Sample no. 1

The powder diffraction data of sample no. 1 for Rietveld analysis was collected at room temperature with a Haoyuan DX-2700BH powder diffractometer (Cu-Kα radiation) and linear detector. The step size of 2θ was 0.01°, and the counting time was 20 sec per 1 deg. All peaks were indexed by cubic cell ($Ia\bar{3}$) with parameters close to Mn_2O_3. Therefore this structure was taken as starting model for Rietveld refinement which was performed using TOPAS 4.2 [1]. Refinement was stable and gave low R-factors (Table 1, Figure 1). Coordinates of atoms and main bond lengths are in Table 2 and Table 3 respectively.

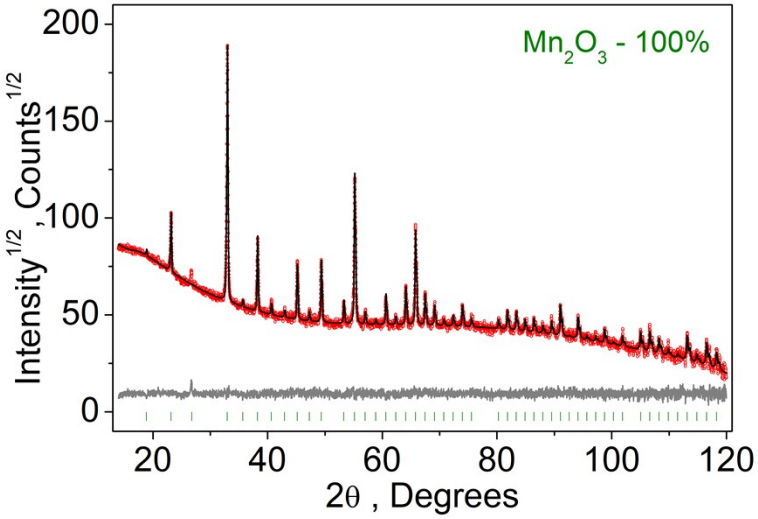

Figure 1. Difference Rietveld plot of Mn_2O_3

Table 1. Main parameters of processing and refinement

Compound	Mn_2O_3
Sp. Gr.	$Ia\bar{3}$
a (Å)	9.41169(23)
V (Å^3)	833.686(61)
Z	16
2θ-interval, º	0-0
R_{wp} ,%	4.69
R_p ,%	3.33

χ^2	2.42
R_B ,%	1.24

Table 2. Fractional atomic coordinates and isotropic displacement parameters (Å^2)

Atom	*x*	*y*	*z*	B_{iso}	*Occ.*
Mn1	0.25	0.25	0.25	0.829(63)	1
Mn2	0.965187(98)	0	0.25	1.008(56)	1
O1	0.38463(38)	1/6	0.39055(35)	0.529(88)	1

Table 3. Main bond lengths (Å)

Mn1—O1^{i}	1.9926(27)	Mn1—O1^{ii}	1.9926(25)
Mn1—O1^{iii}	1.9926(31)	Mn1—O1^{iv}	1.9926(31)
Mn1—O1^{v}	1.9926(25)	Mn1—O1^{vi}	1.9926(27)
Mn2—O1^{vii}	2.0510(30)	Mn2—O1^{viii}	1.9072(29)
Mn2—O1^{ix}	2.1875(23)	Mn2—O1^{x}	2.0510(30)
Mn2—O1^{xi}	1.9072(29)	Mn2—O1^{xii}	2.1875(23)

Symmetry codes: (i) z, x, y; (ii) y, z, x; (iii) x, y, z; (iv) -x+1/2, -y+1/2, -z+1/2; (v) -y+1/2, -z+1/2, -x+1/2; (vi) -z+1/2, -x+1/2, -y+1/2; (vii) -y+1, z+1/2, -x+1/2; (viii) -z+3/2, x+1/2, y; (ix) x+1/2, y, -z+1/2; (x) -y+1, -z+1/2, x; (xi) -z+3/2, -x+1/2, -y+1/2; (xii) x+1/2, -y, z;

References

[1] Bruker AXS TOPAS V4: General profile and structure analysis software for powder diffraction data. – User's Manual. Bruker AXS, Karlsruhe, Germany. 2008.

Sample no. 3

The powder diffraction data of sample no. 3 forRietveld analysis was collected at room temperature with a Haoyuan DX-2700BH powder diffractometer (Cu-Kα radiation) and linear detector. The step size of 2θ was 0.01°, and the counting time was 20 sec per 1 deg. All peaks, besides impurity peaks of Mn_2O_3 and Pt, were indexed by orthorhombic cell with parameters close to Fe_2MnO_4. Therefore these structures were taken as starting model for Rietveld refinement which was performed using TOPAS 4.2 [1]. Refinement was stable and gave low R-factors (Table 1, Figure 1). Coordinates of atoms and main bond lengths are in Table 2 and Table 3 respectively.

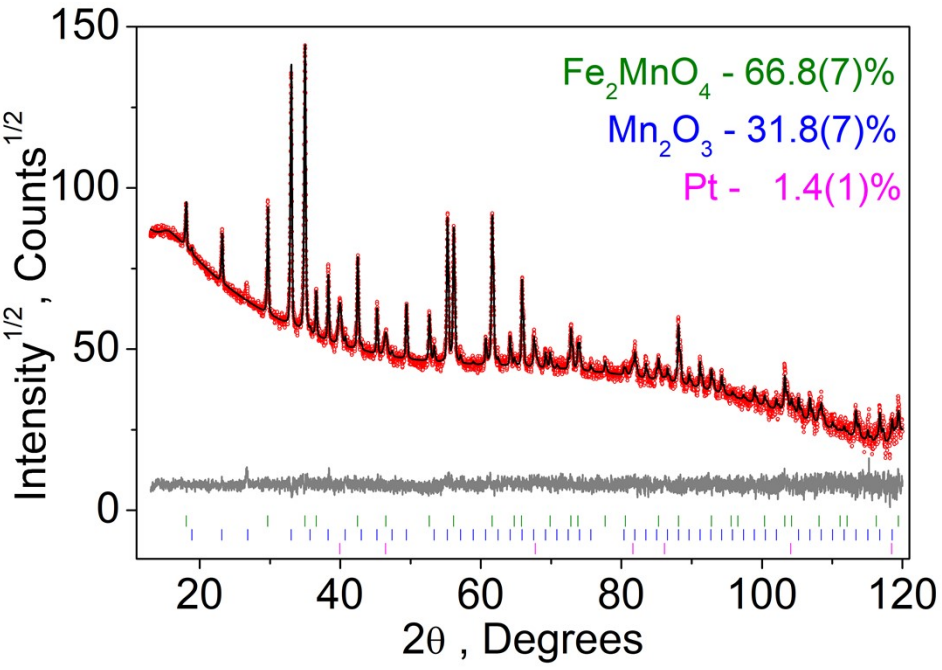

Table 1. Main parameters of processing and refinement of the Fe_2MnO_4 sample

Compound	Fe_2MnO_4
Sp. Gr.	$Fd\bar{3}m$
a (Å)	8.50925(16)
V (Å^3)	616.132(35)
Z	2
2θ-interval, º	7-120
R_{wp} ,%	4.8

R_p ,%	3.33
χ^2	2.49
R_B ,%	1.11

Table 2. Fractional atomic coordinates and isotropic displacement parameters (Å^2)

Atom	*x*	*y*	*z*	B_{iso}	*Occ.*
O1	0.26098(46)	0.26098(46)	0.26098(46)	2.28(15)	1
Fe1	0.5	0.5	0.5	1.000(74)	1
Mn1	0.125	0.125	0.125	1.000(79)	1

Table 3. Main bond lengths (Å)

Fe1—O1^{i}	2.0381(39)	Fe1—O1^{ii}	2.0381(39)
Fe1—O1^{iii}	2.0381(39)	Fe1—O1^{iv}	2.0381(39)
Fe1—O1^{v}	2.0381(39)	Fe1—O1^{vi}	2.0381(39)
Fe1—O1^{vii}	2.0381(39)	Fe1—O1^{viii}	2.0381(39)
Fe1—O1^{ix}	2.0381(39)	Fe1—O1^{x}	2.0381(39)
Fe1—O1^{xi}	2.0381(39)	Fe1—O1^{xii}	2.0381(39)
Fe1—O1^{xiii}	2.0381(39)	Fe1—O1^{xiv}	2.0381(39)
Fe1—O1^{xv}	2.0381(39)	Fe1—O1^{xvi}	2.0381(39)
Fe1—O1^{xvii}	2.0381(39)	Fe1—O1^{xviii}	2.0381(39)
Fe1—O1^{xix}	2.0381(39)	Fe1—O1^{xx}	2.0381(39)
Fe1—O1^{xxi}	2.0381(39)	Fe1—O1^{xxii}	2.0381(39)
Fe1—O1^{xxiii}	2.0381(39)	Fe1—O1^{xxiv}	2.0381(39)
Fe1—O1^{xxv}	2.0381(39)	Fe1—O1^{xxvi}	2.0381(39)
Fe1—O1^{xxvii}	2.0381(39)	Fe1—O1^{xxviii}	2.0381(39)

Fe1—O1^{xxix}	2.0381(39)	Fe1—O1^{xxx}	2.0381(39)
Fe1—O1^{xxxi}	2.0381(39)	Fe1—O1^{xxxii}	2.0381(39)
Fe1—O1^{xxxiii}	2.0381(39)	Fe1—O1^{xxxiv}	2.0381(39)
Fe1—O1^{xxxv}	2.0381(39)	Fe1—O1^{xxxvi}	2.0381(39)
Mn1—O1^{xxxvii}	2.0041(39)	Mn1—O1^{xxxviii}	2.0041(39)
Mn1—O1^{xxxix}	2.0041(39)	Mn1—O1^{xxxx}	2.0041(39)
Mn1—O1	2.0041(39)	Mn1—O1	2.0041(39)
Mn1—O1	2.0041(39)	Mn1—O1	2.0041(39)
Mn1—O1	2.0041(39)	Mn1—O1	2.0041(39)
Mn1—O1	2.0041(39)	Mn1—O1	2.0041(39)
Mn1—O1	2.0041(39)	Mn1—O1	2.0041(39)
Mn1—O1	2.0041(39)	Mn1—O1	2.0041(39)
Mn1—O1	2.0041(39)	Mn1—O1	2.0041(39)
Mn1—O1	2.0041(39)	Mn1—O1	2.0041(39)
Mn1—O1	2.0041(39)	Mn1—O1	2.0041(39)
Mn1—O1	2.0041(39)	Mn1—O1	2.0041(39)

Symmetry codes: (i) -x-3/4, y, -z-3/4; (ii) -x+1, z+1/4, y+1/4; (iii) -y-3/4, z, -x-3/4; (iv) -y+1, x+1/4, z+1/4; (v) -z-3/4, x, -y-3/4; (vi) -z+1, y+1/4, x+1/4; (vii) z, -y-3/4, -x-3/4; (viii) z+1/4, -x+1, y+1/4; (ix) y, -x-3/4, -z-3/4; (x) y+1/4, -z+1, x+1/4; (xi) x, -z-3/4, -y-3/4; (xii) x+1/4, -y+1, z+1/4; (xiii) -x-3/4, -z-3/4, y; (xiv) -x+1, y+1/4, z+1/4; (xv) -y-3/4, -x-3/4, z; (xvi) -y+1, z+1/4, x+1/4; (xvii) -z-3/4, -y-3/4, x; (xviii) -z+1, x+1/4, y+1/4; (xix) z, -x-3/4, -y-3/4; (xx) z+1/4, y+1/4, -x+1; (xxi) y, -z-3/4, -x-3/4; (xxii) y+1/4, x+1/4, -z+1; (xxiii) x, -y-3/4, -z-3/4; (xxiv) x+1/4, z+1/4, -y+1; (xxv) -x-3/4, -y-3/4, z; (xxvi) -x-3/4, z, -y-3/4; (xxvii) -y-3/4, -z-3/4, x; (xxviii) -y-3/4, x, -z-3/4; (xxix) -z-3/4, -x-3/4, y; (xxx) -z-3/4, y, -x-3/4; (xxxi) z+1/4, -y+1, x+1/4; (xxxii) z+1/4, x+1/4, -y+1; (xxxiii) y+1/4, -x+1, z+1/4; (xxxiv) y+1/4, z+1/4, -x+1; (xxxv) x+1/4, -z+1, y+1/4; (xxxvi) x+1/4, y+1/4, -z+1; (xxxvii) z, y, x; (xxxviii) z, x, y; (xxxix) y, z, x; (xxxx) y, x, z; () x, z, y; () x, y, z; () -x+1/4, z, -y+1/4; () -y+1/4, x, -z+1/4; () -z+1/4, y, -x+1/4; () z, -x+1/4, -y+1/4; () y, -z+1/4, -x+1/4; () x, -y+1/4, -z+1/4; () -x+1/4, -y+1/4, z; () -y+1/4, -z+1/4, x; () -z+1/4, -x+1/4, y; () z, -y+1/4, -x+1/4; () y, -x+1/4, -z+1/4; () x, -z+1/4, -y+1/4; () -

x+1/4, -z+1/4, y; () -x+1/4, y, -z+1/4; () -y+1/4, -x+1/4, z; () -y+1/4, z, -x+1/4; () -z+1/4, -y+1/4, x; () -z+1/4, x, -y+1/4;

References

[1] Bruker AXS TOPAS V4: General profile and structure analysis software for powder diffraction data. – User's Manual. Bruker AXS, Karlsruhe, Germany. 2008.

Sample no. 4

The powder diffraction data of sample no. 4 for Rietveld analysis was collected at room temperature with a Haoyuan DX-2700BH powder diffractometer (Cu-Kα radiation) and linear detector. The step size of 2θ was 0.01°, and the counting time was 20 sec per 1 deg. Almost all peaks besides small amount of unknown impurity peaks were indexed by orthorhombic cell with parameters close to $FeGaO_3$. Therefore this structure was taken as starting model for Rietveld refinement which was performed using TOPAS 4.2 [1]. Refinement was stable and gave low R-factors (Table 1, Figure 1). Coordinates of atoms and main bond lengths are in Table 2 and Table 3 respectively.

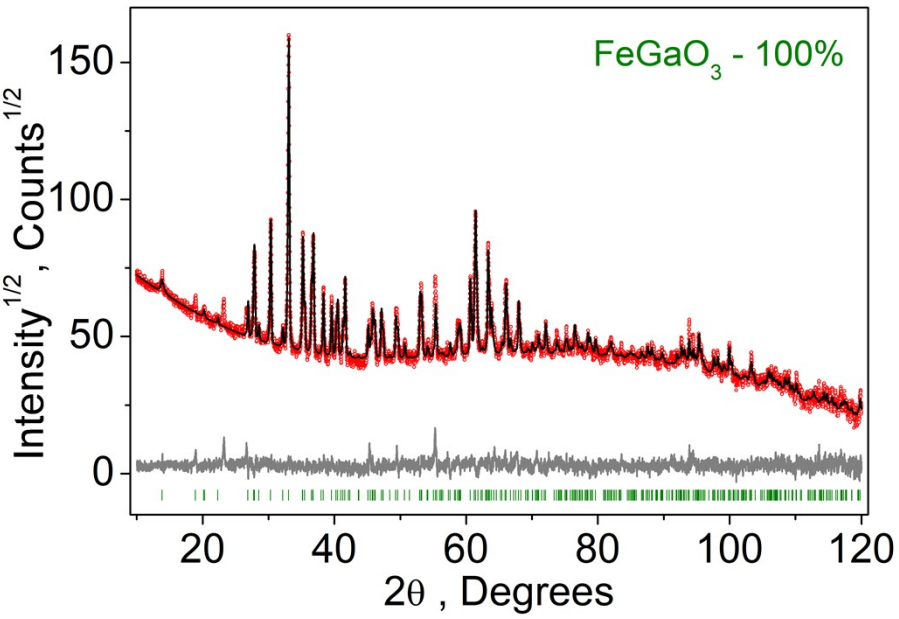

Figure 1. Difference Rietveld plot of $FeGaO_3$

Table 1. Main parameters of processing and refinement

Compound	$FeGaO_3$
Sp. Gr.	$Pc2_1n$
a (Å)	8.7429(4)
b (Å)	9.3958(5)

c (Å)	5.0971(2)
V (Å^3)	418.72(3)
Z	1
2θ-interval, º	10-120
R_{wp} ,%	6.91
R_p ,%	5.01
χ^2	3.33
R_B ,%	3.0

Table 2. Fractional atomic coordinates and isotropic displacement parameters (Å^2)

Atom	x	y	z	B_{iso}	*Occ.*
Fe1	-0.0363(4)	0.124	0.6756(10)	0.61(18)	1.00(7)
Fe2	-0.1492(9)	0.3464(12)	0.1921(15)	2.1(2)	0.21(12)
Ga4	-0.1492(9)	0.3464(12)	0.1921(15)	2.1(2)	0.79(12)
Fe3	0.1593(5)	0.1213(17)	0.1834(9)	1.18(15)	0.58(7)
Ga1	0.1593(5)	0.1213(17)	0.1834(9)	1.18(15)	0.42(7)
Ga2	-0.1537(7)	-0.0845(12)	0.1892(13)	1	1
O1	0.0132(17)	-0.0346(19)	0.014	2.77(10)	1
O2	0.2041(14)	0.0089(19)	0.540(3)	2.77(10)	1
O3	0.2070(13)	0.4383(17)	0.513(2)	2.77(10)	1
O4	-0.0037(15)	0.226(2)	0.383(3)	2.77(10)	1
O5	0.1304(14)	0.2135(14)	-0.201(3)	2.77(10)	1
O6	0.1387(16)	0.7545(14)	0.185(3)	2.77(10)	1

Table 3. Main bond lengths (Å)

Fe1—O1^{i}	2.320(12)	Fe1—O2	2.462(14)
Fe1—O3^{ii}	2.489(13)	Fe1—O3^{iii}	3.255(13)
Fe1—O4	1.795(16)	Fe1—O5^{i}	1.796(13)
Fe1—O6^{ii}	1.676(14)	Fe2—O1^{iv}	1.941(16)
Fe2—O1^{v}	3.493(16)	Fe2—O2^{vi}	2.103(19)
Fe2—O2^{v}	2.318(18)	Fe2—O4	1.960(18)
Fe2—O5	3.398(15)	Fe2—O5^{iv}	3.453(17)
Fe2—O6^{vii}	2.109(17)	Fe2—O6^{ii}	3.291(17)
Fe2—O6^{viii}	2.139(16)	Ga4—O1^{iv}	1.941(16)
Ga4—O1^{v}	3.493(16)	Ga4—O2^{vi}	2.103(19)
Ga4—O2^{v}	2.318(18)	Ga4—O4	1.960(18)
Ga4—O5	3.398(15)	Ga4—O5^{iv}	3.453(17)
Ga4—O6^{vii}	2.109(17)	Ga4—O6^{ii}	3.291(17)
Ga4—O6^{viii}	2.139(16)	Fe3—O1	2.126(19)
Fe3—O2^{ix}	3.467(16)	Fe3—O2	2.138(18)
Fe3—O2^{x}	1.753(18)	Fe3—O3	3.444(20)
Fe3—O3^{x}	3.315(20)	Fe3—O4	2.008(17)
Fe3—O5	2.157(16)	Fe3—O5^{i}	3.264(16)
Fe3—O5^{xi}	2.116(14)	Fe3—O6^{xii}	3.451(20)
Fe3—O6^{vii}	3.446(15)	Ga1—O1	2.126(19)
Ga1—O2^{ix}	3.467(16)	Ga1—O2	2.138(18)
Ga1—O2^{x}	1.753(18)	Ga1—O3	3.444(20)
Ga1—O3^{x}	3.315(20)	Ga1—O4	2.008(17)
Ga1—O5	2.157(16)	Ga1—O5^{i}	3.264(16)
Ga1—O5^{xi}	2.116(14)	Ga1—O6^{xii}	3.451(20)

Ga1—O6^{vii}	3.446(15)	Ga2—O1	1.773(14)
Ga2—O3^{ii}	1.602(12)	Ga2—O3^{viii}	1.609(12)
Ga2—O4	3.347(20)	Ga2—O4^{ii}	3.133(18)
Ga2—O5^{vii}	1.909(17)	Ga2—O6^{xii}	2.970(15)

Symmetry codes: (i) x, y, z+1; (ii) -x, y+1/2, -z+1; (iii) x+1/2, y+1/2, -z+3/2; (iv) -x, y+1/2, -z; (v) x+1/2, y+1/2, -z+1/2; (vi) -x, y+1/2, -z+1; (vii) -x, y+1/2, -z; (viii) x+1/2, y+1/2, -z+1/2; (ix) x, y, z-1; (x) -x+1/2, y, z+1/2; (xi) -x+1/2, y, z+1/2; (xii) x, y-1, z;

References

[1] BrukerAXSTOPAS V4: General profile and structure analysis software for powder diffraction data. – User's Manual. Bruker AXS, Karlsruhe, Germany. 2008.

Sample no. 5

The powder diffraction data of sample no. 5 for Rietveld analysis were collected at room temperature with a Haoyuan DX-2700BH powder diffractometer (Cu-Kα radiation) and linear detector. The step size of 2θ was 0.01°, and the counting time was 20 sec per 1 deg. All peaks were indexed by cubic cell ($Ia\bar{3}$) with parameters close to Mn_2O_3. Therefore this structure was taken as starting model for Rietveld refinement which was performed using TOPAS 4.2 [1]. Refinement was stable and gave low R-factors (Table 1, Figure 1). Coordinates of atoms and main bond lengths are in Table 2 and Table 3 respectively.

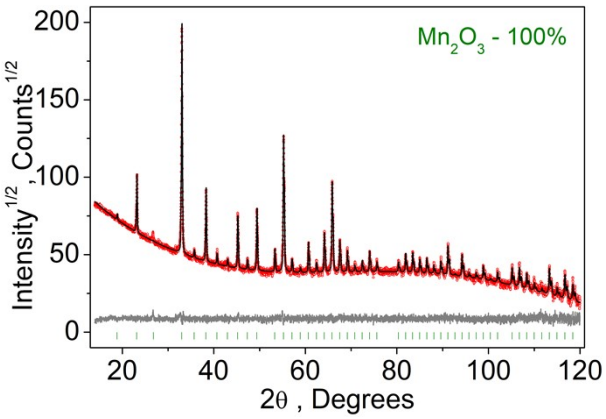

Figure 1. Difference Rietveld plot Mn_2O_3

Table 1. Main parameters of processing and refinement of the sample

Compound	Mn_2O_3
Sp. Gr.	$Ia\bar{3}$
a (Å)	9.404288(96)
V (Å^3)	831.721(25)
Z	16
2θ-interval, º	14-120
R_{wp} ,%	5.171
R_p ,%	3.707
χ^2	2.435

R_B ,%	0.92

Table 2. Fractional atomic coordinates and isotropic displacement parameters (Å^2) of sample

Atom	*x*	*y*	*z*	B_{iso}	*Occ.*
Mn1	0.25	0.25	0.25	0.674(52)	1
Mn2	0.964754(82)	0	0.25	0.781(47)	1
O1	0.38273(34)	1/6	0.39293(31)	0.781(80)	1

Table 3. Main bond lengths (Å)

Mn1—O1^{i}	1.9948(28)	Mn2—O1^{ii}	2.0247(27)
Mn2—O1^{iii}	1.9031(28)	Mn2—O1^{iv}	2.2042(21)

Symmetry codes: (i) z, x, y; (ii) -y+1, z+1/2, -x+1/2; (iii) -z+3/2, x+1/2, y; (iv) x+1/2, y, -z+1/2;

References

[1] Bruker AXS TOPAS V4: General profile and structure analysis software for powder diffraction data. – User's Manual. Bruker AXS, Karlsruhe, Germany. 2008.

Sample no. 6

The powder diffraction data of sample no. 6 for Rietveld analysis was collected at room temperature with a Haoyuan DX-2700BH powder diffractometer (Cu-Kα radiation) and linear detector. The step size of 2θ was 0.01°, and the counting time was 20 sec per 1 deg. All peaks were indexed by cubic cell ($Ia\bar{3}$) with parameters close to Mn_2O_3. Therefore this structure was taken as starting model for Rietveld refinement which was performed using TOPAS 4.2 [1]. Refinement was stable and gave low R-factors (Table 1, Figure 1). Coordinates of atoms and main bond lengths are in Table 2 and Table 3 respectively.

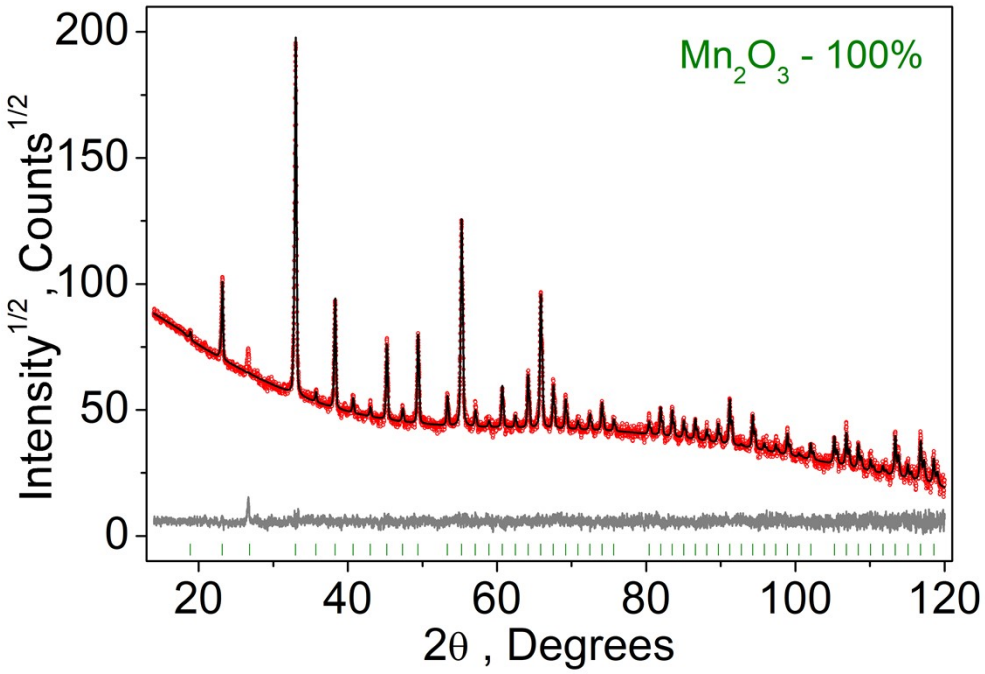

Figure 1. Difference Rietveld plot of Mn_2O_3

Table 1. Main parameters of processing and refinement

Compound	Mn_2O_3
Sp. Gr.	$Ia\bar{3}$
a (Å)	9.39891(13)
V (Å^3)	830.30(4)
Z	16

2θ-interval, º	14-120
R_{wp} ,%	5.1
R_p ,%	3.54
χ^2	2.57
R_B ,%	1.17

Table 2. Fractional atomic coordinates and isotropic displacement parameters (Å^2)

Atom	*x*	*y*	*z*	B_{iso}	*Occ.*
Mn1	0.25	0.25	0.25	0.40(6)	1
Mn2	-0.03448(9)	0	0.25	0.66(6)	1
O1	0.3815(4)	1/6	0.3911(4)	0.56(9)	1

Table 3. Main bond lengths (Å)

Mn1—O1	1.9747(34)	Mn2—O1^{i}	2.0294(32)
Mn2—O1^{ii}	1.9157(31)	Mn2—O1^{iii}	2.1991(26)

Symmetry codes: (i) -y, z+1/2, -x+1/2; (ii) -z+1/2, x+1/2, y; (iii) x+1/2, y, -z+1/2;

References

[1] BrukerAXSTOPAS V4: General profile and structure analysis software for powder diffraction data. – User's Manual. Bruker AXS, Karlsruhe, Germany. 2008.

Sample no. 7

The powder diffraction data of sample no. 7 for Rietveld analysis was collected at room temperature with a Haoyuan DX-2700BH powder diffractometer (Cu-Kα radiation) and linear detector. The step size of 2θ was 0.01°, and the counting time was 20 sec per 1 deg. Almost all peaks besides small impurity peaks were indexed by cubic cell with parameters close to Fe_2MnO_4. Therefore this structure was taken as starting model for Rietveld refinement which was performed using TOPAS 4.2 [1]. Refinement was stable and gave low R-factors (Table 1, Figure 1). Coordinates of atoms and main bond lengths are in Table 2 and Table 3 respectively.

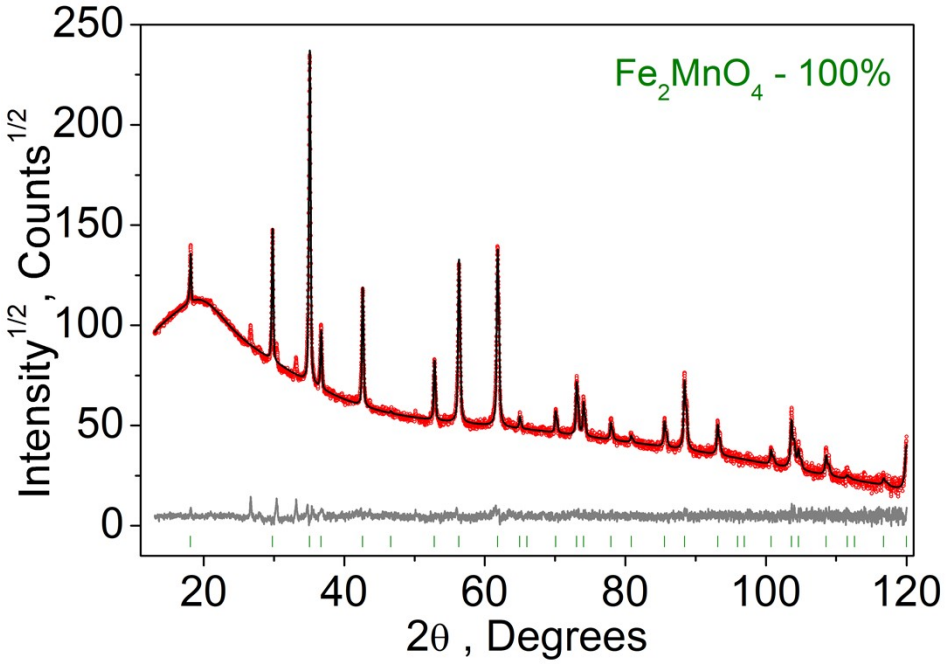

Figure 1. Difference Rietveld plot of Fe_2MnO_4

Table 1. Main parameters of processing and refinement

Compound	Fe_2MnO_4
Sp. Gr.	*Fd*-3*m*
a (Å)	8.48618(16)
V (Å^3)	611.13(3)
Z	2

2θ-interval, º	13-120
R_{wp} ,%	4.5
R_p ,%	3.0
χ^2	2.82
R_B ,%	1.9

Table 2. Fractional atomic coordinates and isotropic displacement parameters (Å^2)

Atom	*x*	*y*	*z*	B_{iso}	*Occ.*
O1	0.2623(2)	0.2623(2)	0.2623(2)	1.85(8)	1
Fe1	0.5	0.5	0.5	1.00(5)	1
Mn1	0.125	0.125	0.125	1.05(5)	1

Table 3. Main bond lengths (Å)

Fe1—O1	3.4938(16)	Fe1—O1^i	2.0225(16)
Mn1—O1	2.0181(16)		

Symmetry codes: (i) -x-3/4, y, -z-3/4

References

[1] BrukerAXSTOPAS V4: General profile and structure analysis software for powder diffraction data. – User's Manual. Bruker AXS, Karlsruhe, Germany. 2008.

Sample no. 8

The powder diffraction data of sample no. 8 for Rietveld analysis was collected at room temperature with a Haoyuan DX-2700BH powder diffractometer (Cu-Kα radiation) and linear detector. The step size of 2θ was 0.01°, and the counting time was 20 sec per 1 deg. Almost all peaks besides small amount of SiO_2 and Ga_2O_3 impurity peaks were indexed by orthorhombic cell with parameters close to $FeGaO_3$. Therefore this structure was taken as starting model for Rietveld refinement which was performed using TOPAS 4.2 [1]. Refinement was stable and gave low R-factors (Table 1, Figure 1). Coordinates of atoms and main bond lengths are in Table 2 and Table 3 respectively.

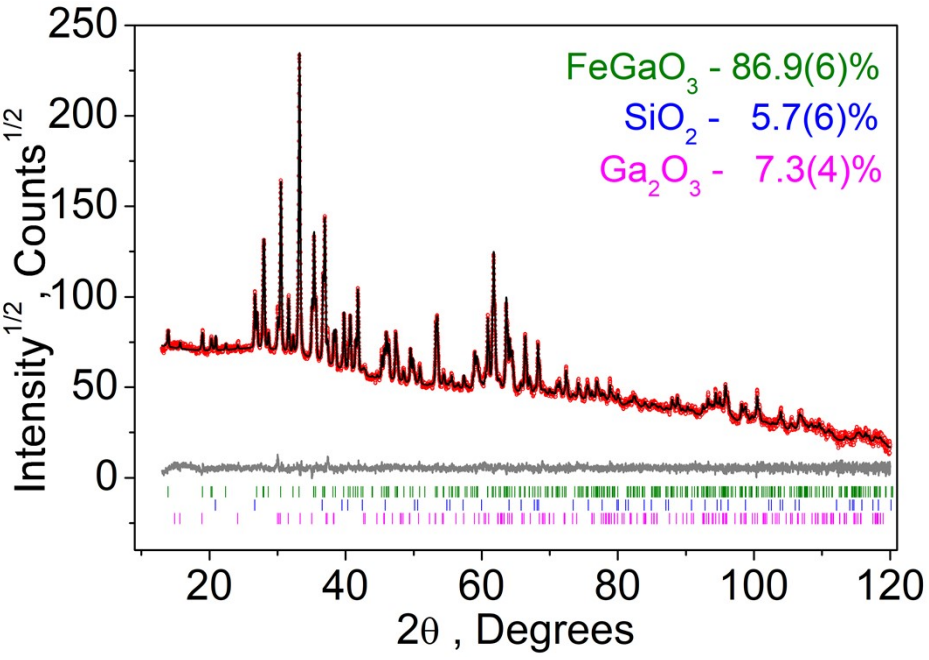

Figure 1. Difference Rietveld plot of $FeGaO_3$

Table 1. Main parameters of processing and refinement

Compound	$FeGaO_3$
Sp. Gr.	$Pc2_1n$
a (Å)	8.7118(2)
b (Å)	9.3479(2)
c (Å)	5.07860(12)

V (Å^3)	413.586(16)
Z	1
2θ-interval, º	13-120
R_{wp} ,%	4.34
R_p ,%	3.09
χ^2	2.48
R_B ,%	0.92

Table 2. Fractional atomic coordinates and isotropic displacement parameters (Å^2)

Atom	x	y	z	B_{iso}	*Occ.*
Fe1	-0.0329(3)	0.1152(7)	0.6789(5)	0.96(8)	0.43(4)
Ga3	-0.0329(3)	0.1152(7)	0.6789(5)	0.96(8)	0.57(4)
Fe2	-0.1534(9)	0.32774(19)	0.1812(9)	1.25(11)	0.32(7)
Ga4	-0.1534(9)	0.32774(19)	0.1812(9)	1.25(11)	0.68(7)
Fe3	0.1615(3)	0.1082(5)	0.1902(5)	1.21(9)	0.56(4)
Ga1	0.1615(3)	0.1082(5)	0.1902(5)	1.21(9)	0.44(4)
Ga2	-0.1533(8)	-0.0855(2)	0.1777(8)	1.22(2)	1
O1	0.0107(14)	-0.0209(13)	0.014	0.47(9)	1
O2	0.1690(15)	-0.0151(11)	0.527(3)	0.47(9)	1
O3	0.1584(17)	0.4687(12)	0.461(2)	0.47(9)	1
O4	-0.0129(14)	0.2129(11)	0.366(3)	0.47(9)	1
O5	0.1464(16)	0.2205(8)	-0.158(3)	0.47(9)	1
O6	0.1806(15)	0.7505(9)	0.151(3)	0.47(9)	1

Table 3. Main bond lengths (Å)

Fe1—O1^{i}	2.1585(86)	Fe1—O2	2.274(13)
Fe1—O3^{ii}	1.890(13)	Fe1—O4	1.841(14)
Fe1—O5^{i}	2.023(13)	Fe1—O6^{ii}	2.000(12)
Fe1—O6^{iii}	3.261(13)	Ga3—O1^{i}	2.1585(86)
Ga3—O2	2.274(13)	Ga3—O3^{ii}	1.890(13)
Ga3—O4	1.841(14)	Ga3—O5^{i}	2.023(13)
Ga3—O6^{ii}	2.000(12)	Ga3—O6^{iii}	3.261(13)
Fe2—O1^{iv}	2.128(11)	Fe2—O2^{v}	2.091(13)
Fe2—O2^{vi}	2.381(13)	Fe2—O3	3.336(15)
Fe2—O4	1.879(13)	Fe2—O4^{vii}	3.488(14)
Fe2—O5	3.285(15)	Fe2—O6^{viii}	1.850(15)
Fe2—O6^{ii}	3.475(15)	Fe2—O6^{iii}	1.827(14)
Ga4—O1^{iv}	2.128(11)	Ga4—O2^{v}	2.091(13)
Ga4—O2^{vi}	2.381(13)	Ga4—O3	3.336(15)
Ga4—O4	1.879(13)	Ga4—O4^{vii}	3.488(14)
Ga4—O5	3.285(15)	Ga4—O6^{viii}	1.850(15)
Ga4—O6^{ii}	3.475(15)	Ga4—O6^{iii}	1.827(14)
Fe3—O1	1.995(11)	Fe3—O2	2.063(14)
Fe3—O2^{ix}	2.048(13)	Fe3—O4	2.015(12)
Fe3—O5	2.060(14)	Fe3—O5^{i}	3.475(14)
Fe3—O5^{x}	2.120(13)	Fe3—O6^{xi}	3.3538(96)
Ga1—O1	1.995(11)	Ga1—O2	2.063(14)
Ga1—O2^{ix}	2.048(13)	Ga1—O4	2.015(12)
Ga1—O5	2.060(14)	Ga1—O5^{i}	3.475(14)
Ga1—O5^{x}	2.120(13)	Ga1—O6^{xi}	3.3538(96)

Ga2—O1	1.759(12)	Ga2—O2	3.385(14)
Ga2—O3^{viii}	3.283(10)	Ga2—O3^{ii}	1.904(10)
Ga2—O3^{iii}	1.855(15)	Ga2—O4	3.192(11)
Ga2—O4^{ii}	3.319(13)	Ga2—O5^{viii}	1.8172(77)
Ga2—O6^{xi}	3.290(13)		

Symmetry codes: (i) x, y, z+1; (ii) -x, y+1/2, -z+1; (iii) x+1/2, y+1/2, -z+1/2; (iv) -x, y+1/2, -z; (v) -x, y+1/2, -z+1; (vi) x+1/2, y+1/2, -z+1/2; (vii) -x+1/2, y, z+1/2; (viii) -x, y+1/2, -z; (ix) -x+1/2, y, z+1/2; (x) -x+1/2, y, z+1/2; (xi) x, y-1, z;

References

[1] BrukerAXSTOPAS V4: General profile and structure analysis software for powder diffraction data. – User's Manual. Bruker AXS, Karlsruhe, Germany. 2008.

Sample no. 9

The powder diffraction data of sample no. 9 for Rietveld analysis was collected at room temperature with a Haoyuan DX-2700BH powder diffractometer (Cu-Kα radiation) and linear detector. The step size of 2θ was 0.01°, and the counting time was 20 sec per 1 deg. All peaks were indexed by orthorhombic cell with parameters close to $FeGaO_3$. Therefore this structure was taken as starting model for Rietveld refinement which was performed using TOPAS 4.2 [1]. Refinement was stable and gave low R-factors (Table 1, Figure 1). Coordinates of atoms and main bond lengths are in Table 2 and Table 3 respectively.

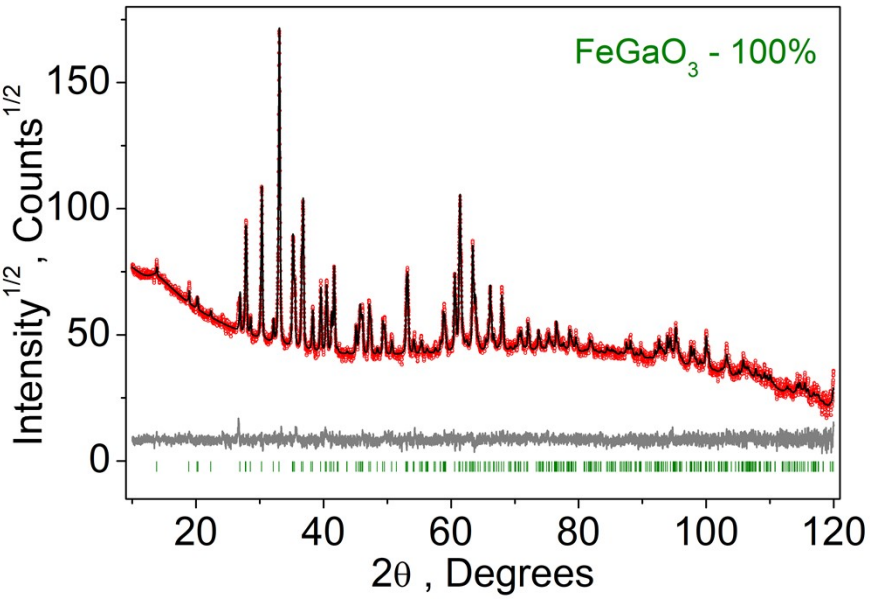

Figure 1. Difference Rietveld plot of $FeGaO_3$

Table 1. Main parameters of processing and refinement

Compound	$FeGaO_3$
Sp. Gr.	$Pc2_1n$
a (Å)	8.75139(45)
b (Å)	9.40233(50)
c (Å)	5.09102(27)
V (Å^3)	418.907(38)

Z	1
2θ-interval, º	7-120
R_{wp} ,%	5.37
R_p ,%	3.92
χ^2	2.69
R_B ,%	1.49

Table 2. Fractional atomic coordinates and isotropic displacement parameters (Å^2)

Atom	*x*	*y*	*z*	B_{iso}	*Occ.*
Fe1	0.96508(35)	0.124	0.67506(85)	0.30(11)	0.968(52)
Ga3	0.96508(35)	0.124	0.67506(85)	0.30(11)	0.032(52)
Fe2	0.8479(11)	0.33676(81)	0.1783(13)	0.30(15)	1.000(66)
Fe3	0.16085(47)	0.1115(11)	0.18953(70)	0.30(12)	1.000(57)
Ga2	0.84915(87)	0.92012(82)	0.1797(12)	1	1
O1	0.0168(18)	0.9873(19)	0.0140(12)	0.66(12)	1
O2	0.1701(20)	0.9969(17)	0.5350(35)	0.66(12)	1
O3	0.1655(24)	0.4857(17)	0.5209(45)	0.66(12)	1
O4	0.9894(19)	0.2163(16)	0.3472(43)	0.66(12)	1
O5	0.1636(22)	0.2245(13)	0.8593(36)	0.66(12)	1
O6	0.1657(26)	0.7519(16)	0.1375(36)	0.66(12)	1

Table 3. Main bond lengths (Å)

Fe1—O1^{i}	2.198(11)	Fe1—O2^{ii}	2.270(17)
Fe1—O3^{iii}	1.998(19)	Fe1—O3^{iv}	3.310(20)
Fe1—O4^{v}	1.893(20)	Fe1—O5^{vi}	2.188(18)

Fe1—O6^{iii}	1.914(19)	Fe1—O6^{vii}	3.292(21)
Ga3—O1^{i}	2.198(11)	Ga3—O2^{ii}	2.270(17)
Ga3—O3^{iii}	1.998(19)	Ga3—O3^{iv}	3.310(20)
Ga3—O4^{v}	1.893(20)	Ga3—O5^{vi}	2.188(18)
Ga3—O6^{iii}	1.914(19)	Ga3—O6^{vii}	3.292(21)
Fe2—O1^{viii}	2.088(17)	Fe2—O2^{iii}	2.102(18)
Fe2—O2^{vii}	2.422(18)	Fe2—O4^{v}	1.885(19)
Fe2—O5^{ix}	3.374(20)	Fe2—O6^{viii}	1.798(19)
Fe2—O6^{vii}	2.014(22)	Fe3—O1^{x}	3.471(15)
Fe3—O1^{xi}	1.936(16)	Fe3—O2^{xii}	1.992(18)
Fe3—O2^{xi}	2.064(18)	Fe3—O3^{xiii}	3.424(21)
Fe3—O4^{xiv}	1.966(18)	Fe3—O5^{xv}	2.058(18)
Fe3—O5^{xvi}	1.988(17)	Fe3—O6^{xi}	3.391(18)
Ga2—O1^{vi}	1.806(16)	Ga2—O2^{vi}	3.417(18)
Ga2—O3^{xvii}	1.649(22)	Ga2—O3^{xviii}	2.001(22)
Ga2—O4^{xix}	3.386(20)	Ga2—O4^{xx}	3.160(17)
Ga2—O5^{xvii}	1.853(14)	Ga2—O5^{xxi}	3.395(18)
Ga2—O6^{vi}	3.197(22)		

Symmetry codes: (i) x+1, y-1, z+1; (ii) x+1, y-1, z; (iii) -x+1, y+1/2, -z+1; (iv) x+1/2, y+1/2, -z+3/2; (v) x, y, z; (vi) x+1, y, z; (vii) x+1/2, y+1/2, -z+1/2; (viii) -x+1, y+1/2, -z; (ix) x+1, y, z-1; (x) -x+1/2, y-1, z+1/2; (xi) x, y-1, z; (xii) -x+1/2, y-1, z+1/2; (xiii) -x, y+1/2, -z+1; (xiv) x-1, y, z; (xv) -x+1/2, y, z+1/2; (xvi) x, y, z-1; (xvii) -x+1, y+1/2, -z+1; (xviii) x+1/2, y+1/2, -z+1/2; (xix) -x+2, y+1/2, -z+1; (xx) x, y+1, z; (xxi) x+1/2, y+1/2, -z+3/2;

References

[1] Bruker AXS TOPAS V4: General profile and structure analysis software for powder diffraction data. – User's Manual. Bruker AXS, Karlsruhe, Germany. 2008.