Supplementary Material to the article
“Study of multiferroics $SmFe_{3-x}Sc_x(BO_3)_4$ (x = 0.17, 0.45) by ^{57}Fe Mössbauer spectroscopy”

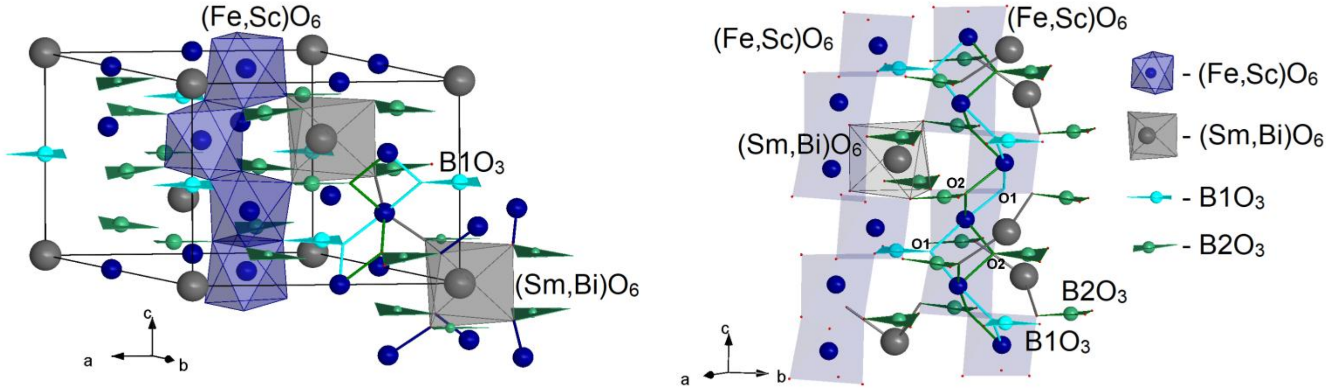

Fig. S1. Crystal structure of the $SmFe_{3-x}Sc_x(BO_3)_4$.

Table S1. Crystallographic parameters and results of structure refinement of the $SmFe_{3-x}Sc_x(BO_3)_4$ single crystals at T = 295 K.

Sc content x	0	0.17	0.45
a, Å	9.5650(1)	9.5879(1)	9.6103(1)
c, Å	7.5869(1)	7.6158(1)	7.6553(1)
V, Å^3	601.13(1)	606.31(1)	612.30(1)
D_x, g/cm^3	4.608	4.554	4.484
μ, mm^{-1}	13.35	6.908	6.702
θ_{max}, degrees	55.86	55.90	55.84
Number of reflections:			
measured	20702	91172	91434
independent	2773	3628	3669
observed [$I > 3\sigma(I)$]	2773	3534	3578
Absolute structure (Flack) parameter	0.480(4)	0.440(7)	0.296(8)
R_{int}	0.027	0.0717	0.1016
R [$F^2 > 2\sigma(F^2)$]	0.011	0.0185	0.0211
$wR(F^2)$	0.015	0.0383	0.0488
$\Delta\rho_{min}$, e/Å^3	-0.88	-1.93	-1.94
$\Delta\rho_{max}$, e/Å^3	0.84	1.35	1.70

a and c– unit cell parameters; V – unit cell volume; D_x – calculated crystal density; μ – absorption coefficient (absorption correction was empirical and numerical based on crystal shape); θ_{max} – maximum diffraction angle; I – reflection intensity; σ – standard deviation; R_{int} – factor of internal agreement; R – refinement factor; wR – weighted refinement factor; Δρ – residual electron density.

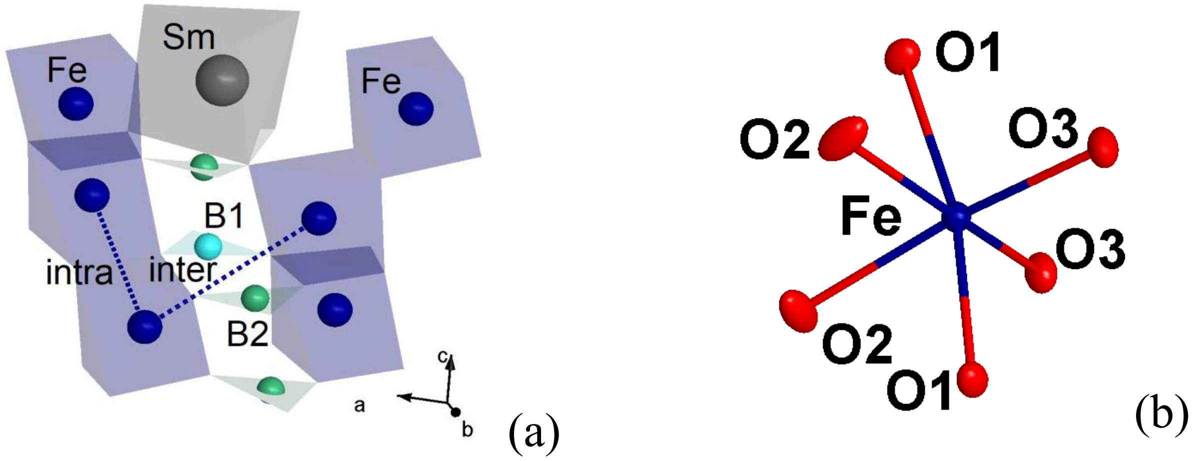

Fig. S2. Local crystal structure of the $SmFe_{3-x}Sc_x(BO_3)_4$. (a) – the diagram of the arrangement of atoms between two adjacent helical chains of FeO_6 octahedra (shown in translucent blue); oxygen atoms at the octahedra vertices are not shown; dotted lines indicate the nearest Fe atoms within the chain (intra) and in adjacent chains (inter). (b) – the diagram of the relative positions of oxygen atoms O1-O6 in the FeO_6 octahedron.

Table S2. Distances between (Fe,Sc) and some nearest atoms

Sc content *x*	0	0.17	0.45
(Fe,Sc) – $(Fe,Sc)_{intra}$ in helicoidal chains	3.1803(1)	3.1818(1)	3.2096(1)
(Fe,Sc) – $(Fe,Sc)_{inter}$ between helicoidal chains	4.3950(1)	4.4058(1)	4.4140(2)
(Fe,Sc) – O_{ave} average in $(Fe,Sc)O_6$ octahedra	2.010(1)	2.017(1)	2.027(1)
(Fe,Sc) – Sm	3.7752(1)	4.3130(1)	4.3274(2)

Table S3. Hyperfine and model parameters calculated from Mössbauer spectra of the $SmFe_{3-x}Sc_x(BO_3)_4$ samples measured at temperatures below the magnetic phase transition point T_N.

				$x = 0.17$					
T (K)	Components	δ (mm/s)	ε (mm/s)	Δ (mm/s)	B_{hf} (T)	*ln*(*R*)	*p*	Γ (mm/s)	*A* (%)
4.0	S	0.508(1)	0.109(1)	–	52.91(6)	13.0(2)	0.41(2)	0.275	100
10.0	S	0.510(1)	0.110(1)	–	51.59(3)	12.1(2)	0.45(1)	0.277	100
15.0	S	0.510(1)	0.111(1)	–	49.27(3)	11.5(2)	0.58(1)	0.287	100
20.0	S	0.510(1)	0.109(1)	–	45.63(4)	12.6(1)	0.73(1)	0.305	100
25.0	S	0.511(2)	0.113(2)	–	39.33(4)	13.0(1)	0.84(2)	0.297	100
28.0	S1	0.518(3)	0.125(3)	–	33.41(8)	13.5(2)	0.92(1)	0.234	69.7
	S2	0.509(4)	0.116(5)	–	30.17(8)	0.0*	0.82(1)	0.356	30.3
29.0	S1	0.504(3)	0.094(3)	–	30.26(13)	14.6(2)	0.93(1)	0.211	68.2
	S2	0.504(6)	0.124(6)	–	25.59(11)	0.0*	0.85(1)	0.415	31.8
30.0	S1	0.504(4)	0.116(4)	–	25.64(17)	16.0(1)	0.95(1)	0.240	67.7
	S2	0.506(16)	0.012(11)	–	14.45(15)	0.1	0.31(2.4)	1.161	32.3
30.5	S1	0.516(7)	0.122(6)	–	21.42(29)	15.4(3)	0.96(1)	0.226	44.8
	S2	0.502(11)	0.090(10)	–	16.21(24)	0.0*	0.89(3)	0.526	24.9
	D	0.511(2)	–	0.309(1)	–	–	–	0.299	30.3
30.8	S1	0.524(10)	0.144(10)	–	16.17(50)	16.4(4)	0.96(1)	0.309	43.1
	S2	0.486(28)	0.038(23)	–	8.59(10)	0.0*	0.0(1.7)	0.969	19.1
	D	0.512(2)	–	0.309(2)	–	–	–	0.297	37.8
31.0	S1	0.500(12)	0.054(23)	–	4.73(29)	16.0(1)	0.0(2.7)	1.391	37.4
	D	0.510(1)	–	0.304(1)	–	–	–	0.306	62.6

x = 0.45									
T (K)	Components	δ (mm/s)	ε (mm/s)	Δ (mm/s)	B_{hf} (T)	*ln*(*R*)	*p*	Γ (mm/s)	*A* (%)
4.2	S	0.519(2)	0.099(2)	–	52.19(6)	13.1(2)	0.67(1)	0.332	100
7.0	S	0.516(2)	0.097(2)	–	51.37(6)	12.6(2)	0.72(1)	0.330	100
10.0	S	0.516(2)	0.098(22)	–	50.70(7)	13.8(1)	0.82(1)	0.310	100
15.0	S	0.525(4)	0.110(4)	–	47.59(11)	14.6(1)	0.90(1)	0.348	100
18.0	S1	0.488(7)	0.102(7)	–	45.53(18	14.3(2)	0.94(1)	0.220	65.5
	S2	0.528(10)	0.09(1)	–	40.17(13)	0.0*	0.88(1)	0.452	34.5
20.0	S1	0.480(9)	0.072(9)	–	42.39(34)	15.3(2)	0.95(1)	0.334	65.4
	S2	0.513(21)	0.144(19)	–	35.14(32)	0.0*	0.94(1)	0.631	34.6
21.0	S1	0.506(10)	0.098(10)	–	40.35(40)	15.2(2)	0.96(1)	0.293	65.4
	S2	0.515(21)	0.128(19)	–	32.72(30)	0.0*	0.95(1)	0.539	34.2
	D	0.516(31)	–	1.04(3)	–	–	–	0.213	0.4
22.0	S1	0.492(15)	0.108(15)	–	38.70(35	15.0(3)	0.98(1)	0.227	65.6
	S2	0.495(21)	0.096(20)	–	30.80(26)	0.0*	0.93(1)	0.539	26.4
	D	0.515(8)	–	0.374(6)	–	–	–	0.379	8.0
22.5	S1	0.509(13)	0.126(15)	–	36.99(50)	15.1(2)	0.99(1)	0.202	65.8
	S2	0.509(15)	0.050(24)	–	28.44(29)	0.0*	0.90(2)	0.542	16.9
	D	0.509(3)	–	0.339(3)	–	–	–	0.366	17.3
23.0	S1	0.497(14)	0.132(14)	–	34.99(34)	15.4(2)	1.00(2)	0.190	65.4
	S2	0.531(27)	0.094(23)	–	24.59(40)	0.0*	0.84(4)	0.801	14.1
	D	0.516(3)	–	0.332(2)	–	–	–	0.339	20.5
23.3	S1	0.495(21)	0.088(21)	–	33.86(60)	15.6(3)	1.00(8)	0.353	65.5
	S2	0.438(29)	0.062(28)	–	24.48(34)	0.0*	0.92(2)	0.404	12.4
	D	0.515(3)	–	0.333(2)	–	–	–	0.338	22.1
24.0	S1	0.517(19)	0.106(22)	–	25.63(50)	15.0(2.0)	1.0	0.976	63.5
	S2	0.318(90)	0.12(8)	–	18.45(80)	0.0*	1.0	0.190	5.3
	D	0.517(2)	–	0.342(2)	–	–	–	0.362	31.2
24.3	S1	0.513(27)	0.222(30)	–	21.45(1.7)	17.7(1.0)	1.0(6)	0.833	62.0
	D	0.517(2)	–	0.341(2)	–	–	–	0.345	38.0
24.5	S1	0.474(32)	0.090(33)	–	13.75(14)	17.0(1.0)	1.0	0.969	58.6
	D	0.518(2)	–	0.332(2)	–	–	–	0.332	41.4
24.7	S1	0.474(16)	0.42(24)	–	2.36(1)	–	–	1.775	38.2
	D	0.515(1)	–	0.322(1)	–	–	–	0.343	61.8

δ – isomer shift, ε – quadrupole shift of the internal spectral lines in the Zeeman sextet, Δ – quadrupole splitting of the paramagnetic doublet, B_{hf} – hyperfine magnetic field at the ^{57}Fe nucleus, *ln(R)* – natural logarithm of the relaxation rate (parameter of the MSR model), *p* – ratio of the populations of successive (adjacent) atomic Zeeman levels (parameter of the MSR model), Γ – width of the spectral line, *A* – the relative area of the component.

* – 0.0 means that the value of *ln*(*R*) is less than 10^{-4}.