Supporting Information

Crystal structure and magnetocaloric effect in non-rare-earth $KBa_8Fe_{12}(Bi_{6-x}Fe_x)O_{38}$

Xuan Wu[a,b], Yanyun Deng[a], Shuting Wu[a,c], Xin Chen[a,c], Xiaolin Hu[a,c,*], Naifeng Zhuang[a,c,*]

[a] College of Chemistry, Fuzhou University, Fuzhou 350108, P.R. China.

[b] Hefei Gongda Vocational and Technical College, Hefei 231135, P.R. China.

[c] Fujian Science & Technology Innovation Laboratory for Optoelectronic Information of China, Fuzhou 350002, P.R. China.

1. Energy dispersion spectrum

The images of the energy dispersion spectrum (EDS) are given in figure S1. The K:Fe:Bi:Ba molar ratio of a crystal is calculated and averaged on the basis of multipoint data on this crystal.

2. Structure information

According to XRD patterns, the crystal structure of $KBa_8Fe_{12}(Bi_{6-x}Fe_x)O_{38}$ (x=0.2,1.1,2.0,2.9,3.8) was analyzed and refined based on the *Rietveld* principle. The structural information, such as the atomic position and the occupancy rate, is listed in Table S1 of the supporting information. From Table S1, the unit cell volume and parameters of $KBa_8Fe_{12}(Bi_{6-x}Fe_x)O_{38}$ (x=0.2,1.1,2.0,2.9,3.8) decrease with the increase of ferric ion. The main reason is that the radius of ferric ion is smaller than bismuth ion. The more ferric ion is substituted for Bi^{3+}, the smaller the unit cell volume and lattice parameters are.

* Corresponding author.

E-mail address: linamethyst@fzu.edu.cn (Xiaolin Hu), nfzhuang@fzu.edu.cn (Naifeng Zhuang)

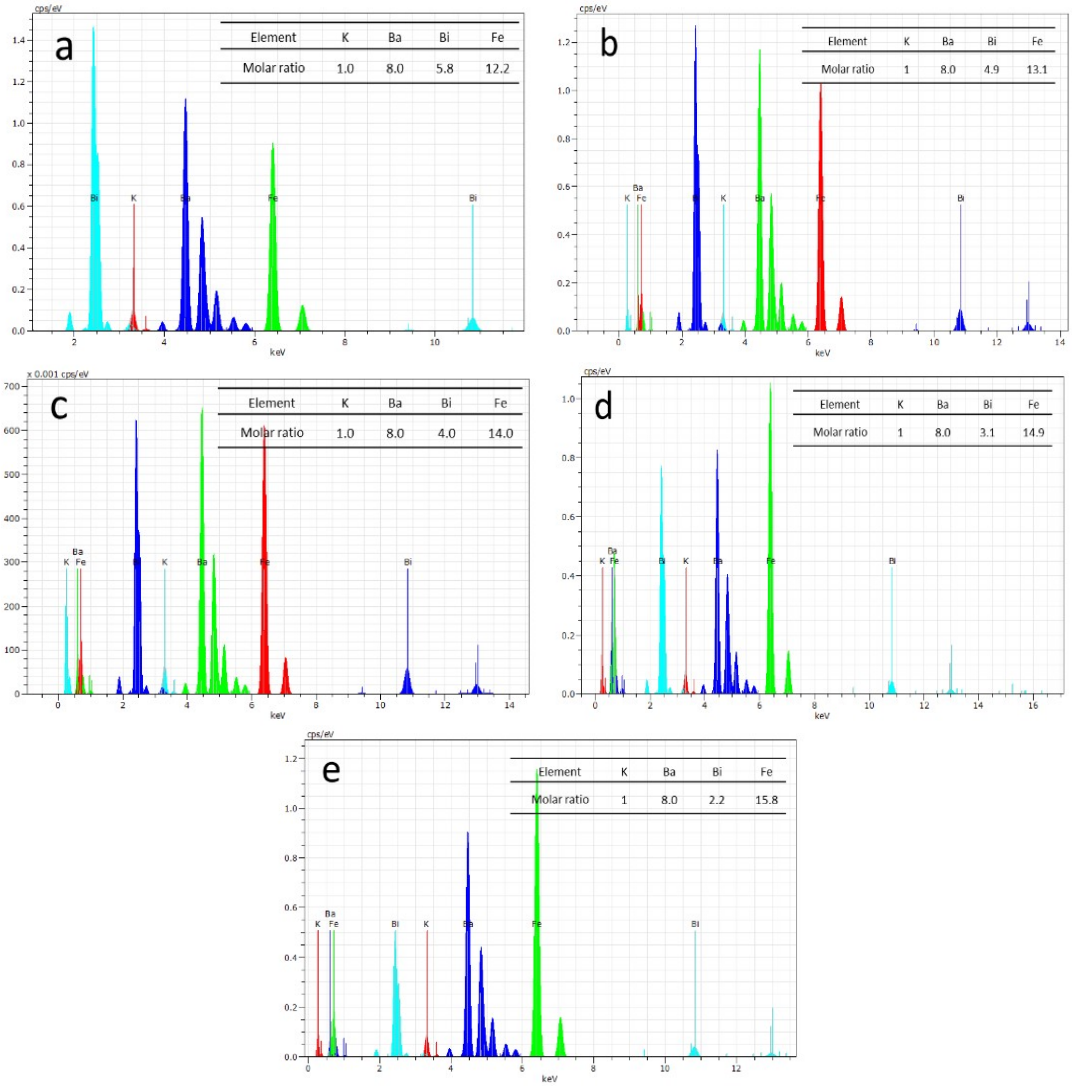

Figure S1 EDS images of $KBa_8Fe_{12}(Bi_{6-x}Fe_x)O_{38}$ crystals. (a) $KBa_8Fe_{12}(Bi_{5.8}Fe_{0.2})O_{38}$, (b) $KBa_8Fe_{12}(Bi_{4.9}Fe_{1.1})O_{38}$, (c) $KBa_8Fe_{12}(Bi_{4.0}Fe_{2.0})O_{38}$, (d) $KBa_8Fe_{12}(Bi_{3.1}Fe_{2.9})O_{38}$, (e) $KBa_8Fe_{12}(Bi_{2.2}Fe_{3.8})O_{38}$.

Table S1 Structure information of $KBa_8Fe_{12}(Bi_{6-x}Fe_x)O_{38}$ (x=0.2,1.1,2.0,2.9,3.8) crystals

Fe1 content	Wyck.	atom	*x*	*y*	*z*	Site Occ	U(eq)
	1b	K	0.5000	0.5000	0.5000	0.95(4)	0.013(13)
	8g	Ba	0.29351(13)	0.29351(13)	0.29351(13)	0.961(9)	0.0000(10)
	6e	Bi	0.0000	0.0000	0.2540(2)	0.8(5)	0.0000(9)
	6e	Fe1	0.0000	0.0000	0.2540(2)	0.02(3)	0.(3)
x=0.2	12h	Fe2	0.5000	0.0000	0.2527(5)	1	0.001(2)
	8g	O1	0.8660(11)	0.1340(11)	0.1340(11)	1	0.000(7)
	6f	O2	0.5000	0.741(2)	0.5000	1	0.000(8)
	12j	O3	0.5000	0.1573(10)	0.1573(10)	1	0.000(10)
	12i	O4	0.3424(10)	0.0000	0.3424(10)	1	0.000(10)
	1b	K	0.5000	0.5000	0.5000	1.00(6)	0.34(6)
	8g	Ba	0.29173(15)	0.29173(15)	0.29173(15)	0.950(7)	0.0383(13)
	6e	Bi	0.0000	0.0000	0.2532(4)	0.615(13)	0.040(8)
	6e	Fe1	0.0000	0.0000	0. 2532(4)	0.12(4)	0.(3)
x=1.1	12h	Fe2	0.5000	0.0000	0.2592(7)	1	0.0168(19)
	8g	O1	0.8660(16)	0.1340(16)	0.1340(16)	1	0.108(11)
	6f	O2	0.5000	0.731(3)	0.5000	1	0.000(9)
	12j	O3	0.5000	0.1491(11)	0.1491(11)	1	0.000(8)
	12i	O4	0.3501(11)	0.0000	0.3501(11)	1	0.000(9)
	1b	K	0.5000	0.5000	0.5000	0.95(4)	0.000(14)
	8g	Ba	0.2891(2)	0.2891(2)	0.2891(2)	0.950(8)	0.0441(19)
	6e	Bi	0.0000	0.0000	0.2582(5)	0.539(13)	0.033(10)
	6e	Fe1	0.0000	0.0000	0.2582(5)	0.27(4)	0.38(13)
x=2.0	12h	Fe2	0.5000	0.0000	0.2572(6)	1	0.000(2)
	8g	O1	0.8660(14)	0.1340(14)	0.1340(14)	1	0.000(8)
	6f	O2	0.5000	0.742(3)	0.5000	1	0.000(10)
	12j	O3	0.5000	0.1686(10)	0.1686(10)	1	0.000(15)
	12i	O4	0.3363(9)	0.0000	0.3363(9)	1	0.000(13)
	1b	K	0.5000	0.5000	0.5000	0.95(6)	0.06(2)
	8g	Ba	0.2894(2)	0.2894(2)	0.2894(2)	0.950(9)	0.0350(19)
	6e	Bi	0.0000	0.0000	0.2578(6)	0.4(4)	0.02(18)
	6e	Fe1	0.0000	0.0000	0.2578(6)	0.40(2)	0.016(10)
x=2.9	12h	Fe2	0.5000	0.0000	0.2559(8)	1	0.000(2)
	8g	O1	0.8660(16)	0.1340(16)	0.1340(16)	1	0.000(9)
	6f	O2	0.5000	0.743(4)	0.5000	1	0.000(12)
	12j	O3	0.5000	0.1526(14)	0.1526(14)	1	0.000(15)
	12i	O4	0.3501(14)	0.0000	0.3501(14)	1	0.000(14)
	1b	K	0.5000	0.5000	0.5000	0.95(5)	0.042(2)
	8g	Ba	0.28978(19)	0.28978 (19)	0.28978 (19)	0.950(8)	0.042(2)
	6e	Bi	0.0000	0.0000	0.2598(7)	0.3(3)	0.0(9)
	6e	Fe1	0.0000	0.0000	0.2598 (7)	0.61(2)	0.33(8)
x=3.8	12h	Fe2	0.5000	0.0000	0.2548(7)	1	0.005(3)
	8g	O1	0.8660(15)	0.1340(15)	0.1340(15)	1	0.000(8)
	6f	O2	0.5000	0.747(3)	0.5000	1	0.000(11)
	12j	O3	0.5000	0.1562(12)	0.1562(12)	1	0.000(15)
	12i	O4	0.3480(12)	0.0000	0.3480(12)	1	0.000(14)