

Table S1. The bond lengths and bond angles of hexaferrite phase obtained from Rietveld refinement (structural model) of the SXR patterns of samples sintered at 1000 °C.

Sample Dopant ionic radii ratio	Undoped	Ba-site doping			Fe-site doping	
	BM10	BMSr10	BMCa10	BMZn10	BMGa10	BMCr10
Ba 2c site						
Coordination Number (12)	12.72	18.63	18.28	13.78	13.04	13.05
$d_{\text{Ba}-\text{O}3} (\text{Å}) \times 6$	2.95214(6)	2.95093(3)	2.95581(6)	2.94808(3)	2.94712(5)	2.95019(8)
$d_{\text{Ba}-\text{O}5} (\text{Å}) \times 6$	2.86792(5)	2.85900(3)	2.87600(4)	2.85455(3)	2.86100(3)	2.87300(4)
Avg. $d_{\text{Ba}-\text{O}5} (\text{Å})$	2.91003(6)	2.90496(3)	2.91591(5)	2.90132(3)	2.90406(4)	2.91159(6)
Distortion (10^{-4})	2.093	2.500	1.862	2.596	2.203	1.742
$\angle \text{O}3 - \text{Ba} - \text{O}3$ (deg)	173.09(7)	173.09(7)	173.09(7)	173.09(7)	173.09(7)	173.09(7)
$\angle \text{O}5 - \text{Ba} - \text{O}5$ (deg)	146.19(5)	146.10(2)	146.30(2)	146.08(3)	146.20(2)	146.30(2)
$\angle \text{O}3 - \text{Ba} - \text{O}3$ (deg)	119.99(9)	119.99(9)	119.99(9)	119.99(9)	119.99(9)	119.99(9)
$\angle \text{O}3 - \text{Ba} - \text{O}5$ (deg)	119.02(1)	119.11(9)	118.97(10)	119.13(6)	119.05(9)	118.94(11)
$\angle \text{O}5 - \text{Ba} - \text{O}5$ (deg)	108.89(2)	108.70(2)	109.00(2)	108.62(3)	108.80(2)	109.10(2)
$\angle \text{O}3 - \text{Ba} - \text{O}5$ (deg)	92.01(9)	92.01(9)	92.01(10)	92.02(6)	92.01(9)	92.00(11)
$\angle \text{O}5 - \text{Ba} - \text{O}5$ (deg)	60.47(3)	60.65(9)	60.36(10)	60.69(4)	60.52(9)	60.30(11)
$\angle \text{O}3 - \text{Ba} - \text{O}3$ (deg)	66.91(3)	66.91(3)	66.91(3)	66.91(3)	66.91(3)	66.91(3)
$\angle \text{O}3 - \text{Ba} - \text{O}5$ (deg)	58.66(6)	58.56(9)	58.71(10)	58.54(12)	58.63(9)	58.74(11)
$\angle \text{O}3 - \text{Ba} - \text{O}3$ (deg)	53.09(8)	53.09(8)	53.09(8)	53.09(8)	53.09(8)	53.09(8)
2a Octahedral site						
Coordination Number (6)	6.31	9.09	9.38	7.51	6.20	6.56
$d_{\text{Fe}1-\text{O}4} (\text{Å}) \times 6$	1.99454(1)	1.99500(20)	1.99100(20)	1.97211(19)	1.99290(20)	1.99100(2)
Distortion (10^{-4})	-0.002	-0.001	0.00	-0.001	0.001	0.000
$\angle \text{O}4 - \text{Fe}1 - \text{O}4$ (deg)	180.00(0)	180.00(18)	180.00(19)	180.00(2)	180.00(18)	180.00(2)
$\angle \text{O}4 - \text{Fe}1 - \text{O}4$ (deg)	86.99(6)	86.93(8)	87.08(9)	88.09(12)	86.92(8)	87.14(10)
2b Bipyramidal site						
Coordination Number (5)	4.10	7.20	5.89	4.35	4.16	4.15
$d_{\text{Fe}2-\text{O}1} (\text{Å}) \times 1$	2.50320(2)	2.44100(8)	2.48900(8)	2.52961(4)	2.50300(8)	2.52200(8)
$d_{\text{Fe}2-\text{O}1} (\text{Å}) \times 1$	2.09919(1)	2.06500(8)	2.08600(8)	1.99457(3)	2.05300(8)	2.09900(8)
$d_{\text{Fe}2-\text{O}3} (\text{Å}) \times 3$	1.89010(1)	1.88790(5)	1.88810(5)	1.89566(2)	1.88980(5)	1.88990(5)
Avg. $d_{\text{Fe}-\text{O}} (\text{Å})$	2.05454(1)	2.04786(6)	2.05264(5)	2.042232(3)	2.04508(6)	2.05814(6)
Distortion ($\times 10^{-4}$)	21.728	111.375	19.580	4.975	13.467	21.833
$\angle \text{O}1 - \text{Fe}2 - \text{O}1$ (deg)	180.00(2)	180.00(6)	180.00(6)	179.97(4)	180.00(6)	180.00(6)
$\angle \text{O}1 - \text{Fe}2 - \text{O}3$ (deg)	83.86(4)	84.30(3)	83.90(3)	81.89(17)	83.20(3)	83.60(3)
4f₁ Tetrahedral site						
Coordination Number (4)	4.25	6.17	6.26	5.06	4.27	4.45
$d_{\text{Fe}3-\text{O}2} (\text{Å}) \times 1$	1.89487(1)	1.90300(5)	1.93300(7)	2.06041(4)	1.88500(5)	1.90600(7)
$d_{\text{Fe}3-\text{O}4} (\text{Å}) \times 3$	1.90682(12)	1.90870(12)	1.90140(12)	1.88267(2)	1.90620(11)	1.90160(14)
Avg. $d_{\text{Fe}-\text{O}} (\text{Å})$	1.90383(12)	1.90728(10)	1.90930(5)	1.92710(2)	1.90090(10)	1.90270(12)
Distortion ($\times 10^{-4}$)	0.074	0.014	0.508	15.951	0.242	0.008
$\angle \text{O}4 - \text{Fe}3 - \text{O}4$ (deg)	111.25(5)	111.02(5)	111.56(5)	113.20(16)	111.06(5)	111.60(6)
$\angle \text{O}2 - \text{Fe}3 - \text{O}4$ (deg)	107.62(4)	107.90(3)	107.30(4)	105.42(2)	107.80(3)	107.20(4)
4f₂ Octahedral site						
Coordination Number (6)	6.36	9.31	9.14	6.89	6.52	6.53
$d_{\text{Fe}4-\text{O}3} (\text{Å}) \times 3$	2.05854(11)	2.06110(11)	2.04670(12)	2.02815(2)	2.05860(11)	2.05680(14)
$d_{\text{Fe}4-\text{O}5} (\text{Å}) \times 3$	1.97743(11)	1.97000(2)	1.98500(2)	1.98913(5)	1.97100(2)	1.98100(2)
Avg. $d_{\text{Fe}-\text{O}} (\text{Å})$	2.01799(11)	2.01555(18)	2.01585(12)	2.00864(4)	2.01480(6)	2.01890(8)
Distortion (10^{-4})	4.038	5.140	2.322	0.938	4.737	3.552
$\angle \text{O}3 - \text{Fe}4 - \text{O}5$ (deg)	166.40(13)	165.93(15)	167.22(16)	168.02(2)	166.12(15)	166.66(17)
$\angle \text{O}3 - \text{Fe}4 - \text{O}3$ (deg)	79.71(4)	79.56(4)	80.17(5)	81.02(12)	79.57(4)	79.73(6)
12k Octahedral site						
Coordination Number (6)	6.36	9.19	9.22	7.12	6.44	6.63
$d_{\text{Fe}5-\text{O}1} (\text{Å}) \times 1$	1.98580(11)	2.00400(4)	1.98200(3)	1.99274(2)	1.99300(4)	1.97900(3)
$d_{\text{Fe}5-\text{O}2} (\text{Å}) \times 1$	2.09619(11)	2.08700(3)	2.07800(4)	2.02966(7)	2.09600(3)	2.09300(4)
$d_{\text{Fe}5-\text{O}4} (\text{Å}) \times 2$	2.10937(9)	2.10800(2)	2.11100(2)	2.13659(4)	2.10600(2)	2.11100(3)
$d_{\text{Fe}5-\text{O}5} (\text{Å}) \times 2$	1.928325(8)	1.92700(2)	1.91600(2)	1.92316(4)	1.92800(2)	1.92200(2)
Avg. $d_{\text{Fe}-\text{O}} (\text{Å})$	2.02623(9)	2.02683(3)	2.01900(3)	2.02365(4)	2.02617(3)	2.02300(4)
Distortion (10^{-4})	16.055	15.074	17.467	19.019	15.483	17.369
$\angle \text{O}1 - \text{Fe}5 - \text{O}2$ (deg)	173.16(13)	174.40(3)	173.70(3)	176.12(5)	173.60(3)	172.90(3)
$\angle \text{O}1 - \text{Fe}5 - \text{O}4$ (deg)	85.74(8)	86.50(3)	85.80(3)	86.81(8)	85.10(3)	85.60(3)
$\angle \text{Fe}2 - \text{O}1 - \text{Fe}5$ (deg)	119.86(6)	120.80(3)	119.80(3)	120.34(7)	120.40(3)	119.60(3)
$\angle \text{Fe}3 - \text{O}2 - \text{Fe}5$ (deg)	126.70(4)	126.40(2)	126.10(3)	124.22(2)	126.81(20)	126.60(3)
$\angle \text{Fe}5 - \text{O}2 - \text{Fe}5$ (deg)	87.94(4)	88.39(11)	88.82(16)	91.46(3)	87.80(11)	88.06(16)
$\angle \text{Fe}2 - \text{O}3 - \text{Fe}4$ (deg)	143.86(8)	143.34 (12)	144.16(12)	146.71(2)	144.47(11)	144.16(13)
$\angle \text{Fe}4 - \text{O}3 - \text{Fe}4$ (deg)	84.53(2)	84.74(10)	83.93(11)	82.80(4)	84.73(10)	84.51(12)
$\angle \text{Fe}1 - \text{O}4 - \text{Fe}3$ (deg)	125.01(7)	124.72(7)	125.38(7)	127.96(9)	124.75(7)	125.50(8)
$\angle \text{Fe}1 - \text{O}4 - \text{Fe}5$ (deg)	95.87(3)	95.90(9)	95.93(9)	96.03(7)	95.91(9)	95.86(11)
$\angle \text{Fe}4 - \text{O}5 - \text{Fe}5$ (deg)	127.91(8)	127.81(10)	127.93(11)	128.09(5)	127.90(10)	127.92(12)