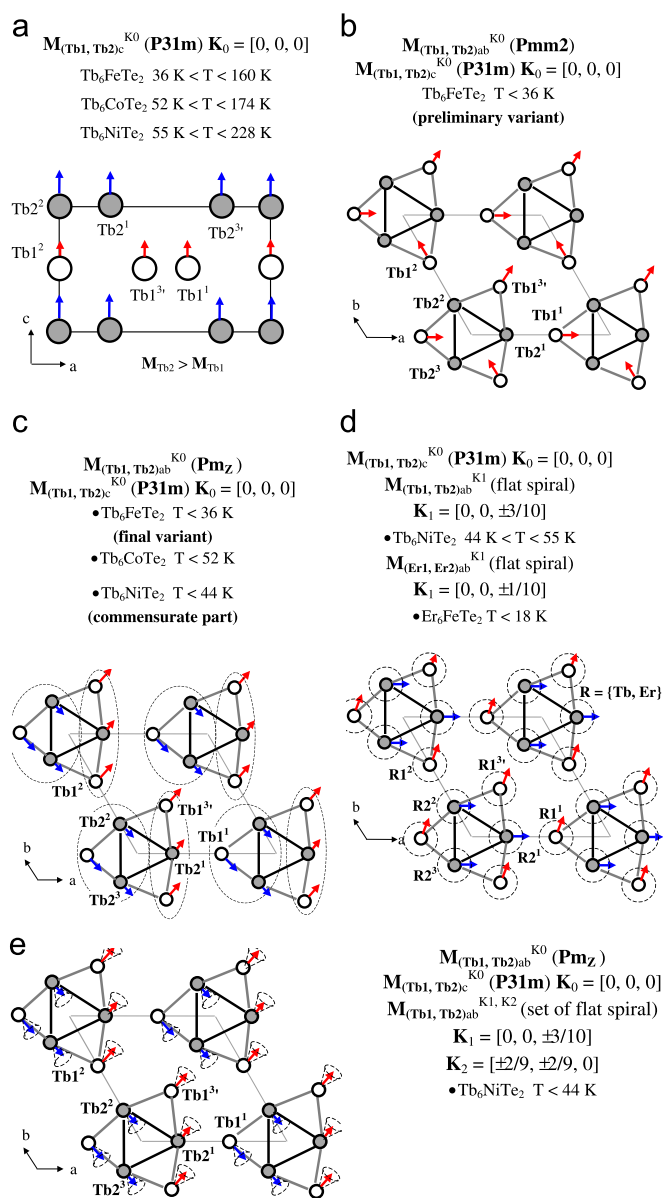


Fig. 11. (a) Magnetic structure of Tb_6FeTe_2 , Tb_6CoTe_2 and Tb_6NiTe_2 below the high-temperature ferromagnetic transitions, (b) a preliminary variant of Tb_6FeTe_2 , (c) the final variants of Tb_6FeTe_2 , Tb_6CoTe_2 and commensurate part of Tb_6FeTe_2 below the low-temperature AF–F transition, (d) the final variants of Tb_6NiTe_2 below $T_{CN}=44$ K and $T_N=55$ K of Er_6FeTe_2 below $T_N=18$ K and (e) of Tb_6NiTe_2 below $T_{CN}=44$ K (the cone axes coincide with the directions of the commensurate magnetic moments).

nature of the transition metals : $T_C^{R6NiTe_2} > T_C^{R6CoTe_2} > T_C^{R6FeTe_2}$ (Tables 1 and 2).

The magnetocaloric effect of Tb_6NiTe_2 ($\Delta S_{mag} = -4.86$ J/kg K at 229 K for the field change $\Delta \mu_0 H = 0-5$ T) corresponds to the decrease in the symmetry of the Tb sublattice from $P6_2m$ (paramagnetic state) \rightarrow $\mathbf{P31m}$ (collinear ferromagnetic ordering).

4. Conclusion

Formation of the Fe_2P -type compounds from the Mg-type rare-earth metals [6] is shown to modify the magnetic structure of the parent elements. While the magnetic ordering temperature of R_6Te_2 is lower than those of the pure rare-earth metals, the current modification of the Mg-type lattice facilitates ferromagnetic orderings and suppresses antiferromagnetic ones. In general, the

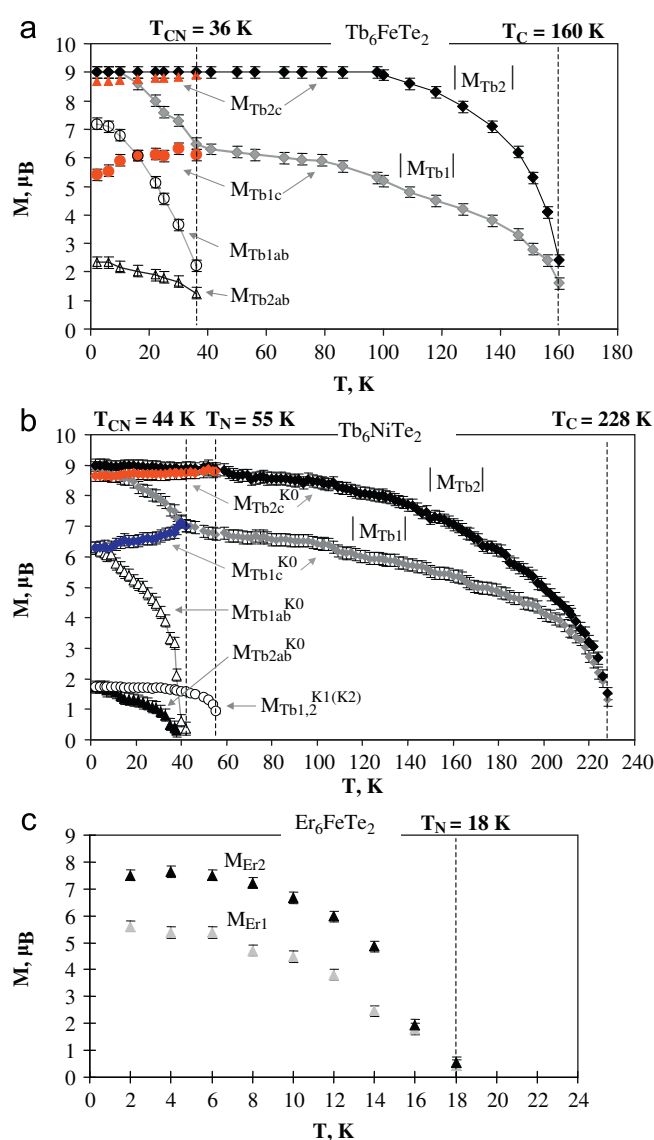


Fig. 12. Thermal variation of the magnetic moments for the R1 and R2 sites in (a) Tb_6FeTe_2 , (b) Tb_6NiTe_2 and (c) Er_6FeTe_2 .

high-temperature magnetic transitions are ferromagnetic in nature and the low-temperature ones coincide with the reorientation of magnetic moments and increase in the antiferromagnetic component.

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Tb₆FeTe₂, Ho₆FeTe₂, Zr₆FeTe₂ and Hf₆FeTe₂ were used with permission—© JCPDS—International Centre for Diffraction Data.

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