Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.
This journal is © the Partner Organisations 2022

Electronic Supporting Information (ESI)

for

Nanocrystalline triple perovskite compounds $A_3Fe_2BO_9$ (A = Sr, Ba; B= W, Te) with ferromagnetic and dielectric properties for triboelectric energy harvesting

Jelena Kojčinović[1, ‡], Sugato Hajra[2, ‡], Manisha Sahu[2, ‡], Dalibor Tatar[1], Teodoro Klaser[3], Željko Skoko[3], Zvonko Jagličić[4,5], Elaheh Sadrollahi[6,7], Fred Jochen Litterst[6], Hoe Joon Kim[2,*] and Igor Djerdj[1,*]

[1]*Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Cara Hadrijana 8/A, 31000 Osijek, Croatia*

[2]*Department of Robotics Engineering, Daegu Gyeongbuk Institute of Science and Technology, Daegu-42988, Republic of Korea*

[3]*Department of Physics, Faculty of Science, University of Zagreb, Bijenička cesta 32, 10000 Zagreb, Croatia*

[4]*Institute of mathematics, physics and mechanics, University of Ljubljana, Jamova 2, 1000 Ljubljana, Slovenia*

[5]*Faculty of Civil & Geodetic Engineering, University of Ljubljana, Jadranska 19, 1000 Ljubljana, Slovenia*

[6]*Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany*

[7]*Institut für Festkörper- und Materialphysik, Technische Universität Dresden, Haeckelstr.3, 01069 Dresden, Germany*

***Corresponding authors:**

Prof. Dr. Igor Djerdj | e-mail: igor.djerdj@kemija.unios.hr

Prof. Dr. Hoe Joon Kim | e-mail: joonkim@dgist.ac.kr

‡Equal contribution:

Jelena Kojčinović (J. K.), Sugato Hajra (S. H.) and Manisha Sahu (M. S.)

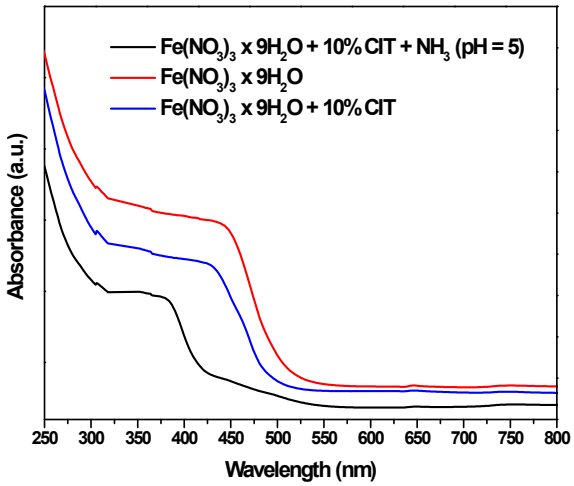

Figure S1. UV/Vis absorption spectra of aqueous solution of iron(III) nitrate nonahydrate (c = $8.1 \cdot 10^{-3}$ mol dm^{-3}) without addition of citric acid (red), with addition of citric acid, w = 10 % (blue), with addition of both citric acid (c = 10%) and concentrated ammonia solution (pH = 5) (black).

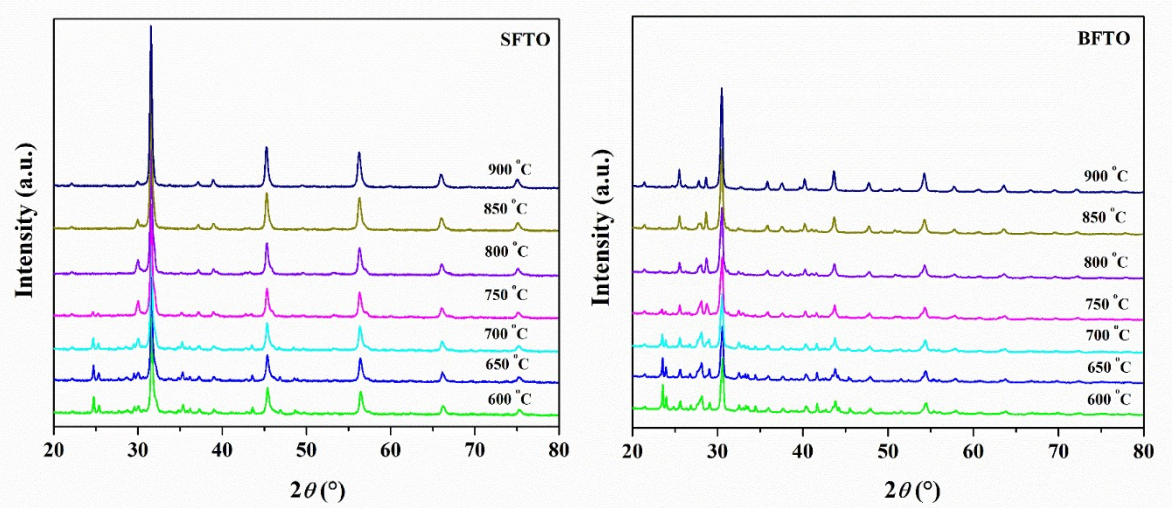

Figure S2. Temperature-dependent powder XRD patterns of SFTO (left) and BFTO (right) taken from 600 to 900 °C.

Table S1. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the SFTO (after the first step of calcination at 600 ℃) collected 600 ℃.

Chemical formula	**SrO**	**$SrCO_3$**	**Fe_3O_4**	**$Sr_3Fe_2TeO_9$**
Space group	*I*4/*mmm* (139)	*Pnma* (62)	*Fd*-3*m* (227)	*I*4/*m* (87)
Molecular weight	103.62	147.63	231.54	646.15
Crystal system	tetragonal	orthorhombic	cubic	tetragonal
Lattice parameters (Å)	*a* = 3.3984 *c* = 6.5149	*a* = 6.1913 *b* = 5.1402 *c* = 8.4786	*a* = 8.3944	*a* = 5.6288 *c* = 7.9612
Cell volume ($Å^3$)	75.24	269.83	591.52	252.24
Calculated density (g/cm^3)	5.280	3.634	5.200	5.650
Data collection range	20 to 80 °			
No. of parameters refined	40			
Average apparent crystallite size (nm)	44.1	61.7	28.7	26.9
Average apparent microstrain ($\times 10^{-4}$)	4.23	4.23	4.23	4.23
Phase composition (wt %)	2.86	15.99	13.48	67.67
R_B (%)	18.0	15.7	14.5	2.88
Conventional R_p, R_{wp}, R_e (%)	23.0, 15.2, 9.10			
GoF	1.6			

Table S2. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the SFTO (after the first step of calcination at 600 ℃) collected at 650 ℃.

Chemical formula	**SrO**	**$SrCO_3$**	**Fe_3O_4**	**$Sr_3Fe_2TeO_9$**
Space group	*I*4/*mmm* (139)	*Pnma* (62)	*Fd*-3*m* (227)	*I*4/*m* (87)
Molecular weight	103.62	147.63	231.54	646.15
Crystal system	tetragonal	orthorhombic	cubic	tetragonal
Lattice parameters (Å)	*a* = 3.4037 *c* = 6.5156	*a* = 6.2100 *b* = 5.1439 *c* = 8.4863	*a* = 8.4022	*a* = 5.6912 *c* = 8.0187
Cell volume ($Å^3$)	75.49	271.08	593.16	259.72
Calculated density (g/cm^3)	5.263	3.617	5.185	5.637
Data collection range	20 to 80 °			
No. of parameters refined	40			
Average apparent crystallite size (nm)	58.3	62.2	25.7	23.6
Average apparent microstrain ($\times 10^{-4}$)	4.23	4.23	4.23	4.23
Phase composition (wt %)	2.55	14.24	13.97	69.24
R_B (%)	18.6	16.9	17.3	3.02
Conventional R_p, R_{wp}, R_e (%)	23.4, 15.0, 8.91			
GoF	1.7			

Table S3. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the SFTO (after the first step of calcination at 600 ℃) collected at 700 ℃.

Chemical formula	**SrO**	**$SrCO_3$**	**Fe_3O_4**	**$Sr_3Fe_2TeO_9$**
Space group	*I*4/*mmm* (139)	*Pnma* (62)	*Fd*-3*m* (227)	*I*4/*m* (87)
Molecular weight	103.62	147.63	231.54	646.15
Crystal system	tetragonal	orthorhombic	cubic	tetragonal
Lattice parameters (Å)	*a* = 3.4051 *c* = 6.5241	*a* = 6.2292 *b* = 5.1449 *c* = 8.4919	*a* = 8.3963	*a* = 5.7502 *c* = 8.0764
Cell volume ($Å^3$)	75.65	272.16	591.93	267.04
Calculated density (g/cm^3)	5.252	3.603	5.196	5.628
Data collection range	20 to 80 °			
No. of parameters refined	40			
Average apparent crystallite size (nm)	64.8	65.5	21.6	22.7
Average apparent microstrain ($\times 10^{-4}$)	4.23	4.23	4.23	4.23
Phase composition (wt %)	1.96	10.89	15.66	71.48
R_B (%)	17.5	20.3	20.4	2.97
Conventional R_p, R_{wp}, R_e (%)	25.3, 15.8, 8.74			
GoF	1.8			

Table S4. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the SFTO (after the first step of calcination at 600 ℃) collected at 750 ℃.

Chemical formula	**$SrCO_3$**	**Fe_3O_4**	**$Sr_3Fe_2TeO_9$**
Space group	*Pnma* (62)	*Fd*-3*m* (227)	*I*4/*m* (87)
Molecular weight	147.63	231.54	646.15
Crystal system	orthorhombic	cubic	tetragonal
Lattice parameters (Å)	a = 6.2391 b = 5.1487 c = 8.4965	a = 8.3954	a = 5.8064 c = 8.1341
Cell volume ($Å^3$)	272.94	591.73	274.24
Calculated density (g/cm^3)	3.593	5.198	5.624
Data collection range		20 to 80 °	
No. of parameters refined		33	
Average apparent crystallite size (nm)	88.2	19.1	21.7
Average apparent microstrain ($\times 10^{-4}$)	4.23	4.23	4.23
Phase composition (wt %)	3.84	15.01	81.15
R_B (%)	29.7	31.7	2.97
Conventional R_p, R_{wp}, R_e (%)		28.2, 17.5, 8.39	
GoF		2.1	

Table S5. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the SFTO (after the first step of calcination at 600 ℃) collected at 800 ℃.

Chemical formula	**Fe_3O_4**	**$Sr_3Fe_2TeO_9$**
Space group	*Fd*-3*m* (227)	*I*4/*m* (87)
Molecular weight	231.54	646.15
Crystal system	cubic	tetragonal
Lattice parameters (Å)	a = 8.3922	a = 5.8462 c = 8.1819
Cell volume (Å^3)	591.06	279.64
Calculated density (g/cm^3)	5.204	5.623
Data collection range	20 to 80 °	
No. of parameters refined	18	
Average apparent crystallite size (nm)	18.4	22.7
Average apparent microstrain ($\times 10^{-4}$)	4.23	4.23
Phase composition (wt %)	13.26	86.74
R_B (%)	31.0	3.51
Conventional R_p, R_{wp}, R_e (%)	24.6, 15.7, 7.95	
GoF	1.9	

Table S6. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the SFTO (after the first step of calcination at 600 ℃) collected at 850 ℃.

Chemical formula	**Fe_3O_4**	**Sr_3Fe_2TeO**
Space group	*Fd*-3*m*	*I*4/*m* (87)
Molecular weight	231.54	646.15
Crystal system	cubic	tetragonal
Lattice parameters (Å)	a = 8.4026	a = 5.9036 c = 8.2393
Cell volume (Å^3)	593.24	287.16
Calculated density (g/cm^3)	5.185	5.612
Data collection range	20 to 80 °	
No. of parameters refined	18	
Average apparent crystallite size	19.2	26.2
Average apparent microstrain ($\times 10^{-4}$)	4.23	4.23
Phase composition (wt %)	9.45	90.55
R_B (%)	36.0	2.68
Conventional R_p, R_{wp}, R_e (%)	20.6, 12.7, 7.47	
GoF	1.7	

Table S7. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the SFTO (after the first step of calcination at 600 ℃) collected at 900 ℃.

Chemical formula	**Fe_3O_4**	**Sr_3Fe_2TeO**
Space group	*Fd*-3*m*	*I*4/*m* (87)
Molecular weight	231.54	646.15
Crystal system	cubic	tetragonal
Lattice parameters (Å)	a = 8.4068	a = 5.9612 c = 8.2968
Cell volume (Å^3)	594.15	294.83
Calculated density (g/cm^3)	5.177	5.599
Data collection range	20 to 80 °	
No. of parameters refined	18	
Average apparent crystallite size	21.1	29.0
Average apparent microstrain ($\times 10^{-4}$)	4.23	4.23
Phase composition (wt %)	5.46	94.54
R_B (%)	44.9	3.53
Conventional R_p, R_{wp}, R_e (%)	21.3, 13.3, 7.27	
GoF	1.8	

Table S8. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the BFTO (after the first step of calcination at 600 ℃) collected 600 ℃.

Chemical formula	**$Ba_3Fe_2TeO_9$**	**$BaCO_3$**	**$BaFe_2O_4$**	**Ba_3TeO_6**
Space group	$P6_3/mmc$ (194)	$Pnma$ (62)	$Bb2_1m$ (36)	$I4_1/a$ (88)
Molecular weight	795.27	197.34	313.02	635.58
Crystal system	hexagonal	orthorhombic	orthorhombic	tetragonal
Lattice parameters (Å)	a = 5.8267 c = 14.3257	a = 6.6262 b = 5.3319 c = 8.9245	a = 19.1837 b = 5.3700 c = 8.6215	a = 19.3949 c = 34.6262
Cell volume ($Å^3$)	421.20	315.30	888.16	13025.11
Calculated density (g/cm^3)	12.542	4.157	4.682	6.483
Data collection range	20 to 80 °			
No. of parameters refined	71			
Average apparent crystallite size (nm)	26.2	90.3	16.8	60.4
Average apparent microstrain ($\times 10^{-4}$)	4.23	4.23	4.23	4.23
Phase composition (wt %)	33.40	18.84	44.35	3.41
R_B (%)	5.84	15.0	10.6	14.5
Conventional R_p, R_{wp}, R_e (%)	21.1, 20.3, 9.09			
GoF	2.2			

Table S9. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the BFTO (after the first step of calcination at 600 ℃) collected at 650 ℃.

Chemical formula	**$Ba_3Fe_2TeO_9$**	**$BaCO_3$**	**$BaFe_2O_4$**	**Ba_3TeO_6**
Space group	$P6_3/mmc$ (194)	$Pnma$ (62)	$Bb2_1m$ (36)	$I4_1/a$ (88)
Molecular weight	795.27	197.34	313.02	635.58
Crystal system	hexagonal	orthorhombic	orthorhombic	tetragonal
Lattice parameters (Å)	a = 5.8267 c = 14.3257	a = 6.6262 b = 5.3319 c = 8.9245	a = 19.1838 b = 5.3699 c = 8.6217	a = 19.3950 c = 34.6262
Cell volume ($Å^3$)	421.20	315.30	888.17	13025.16
Calculated density (g/cm^3)	12.542	4.157	4.682	6.483
Data collection range	20 to 80 °			
No. of parameters refined	71			
Average apparent crystallite size (nm)	24.8	101.2	17.2	57.5
Average apparent microstrain ($\times 10^{-4}$)	4.23	4.23	4.23	4.23
Phase composition (wt %)	33.79	14.11	48.23	3.87
R_B (%)	5.87	16.1	11.1	16.4
Conventional R_p, R_{wp}, R_e (%)	22.5, 21.2, 9.20			
GoF	2.3			

Table S10. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the BFTO (after the first step of calcination at 600 ℃) collected at 700 ℃.

Chemical formula	**$Ba_3Fe_2TeO_9$**	**$BaCO_3$**	**$BaFe_2O_4$**	**Ba_3TeO_6**
Space group	$P6_3/mmc$ (194)	$Pnma$ (62)	$Bb2_1m$ (36)	$I4_1/a$ (88)
Molecular weight	795.27	197.34	313.02	635.58
Crystal system	hexagonal	orthorhombic	orthorhombic	tetragonal
Lattice parameters (Å)	a = 5.8304 c = 14.3305	a = 6.6489 b = 5.3331 c = 8.9275	a = 19.1929 b = 5.3806 c = 8.6208	a = 19.4347 c = 34.6590
Cell volume ($Å^3$)	421.88	316.56	890.26	13091.00
Calculated density (g/cm^3)	12.522	4.141	4.671	6.450
Data collection range	20 to 80 °			
No. of parameters refined	71			
Average apparent crystallite size (nm)	22.6	85.6	20.2	33.4
Average apparent microstrain ($\times 10^{-4}$)	4.23	4.23	4.23	4.23
Phase composition (wt %)	38.93	10.28	44.26	6.53
R_B (%)	5.59	18.6	12.1	14.7
Conventional R_p, R_{wp}, R_e (%)	22.9, 21.7, 9.23			
GoF	2.3			

Table S11. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the BFTO (after the first step of calcination at 600 ℃) collected at 750 ℃.

Chemical formula	**$Ba_3Fe_2TeO_9$**	**$BaCO_3$**	**$BaFe_2O_4$**	**Ba_3TeO_6**
Space group	$P6_3/mmc$ (194)	$Pnma$ (62)	$Bb2_1m$ (36)	$I4_1/a$ (88)
Molecular weight	795.27	197.34	313.02	635.58
Crystal system	hexagonal	orthorhombic	orthorhombic	tetragonal
Lattice parameters (Å)	a = 5.8363 c = 14.3439	a = 6.6760 b = 5.3390 c = 8.9336	a = 19.1942 b = 5.4015 c = 8.6121	a = 19.6117 c = 34.6257
Cell volume (Å^3)	423.13	318.42	892.89	13317.63
Calculated density (g/cm^3)	12.485	4.117	4.657	6.340
Data collection range	20 to 80 °			
No. of parameters refined	71			
Average apparent crystallite size (nm)	20.1	65.0	25.6	29.7
Average apparent microstrain ($\times10^{-4}$)	4.23	4.23	4.23	4.23
Phase composition (wt %)	49.95	5.32	34.96	9.77
R_B (%)	5.91	23.1	12.5	14.7
Conventional R_p, R_{wp}, R_e (%)	22.2, 20.7, 9.21			
GoF	2.2			

Table S12. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the BFTO (after the first step of calcination at 600 ℃) collected at 800 ℃.

Chemical formula	**$Ba_3Fe_2TeO_9$**	**$BaCO_3$**	**$BaFe_2O_4$**	**Ba_3TeO_6**
Space group	*P*6$_3$/*mmc* (194)	*Pnma* (62)	*Bb*2$_1$*m* (36)	*I*4$_1$/*a* (88)
Molecular weight	795.27	197.34	313.02	635.58
Crystal system	hexagonal	orthorhombic	orthorhombic	tetragonal
Lattice parameters (Å)	*a* = 5.8440 *c* = 14.3705	*a* = 6.8221 *b* = 5.3747 *c* = 8.7994	*a* = 19.2088 *b* = 5.4216 *c* = 8.6328	*a* = 19.6847 c = 35.0259
Cell volume (Å^3)	425.03	322.64	899.04	13572.02
Calculated density (g/cm^3)	12.429	4.063	4.626	6.222
Data collection range	20 to 80 °			
No. of parameters refined	70			
Average apparent crystallite size (nm)	19.7	18.6	19.3	38.9
Average apparent microstrain (×10^{-4})	4.23	4.23	4.23	4.23
Phase composition (wt %)	58.80	3.42	27.08	10.70
R_B (%)	5.14	21.7	15.0	14.7
Conventional R_p, R_{wp}, R_e (%)	19.6, 18.5, 8.65			
GoF	2.1			

Table S13. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the BFTO (after the first step of calcination at 600 ℃) collected at 850 ℃.

Chemical formula	**$Ba_3Fe_2TeO_9$**	**$BaFe_2O_4$**	**Ba_3TeO_6**
Space group	$P6_3/mmc$ (194)	$Bb2_1m$ (36)	$I4_1/a$ (88)
Molecular weight	795.27	313.02	635.58
Crystal system	hexagonal	orthorhombic	tetragonal
Lattice parameters (Å)	a = 5.8443 c = 14.3755	a = 19.1754 b = 5.4273 c = 8.6423	a = 19.6907 c = 35.0747
Cell volume ($Å^3$)	425.23	899.40	13599.34
Calculated density (g/cm^3)	12.423	4.624	6.209
Data collection range		20 to 80 °	
No. of parameters refined		56	
Average apparent crystallite size (nm)	26.0	18.9	53.6
Average apparent microstrain ($\times 10^{-4}$)	4.23	4.23	4.23
Phase composition (wt %)	67.43	21.92	10.65
R_B (%)	4.62	14.5	14.5
Conventional R_p, R_{wp}, R_e (%)		17.8, 16.0, 8.4	
GoF		1.9	

Table S14. Crystallographic data and refinement parameters obtained from the temperature-dependent X-ray powder diffraction for the BFTO (after the first step of calcination at 600 ℃) collected at 900 ℃.

Chemical formula	**$Ba_3Fe_2TeO_9$**	**$BaFe_2O_4$**	**Ba_3TeO_6**
Space group	$P6_3/mmc$ (194)	$Bb2_1m$ (36)	$I4_1/a$ (88)
Molecular weight	795.27	313.02	635.58
Crystal system	hexagonal	orthorhombic	tetragonal
Lattice parameters (Å)	a = 5.8438 c = 14.3804	a = 18.9789 b = 5.4376 c = 8.6923	a = 19.6799 c = 35.0307
Cell volume ($Å^3$)	425.30	897.04	13567.35
Calculated density (g/cm^3)	12.422	4.636	6.224
Data collection range		20 to 80 °	
No. of parameters refined		56	
Average apparent crystallite size (nm)	35.2	34.9	80.8
Average apparent microstrain ($\times 10^{-4}$)	4.23	4.23	4.23
Phase composition (wt %)	78.92	14.46	6.62
R_B (%)	4.38	16.5	15.9
Conventional R_p, R_{wp}, R_e (%)		15.5, 13.0, 8.1	
GoF		1.6	

Table S15. Phase composition obtained from the Rietveld refinement of PXRD data of BFTO collected from 600 °C to 900 °C after the first step of calcination (600 °C, 2 °C/min, 8 h).

Phase (wt.%) / Temp. (°C)	$BaFe_2O_4$	$BaCO_3$	Ba_3TeO_6	$Ba_3Fe_2TeO_9$
600	44.4(14)	18.8(4)	3.4(1)	33.4(6)
650	48.2(17)	14.1(4)	3.9(1)	33.8(7)
700	44.3(15)	10.3(4)	6.5(2)	38.9(7)
750	35.0(12)	5.3(3)	9.8(3)	49.9(8)
800	27.1(12)	3.4(4)	10.7(2)	58.8(9)
850	21.9(9)	-	10.7(2)	67.4(8)
900	14.5(6)	-	6.6(1)	78.9(7)

Table S16. Phase composition obtained from Rietveld refinement of PXRD data of SFTO collected from 600 °C to 900 °C after the first step of calcination (600 °C, 2 °C/min, 8 h).

Phase (wt.%) / Temp. (°C)	SrO	$SrCO_3$	Fe_3O_4	$Sr_3Fe_2TeO_9$
600	2.9(1)	16.0(4)	13.5(8)	67.7(8)
650	2.6(1)	14.2(4)	14.0(8)	69.2(8)
700	1.9(1)	10.9(4)	15.7(9)	71.5(8)
750	-	3.8(4)	15.0(4)	81.2(8)
800	-	-	13.3(4)	86.7(7)
850	-	-	9.5(3)	90.5(6)
900	-	-	5.5(3)	94.5(6)

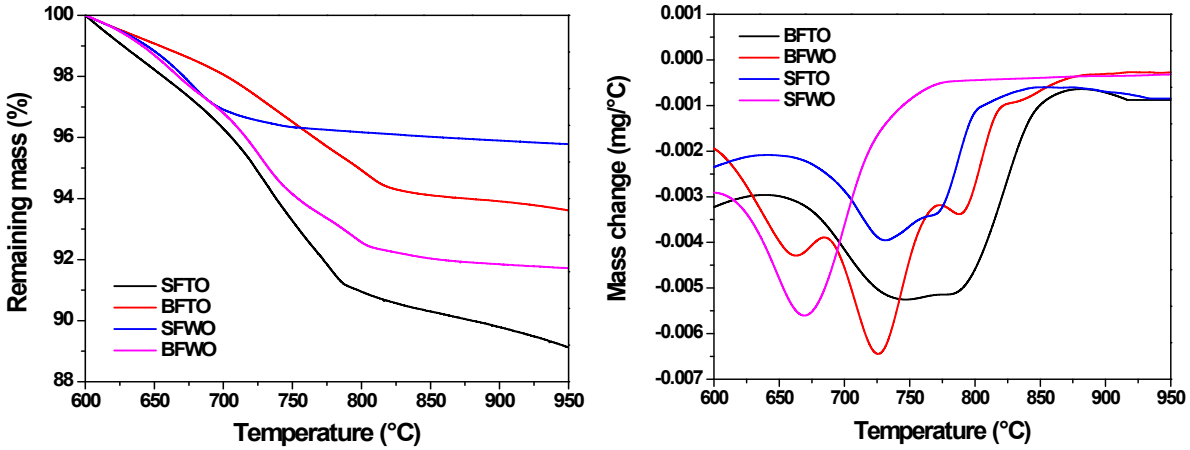

Figure S3. TGA (left) and DTG (right) curves of SFTO, BFTO, SFWO, and BFWO compounds recorded after the first step of calcination at 600°C.

Table S17. Parameters obtained from the Rietveld refinement of PXRD patterns for $Sr_3Fe_2TeO_9$, $Ba_3Fe_2TeO_9$, $Sr_3Fe_2WO_9$ and $Ba_3Fe_2WO_9$ compounds collected at room temperature and ambient pressure.

Chemical formula	**$Sr_3Fe_2TeO_9$**	**$Ba_3Fe_2TeO_9$**	**$Sr_3Fe_2WO_9$**	**$Ba_3Fe_2WO_9$**
Space group	*I*4/*m* (87)	*P*6$_3$/*mmc* (194)	*I*4/*m* (87)	*P*6$_3$/*mmc* (194)
Molecular weight	646.15	795.271	702.38	851.51
Z	4	2	4	2
Crystal system	tetragonal	hexagonal	tetragonal	hexagonal
Lattice parameters (Å)	*a* = 5.5712(3) *c* = 7.9026(3)	*a* = 5.7691(2) *c* = 14.2056(2)	*a* = 5.5726(2) *c* = 7.9038(1)	*a* = 5.7757(2) *c* = 14.1415(7)
Unit cell volume (Å^3)	245.284(2)	409.453(2)	245.4412(4)	408.543(2)
Calculated density (g/cm^3)	13.255	12.902	6.274	6.923
Data collection range	10 – 100°			
No. of refined parameters	19	23	16	31
Average apparent crystallite size (nm)	37.1	51.4	35.8	31.8
Average apparent microstrain (×10^{-4})	30.85	10.56	15.72	4.23
R_B (%)	4.67	9.38	3.58	3.99
R_p, R_{wp}, R_e (%)	12.5, 9.72, 6.39	20.7, 16.4, 9.35	14.2, 15.2, 10.5	16.1, 12.3, 9.66
GoF	1.5	1.7	1.4	1.2

Table S18. Structural parameters for $Sr_3Fe_2TeO_9$ extracted at room temperature (292 K). The refined occupancies are expressed in terms of the ratio m/M: site multiplicity/multiplicity of a general position (48).

Atom	**Wyckoff position**	***x***	***y***	***z***	**Occupancy**
Sr	4*d*	0	1/2	1/4	0.25000

Fe1	2*a*	0	0	0	0.07125
Fe2	2*b*	0	0	1/2	0.11250
Te1	2*a*	0	0	0	0.05375
Te2	2*b*	0	0	1/2	0.01250
O1	4*e*	0	0	0.24368(6)	0.25000
O2	8*h*	0.27788(9)	0.22927(1)	0	0.50000

Table S19. Structural parameters for $Ba_3Fe_2TeO_9$ extracted at room temperature (292 K). The refined occupancies are expressed in terms of the ratio m/M: site multiplicity/multiplicity of a general position (24).

Atom	Wyckoff position	*x*	*y*	*z*	Occupancy
Ba1	2*b*	0	0	1/4	0.08333
Ba2	4*f*	1/3	2/3	0.09299(1)	0.16667
Fe1	2*a*	0	0	0	0.08333
Te	4*f*	1/3	2/3	0.84625(1)	0.08333
Fe2	4*f*	1/3	2/3	0.84625(1)	0.08333
O1	6*h*	0.50480(2)	0.00960(8)	1/4	0.25000
O2	24*l*	0.84200(6)	0.68380(1)	0.07760(4)	0.50000

Table S20. Structural parameters for $Sr_3Fe_2WO_9$ extracted at room temperature (292 K). The refined occupancies are expressed in terms of the ratio m/M: site multiplicity/multiplicity of a general position (48).

Atom	Wyckoff position	*x*	*y*	*z*	Occupancy
Sr1	4*d*	0	1/2	1/4	0.25
Fe1	2*a*	0	0	0	0.09716
W1	2*a*	0	0	0	0.02784
Fe2	2*b*	0	0	1/2	0.07401
W2	2*b*	0	0	1/2	0.05099
O1	8*h*	0.26987	0. 22183	0	0.5
O2	4*e*	0	0	0.24498	0.25

Table S21. Structural parameters for $Ba_3Fe_2WO_9$ extracted at room temperature (292 K). The refined occupancies are expressed in terms of the ratio m/M: site multiplicity/multiplicity of a general position (24).

Atom	Wyckoff position	*x*	*y*	*z*	Occupancy
Ba1	2*b*	0	0	1/4	0.08333
Ba2	4*f*	1/3	2/3	0.094(5)	0.16667
Fe1	4*f*	1/3	2/3	0.846(5)	0.0954
W1	4*f*	1/3	2/3	0.846(5)	0.0713

Fe2	2*a*	0	0	0	0.0713
W2	2*a*	0	0	0	0.0121
O1	6*h*	0.482(1)	0.019(7)	1/4	0.25
O2	4*e*	0.830(4)	0.661(8)	0.082(2)	0.50

Table S22. Crystallographic data and refinement parameters of byphase $BaWO_4$ obtained from the X-ray diffraction pattern of BFWO powder collected at room temperature.

Chemical formula:	**$BaWO_4$**
Space group	$I4_1/a$
Molecular weight	385.17
Z	4
Crystal system	tetragonal
Lattice parameters (Å)	a = 5.6188(2)
	c = 12.7931(8)
Unit cell volume (Å^3)	403.891(2)
Calculated density (g/cm^3)	6.335
Average apparent crystallite size (nm)	36.8
Average apparent microstrain ($\times 10^{-4}$)	22.8
R_B (%)	11.1

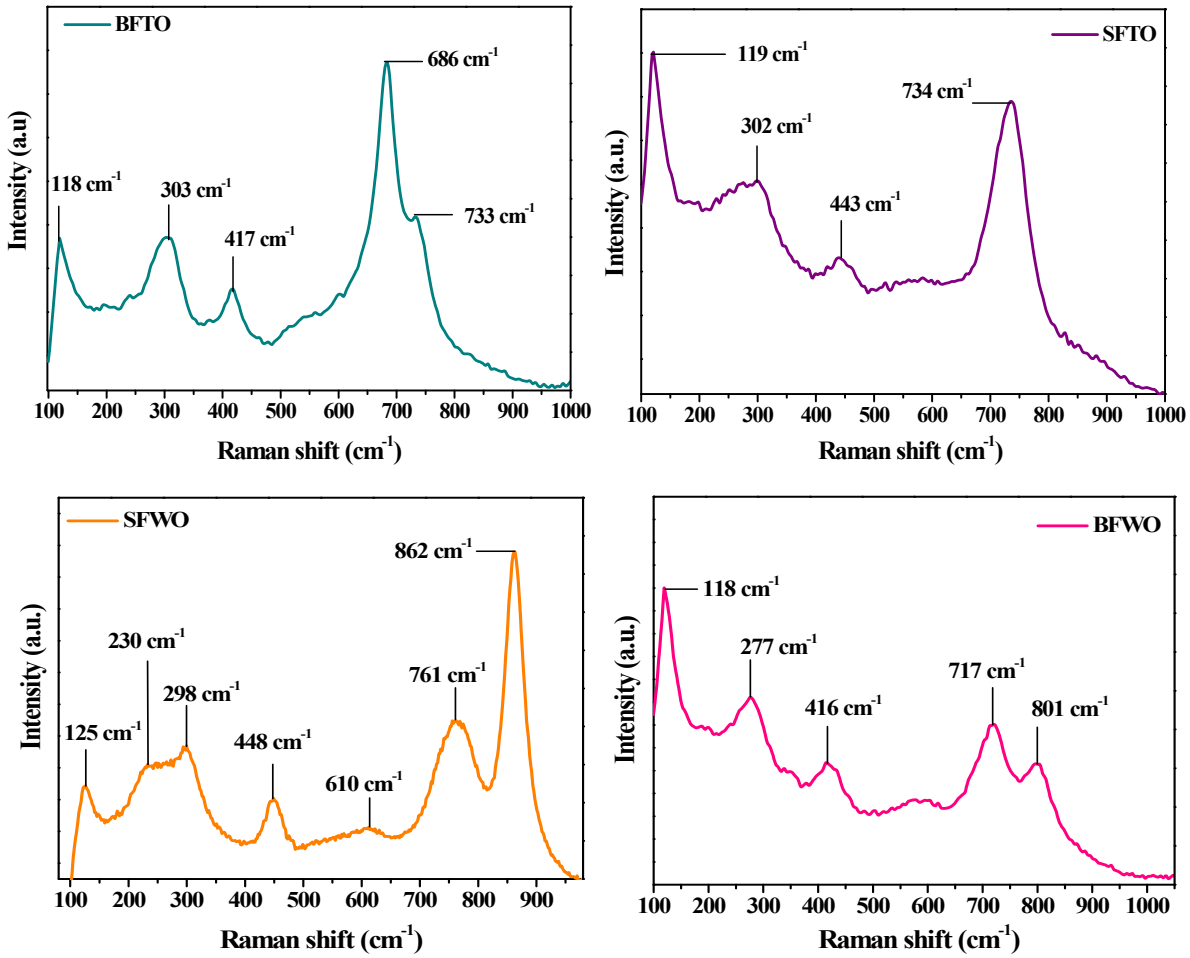

Figure S4. Raman spectra of synthesized compounds BFTO, SFTO, SFWO, and BFWO.

Table S23. Assigned Raman modes for synthesized compounds: BFTO, SFTO, SFWO and BFWO.

Compound	Raman shift (cm^{-1})	Assignation
$Ba_3Fe_2WO_9$	118	T-translational
	277	L-librational
	416	ν_2
	717	ν_1
	801	
$Sr_3Fe_2WO_9$	125	T-translational
	230	L-librational
	298	
	448	ν_5
	610	ν_2
	761	ν_1
	862	
$Sr_3Fe_2TeO_9$	119	T-translational
	302	L-librational
	443	ν_5
	734	ν_1
$Ba_3Fe_2TeO_9$	118	T-translational
	303	L-librational
	417	ν_2
	686	ν_1
	733	

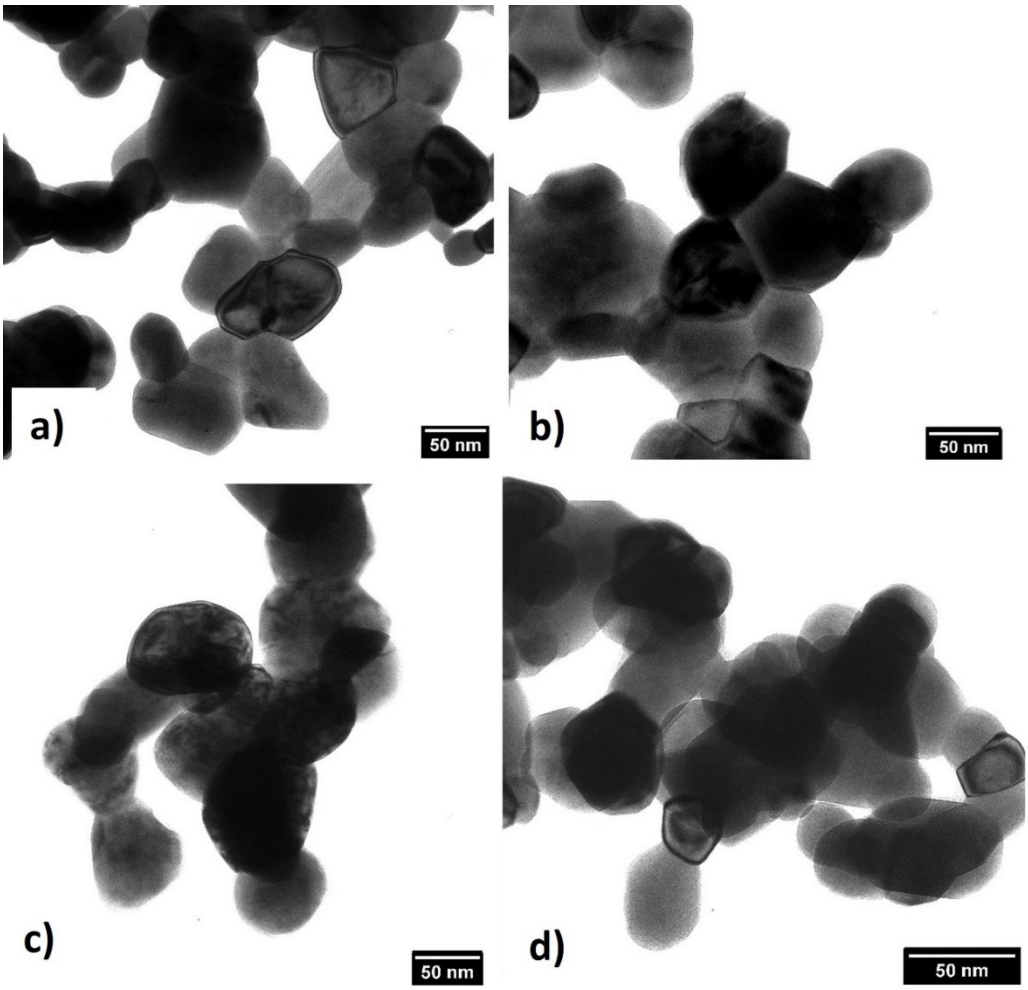

Figure S5. TEM images of a) BFTO, b) BFWO, c) SFTO and d) SFWO powders.

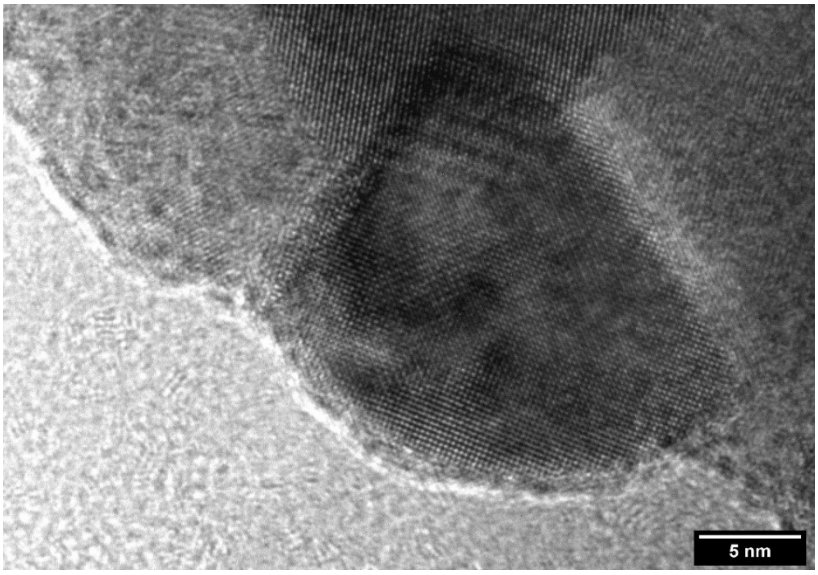

Figure S6. Selected HRTEM image of SFWO powder.

Table S24. Results of the quantitative EDX analysis of SFWO, BFWO, SFTO and BFTO pellets.

Compound	Elements	*α* series	Energy (eV)	Atomic percent (at. %)	Nominal chemical composition (at. %)
$Sr_3Fe_2WO_9$	Sr	K	14.1	22.3	20
	Fe	K	6.4	15.0	13.3
	W	L	8.4	7.1	6.7
	O	K	0.5	55.6	60
$Ba_3Fe_2WO_9$	Ba	L	4.5	22.8	20
	Fe	K	6.4	14.5	13.3
	W	L	8.4	7.2	6.7
	O	K	0.5	55.6	60
$Sr_3Fe_2TeO_9$	Sr	K	14.1	21.8	20
	Fe	K	6.4	14.9	13.3
	Te	L	3.8	6.8	6.7
	O	K	0.5	56.5	60
$Ba_3Fe_2TeO_9$	Ba	L	4.5	23.5	20
	Fe	K	6.4	14.7	13.3
	Te	L	3.8	7.2	6.7
	O	K	0.5	54.7	60

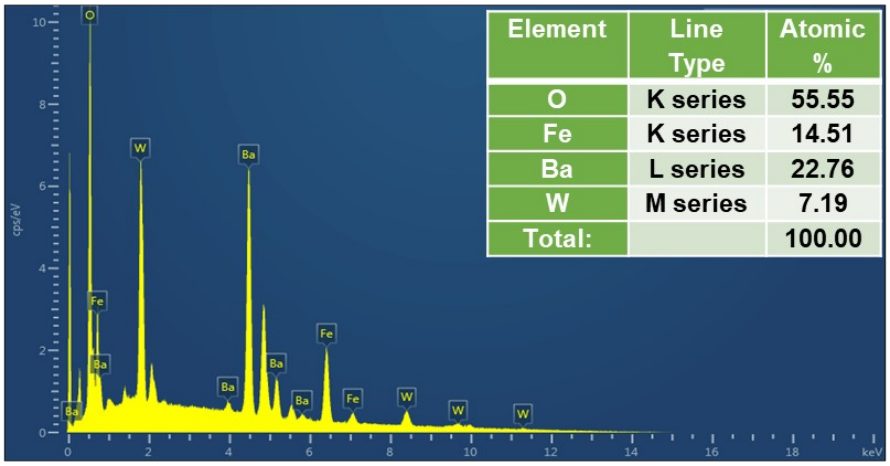

Figure S7. EDX spectrum of BFWO pellet.

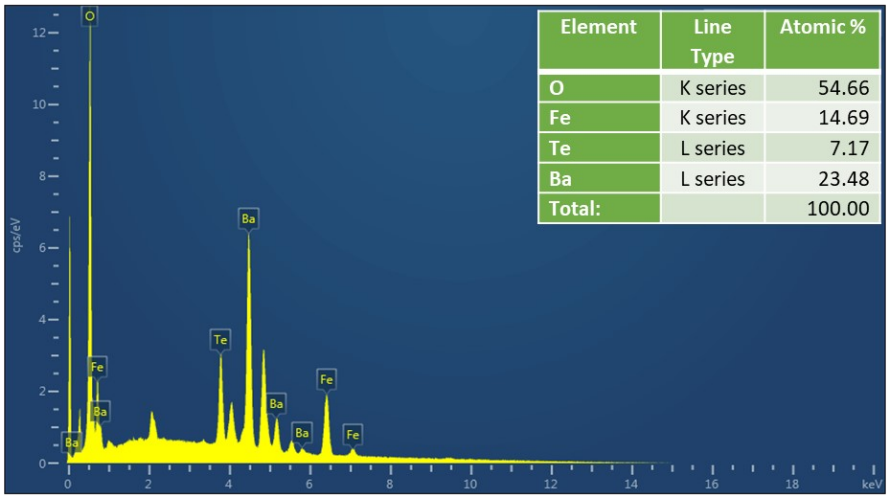

Figure S8. EDX spectrum of BFTO pellet.

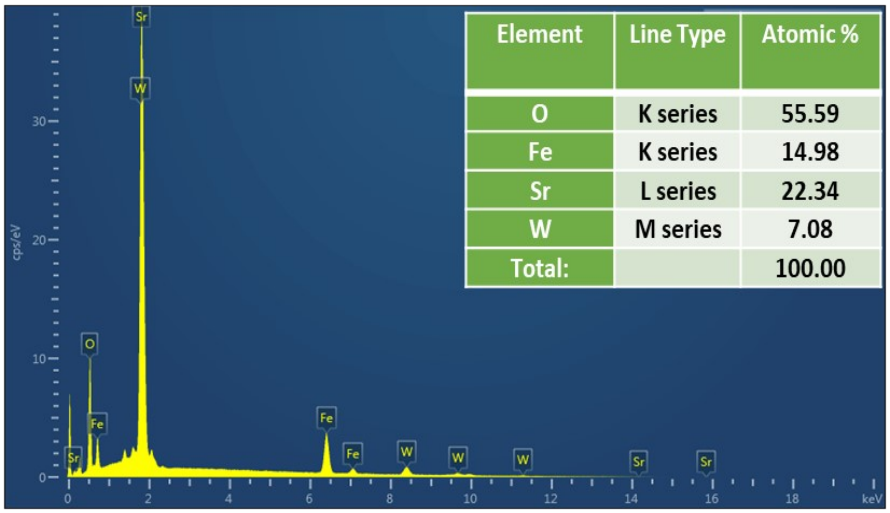

Figure S9. EDX spectrum of SFWO pellet.

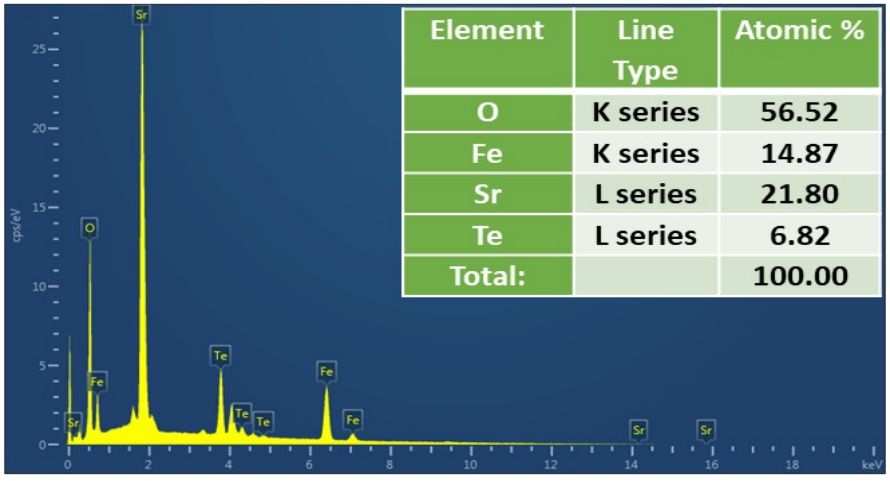

Figure S10. EDX spectrum of SFTO pellet.

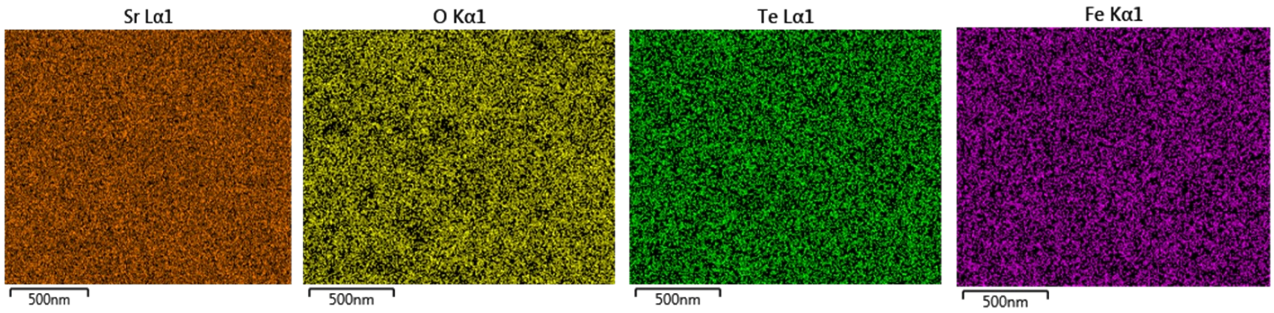

Figure S11. Qualitative elemental maps of SFTO pellet.

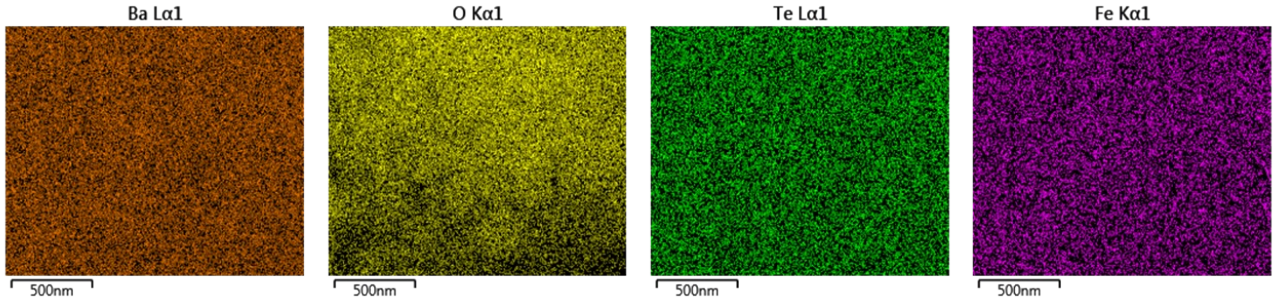

Figure S12. Qualitative elemental maps of BFTO pellet.

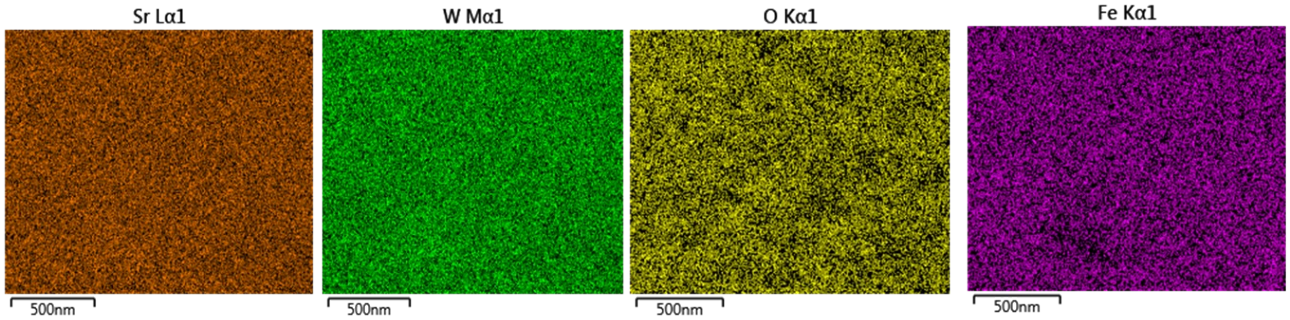

Figure S13. Qualitative elemental maps of SFWO pellet.

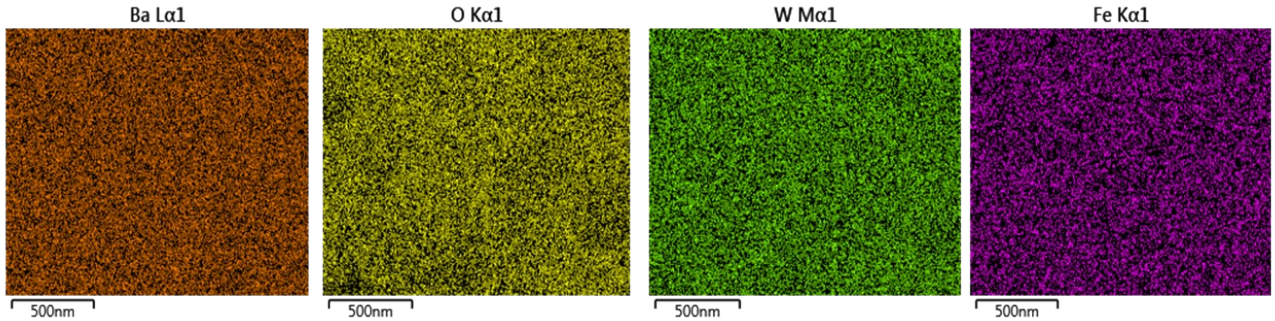

Figure S14. Qualitative elemental maps of BFWO pellet.

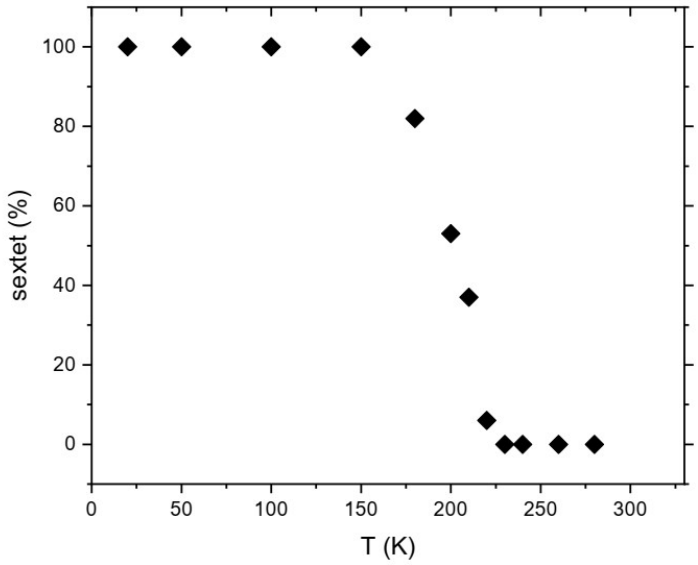

Figure S15. Temperature dependence of the magnetic contributions (sextets) in Mössbauer spectra of BFWO.

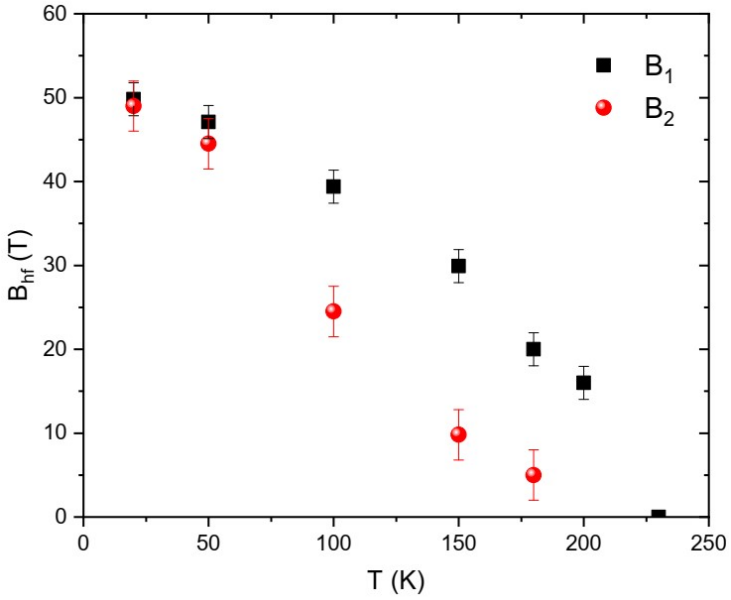

Figure S16. Temperature dependence of the mean magnetic hyperfine fields B_1 and B_2 of the two magnetic patterns in BFWO.

Table S25. The essential characteristics of Mössbauer spectra of synthesized compounds.

Sample	*T* (K)	Type of spectrum	Relative area (%)	Center shift (mm/s)	Quadrupole splitting (mm/s)	Mean magnetic hyperfine field B_{hf} (T)	Gaussian width of B_{hf} (T)	Lorentzian width (mm/s)
BFWO	20	sextet	60(2)	0.48(1)	0.20(2)	49.8(1)	1.3(1)	0.54(5)
	20	sextet	40(29	0.48(1)	0.00(2)	49.0(1)	1.7(1)	0.54(5)
	300	doublet	78(2)	0.37(1)	0.61(1)			0.42(2)
		doublet	22(2)	0.40(1)	1.06(1)			0.42(2)
SFWO	20	sextet	50(2)	0.40(2)	0.21(1)	51.4(1)	2.5(1)	0.25(5)
		sextet	44(2)	0.53(2)	-0.22(1)	52.0(1)	2.0(1)	0.25(5)
		sextet	6(2)	0.33(2)	0.19(2)	25.5(1)	1.6(1)	0.25(5)
	300	sextet	63(2)	0.35(1)	-0.02(2)	31.6(1)	4.4(2)	0.66(5)
		sextet	37(2)	0.36(1)	0.18(2)	14.4(2)	10(1)	0.46(5)
BFTO	20	sextet	42(2)	0.47(1)	0.53(2)	51.4(2)	1.5(1)	0.27(3)
		sextet	33(2)	0.46(1)	0.25(2)	46.4(2)	3.5(1)	0.43(5)
		sextet	13(2)	0.47(1)	0.26(2)	19.0(2)	10(1)	0.27(5)
		sextet	12(2)	0.48(1)	-0.12(2)	50.1(2)	0.0(2)	0.43(2)
	300	sextet	43(4)	0.36(2)	0.9(1)	22(1)	10(1)	0.40(5)
		doublet	30(4)	0.36(2)	0.52(2)			0.40(2)
		doublet	26(4)	0.37(2)	1.17(2)			0.40(2)
SFTO	20	sextet	46(2)	0.48(1)	0.01(2)	49.1(2)	2.6(1)	0.50(2)
		sextet	42(2)	0.48(1)	0.02(2)	52.5(2)	1.2(1)	0.50(2)
		sextet	12(2)	0.48(1)	0.09(2)	23.1(2)	4.3(2)	0.50(2)
	300	sextet	11(4)	0.35(2)	0.27(2)	42.0(2)	2.0(1)	0.47(5)
		doublet	48(4)	0.23(1)	0.51(1)			0.62(4)
		doublet	41(4)	0.38	1.14(1)			0.52(3)

Table S26. Optical band gap values for $Sr_3Fe_2WO_9$, $Sr_3Fe_2TeO_9$, $Ba_3Fe_2WO_9$ and $Ba_3Fe_2TeO_9$.

Compound	Indirect bandgap (eV)	Direct band gap (eV)
$Sr_3Fe_2TeO_9$	1.97	2.45
$Ba_3Fe_2TeO_9$	2.02	2.74
$Sr_3Fe_2WO_9$	1.88	2.53
$Ba_3Fe_2WO_9$	1.61	2.36

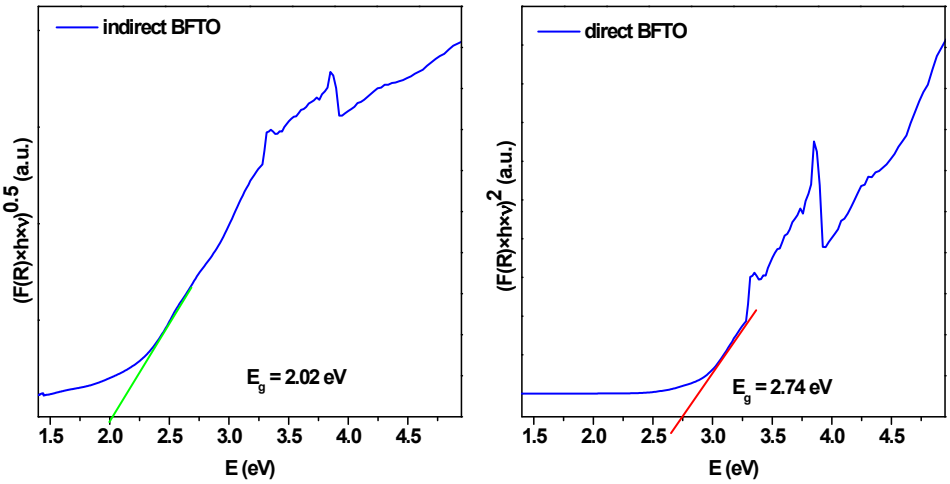

Figure S17. Tauc plot for direct and indirect band gap estimation of BFTO powder.

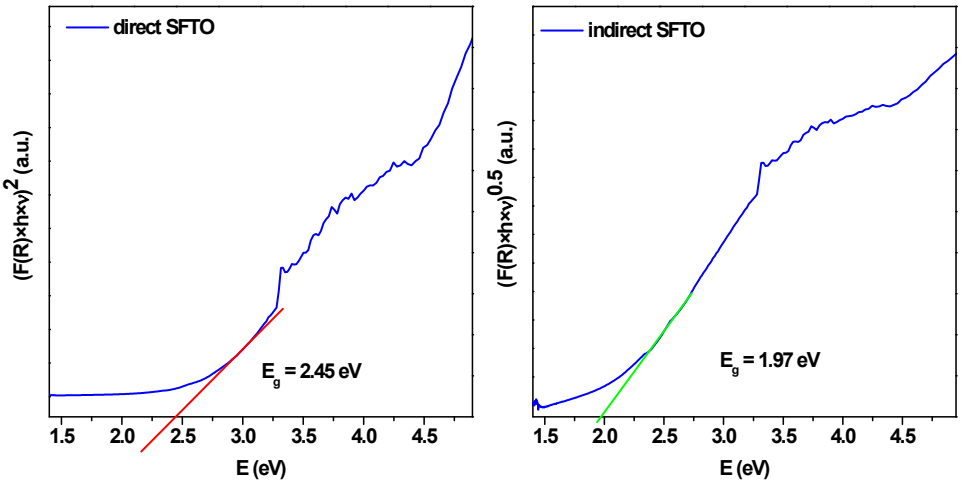

Figure S18. Tauc plot for direct and indirect band gap estimation of SFTO powder.

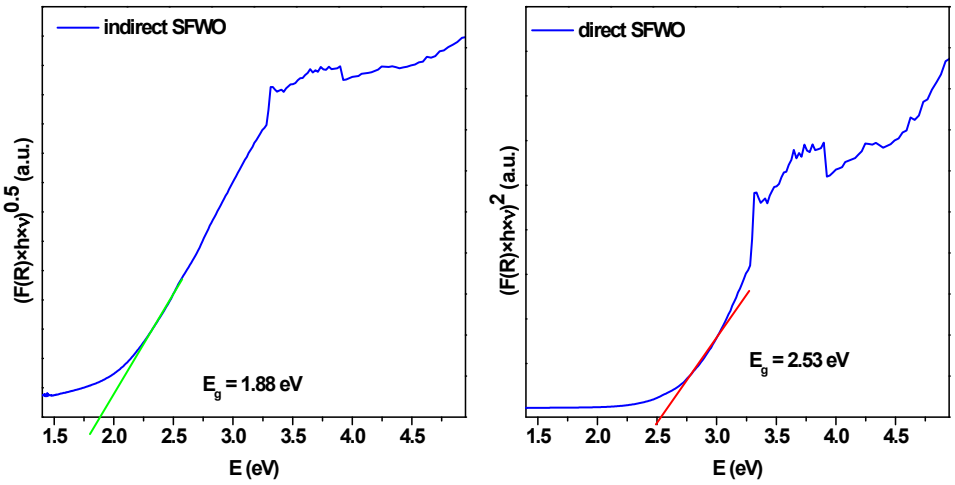

Figure S19. Tauc plot for direct and indirect band gap estimation of SFWO powder.

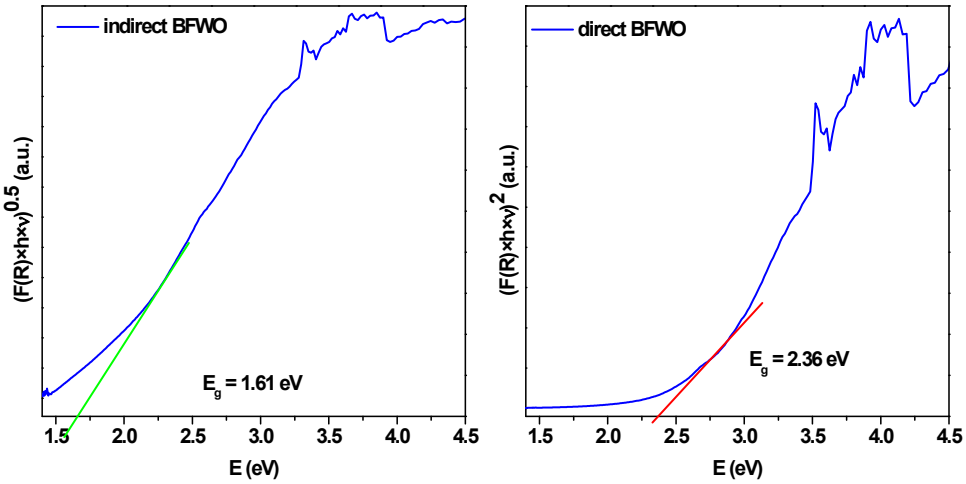

Figure S20. Tauc plot for direct and indirect band gap estimation of BFWO powder.

Table S27. Parameters obtained from the Rietveld refinement of XRD patterns for $Sr_3Fe_2TeO_9$, $Ba_3Fe_2TeO_9$, $Sr_3Fe_2WO_9$ and $Ba_3Fe_2WO_9$ pellets collected at room temperature and ambient pressure.

Chemical formula:	**$Sr_3Fe_2TeO_9$**	**$Ba_3Fe_2TeO_9$**	**$Sr_3Fe_2WO_9$**	**$Ba_3Fe_2WO_9$**
Space group	*I*4/*m* (87)	*P*6$_3$/*mmc* (194)	*I*4/*m* (87)	*P*6$_3$/*mmc* (194)
Molecular weight	646.15	795.271	702.38	851.51
Z	4	2	4	2
Crystal system	tetragonal	hexagonal	tetragonal	hexagonal
Lattice parameters (Å)	*a* = 5.5770(2) *c* = 7.8870(1)	*a* = 5.7682(2) *c* = 14.2097(7)	*a* = 5.5648(2) *c* = 7.8685(1)	*a* = 5.7471(2) *c* = 14.0842(7)
Unit cell volume (Å^3)	245.3064(4)	409.4449(2)	243.6624(4)	402.873(2)
Calculated density (g/cm^3)	13.254	12.902	6.383	7.020
Data collection range	10 – 80°			
No. of refined parameters	17	21	18	21
Average apparent crystallite size (nm)	45.2	53.6	40.2	44.0
Average apparent microstrain (×10^{-4})	22.42	16.81	22.61	21.72
R_B (%)	4.78	7.79	3.46	8.04
R_p, R_{wp}, R_e (%)	25.0, 18.4, 9.7	21.8, 16.8, 13.1	25.6, 18.8, 9.12	26.2, 23.3, 11.8
GoF	1.9	1.3	2.1	2.0

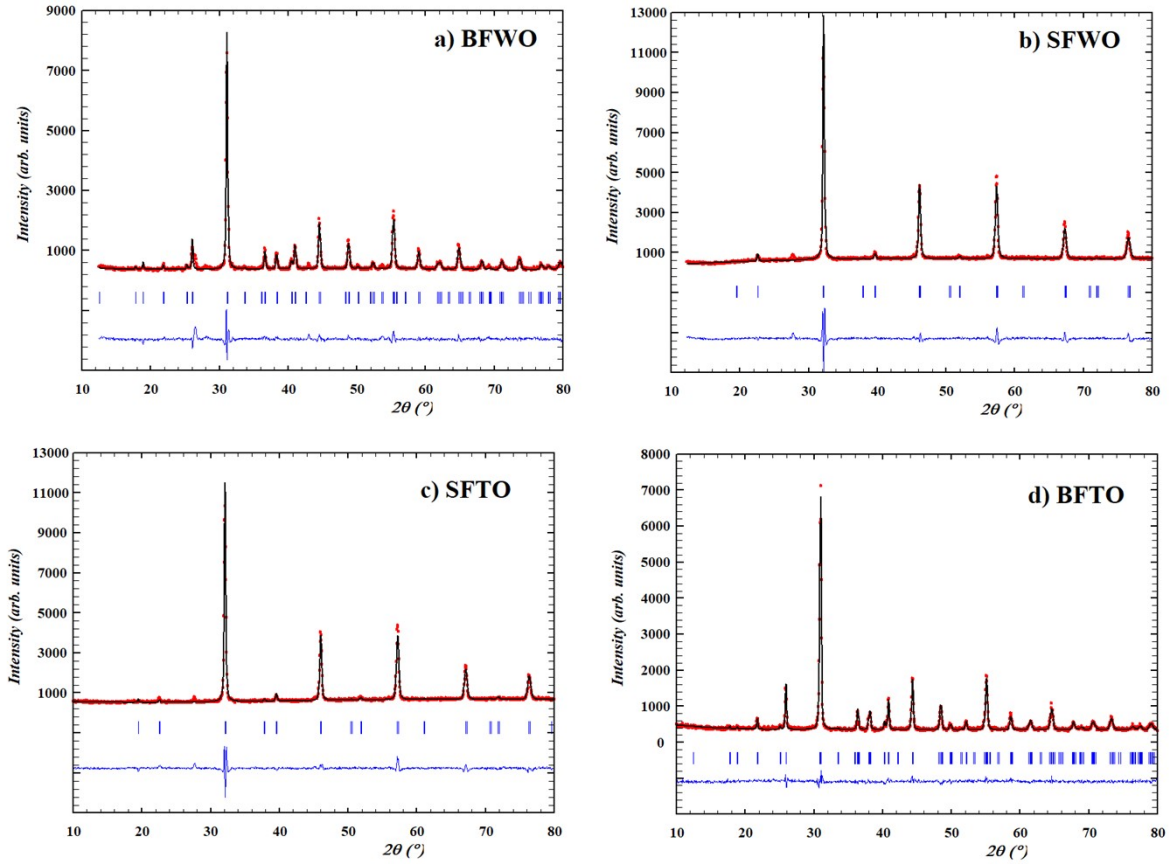

Figure S21. Rietveld plots of refined X-ray diffraction patterns of BFWO (a), SFWO (b), SFTO (c) and BFTO (d) pellets collected at room temperature and ambient pressure: experimental (red), calculated (black), difference (blue).