Supporting information

Controllable Thermal Expansion and Magnetic Structure in $Er_2(Fe,Co)_{14}B$ Intermetallic Compounds

Yongqiang Qiao, [a] Yuzhu Song, [a] Meng Xu, [a] Qilong Gao, [b] Yang Ren, [c] Xianran Xing [a] and Jun Chen*[a]

[a] Beijing Advanced Innovation Center for Materials Genome Engineering, and Department of Physical Chemistry, University of Science and Technology Beijing, Beijing 100083, China

[b] School of Physical Science, Zhengzhou University, Zhengzhou, China

[c] X-Ray Science Division, Argonne National Laboratory, Argonne, Illinois 60439, United States

Supplementary Figure

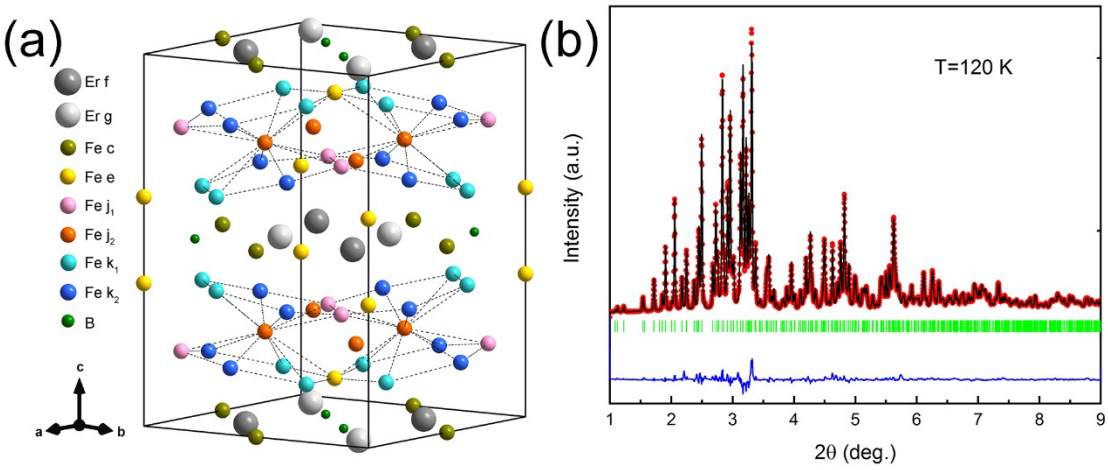

Figure S1. (a) The crystal structure of $Er_2Fe_{14}B$. (b) The refinement of the SXRD pattern with the space group $P4_2/mnm$ at 120 K.

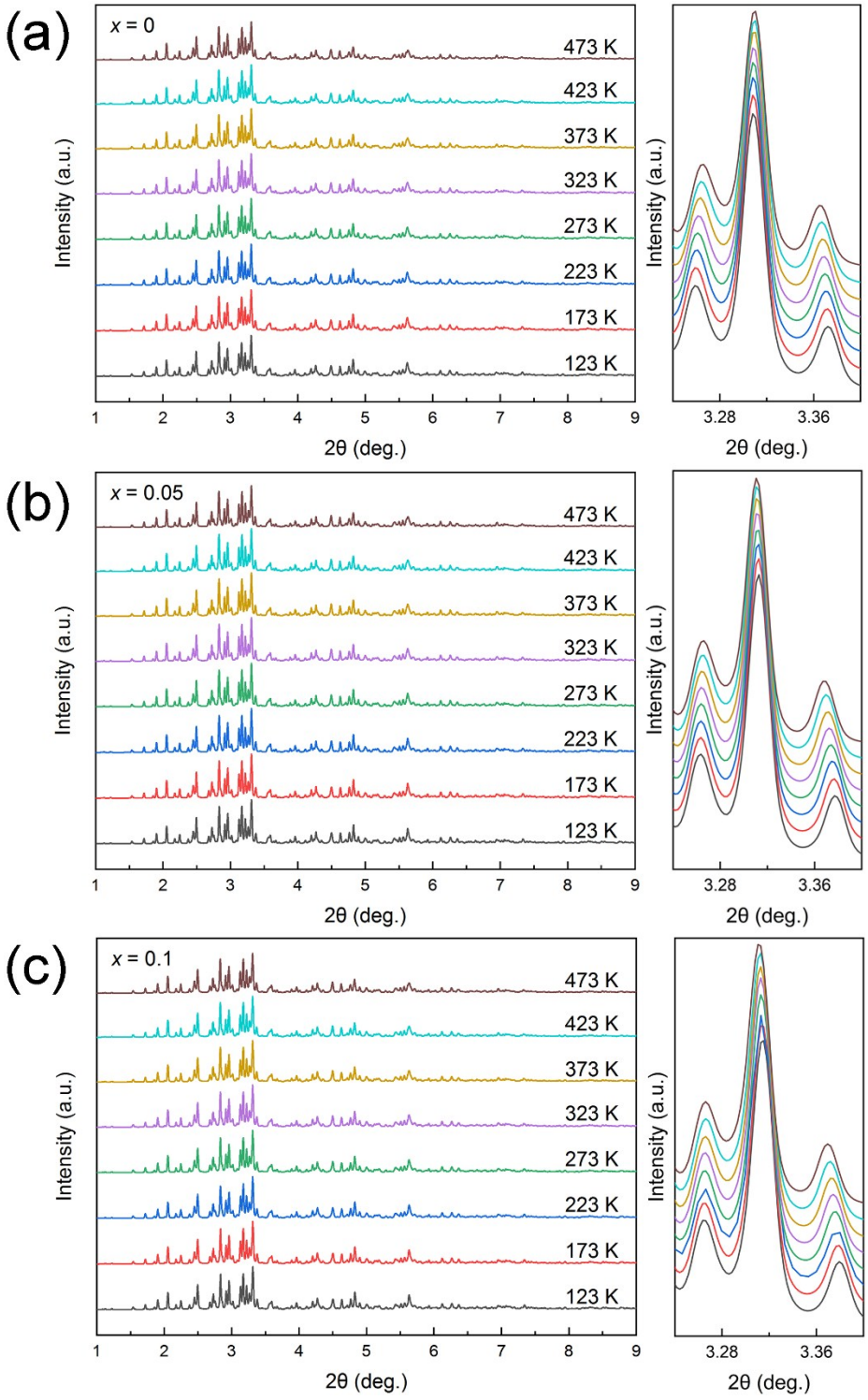

Figure S2. The variable temperature SXRD datasets for the $Er_2(Fe_{1-x}Co_x)_{14}B$ intermetallic compounds (x = 0, 0.05, and 0.1) and the enlarged image is on the right.

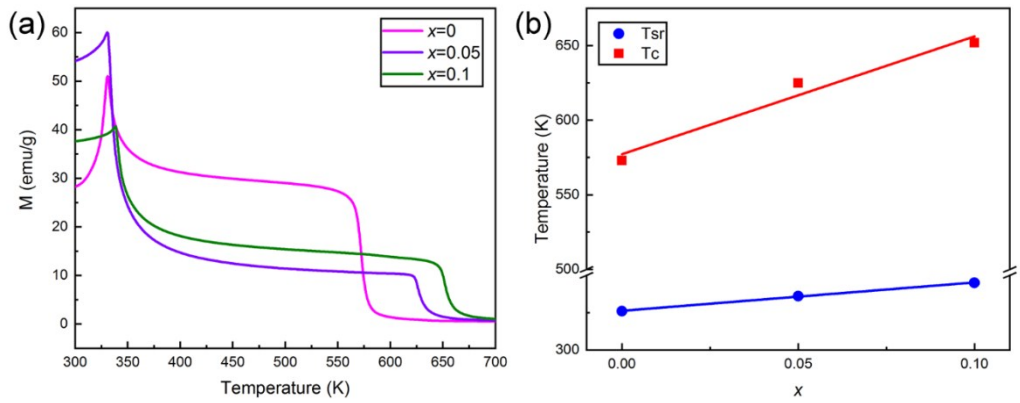

Figure S3. (a) Temperature dependence of magnetizations at magnetic field of 0.1 T for $Er_2(Fe_{1-x}Co_x)_{14}B$ intermetallic compounds (x = 0, 0.05, and 0.1). (b) The temperature of spin reorientation (T_{SR}) and Curie point (T_C) as function of Co content.

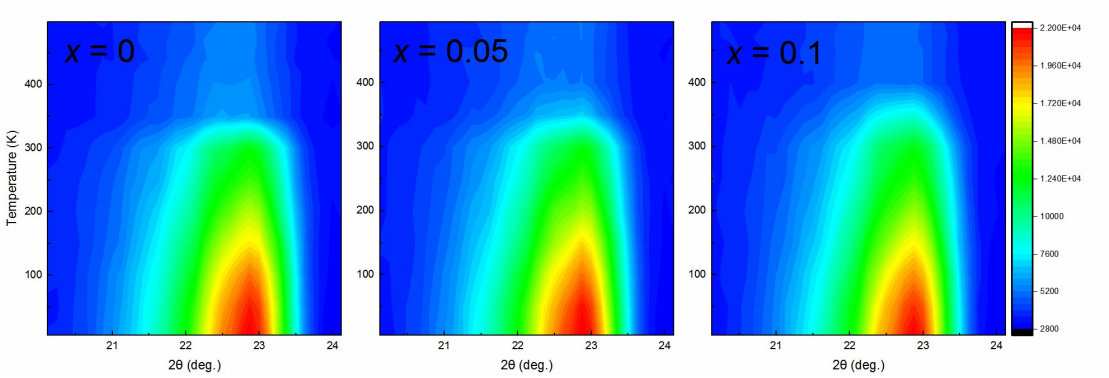

Figure S4. The temperature dependence of contour plots of the (002) NPD peak intensity for various x.

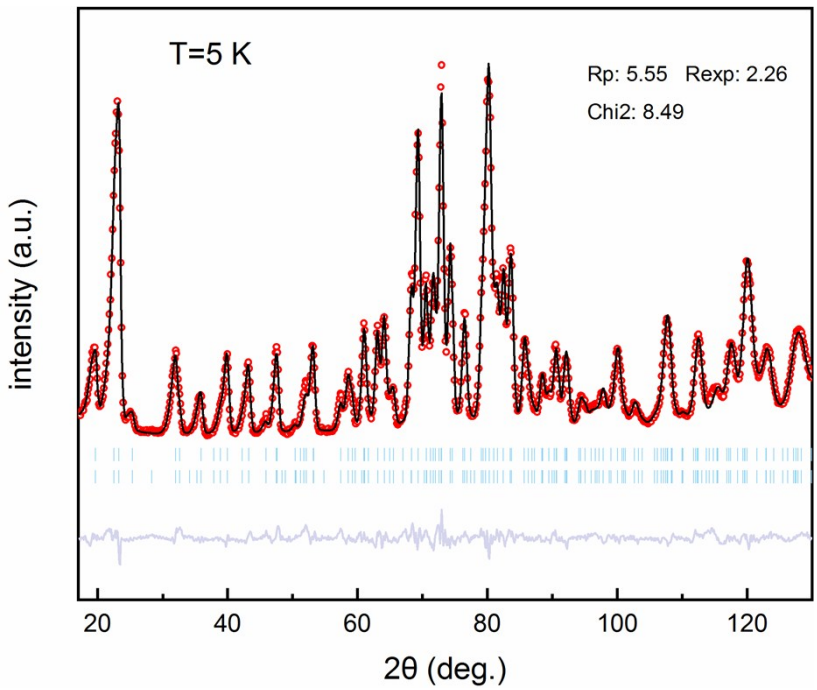

Figure S5. The refinement of the NPD pattern at 5 K for $Er_2Fe_{14}B$.

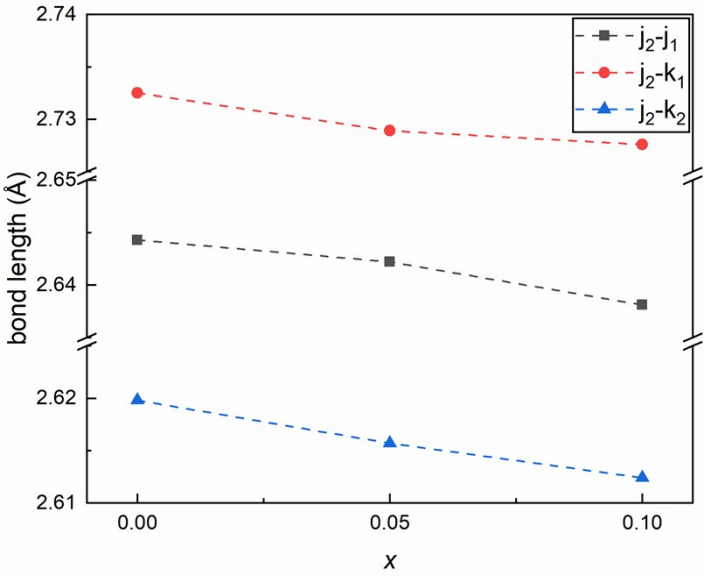

Figure S6. The band lengths between Fe(j_2) and Fe(j_1), Fe(k_1), Fe(k_2) with various Co contents.

Table S1. The structural parameters obtained by the SXRD and NPD refinement of $Er_2(Fe_{0.9}Co_{0.1})_{14}B$.

SXRD					NPD					
Atom	123 K				Atom	5 K				
	x	*y*	*z*	Occ		*x*	*y*	*z*	Occ	M(μ_B)
Er(4f)	0.2677(1)	0.2677(1)	0	1	Er(4f)	0.2682(4)	0.2682(4)	0	1	7.774(130)
Er(4g)	0.1438(1)	0.8561(1)	0	1	Er(4g)	0.1446(5)	0.8553(5)	0	1	7.774(130)
Fe($16k_1$)	0.2235(1)	0.5665(1)	0.1259(1)	0.9	Fe($16k_1$)	0.2214(6)	0.5646(5)	0.1270(4)	0.863(12)	2.469(94)
Fe($16k_2$)	0.0380(1)	0.3573(1)	0.1737(1)	0.9	Fe($16k_2$)	0.0394(5)	0.3589(5)	0.1750(3)	0.827(10)	2.499(88)
Fe($8j_1$)	0.0981(1)	0.0981(1)	0.1995(1)	0.9	Fe($8j_1$)	0.0964(4)	0.0964(4)	0.1997(4)	0.832(10)	2.689(94)
Fe($8j_2$)	0.3177(1)	0.3177(1)	0.2458(1)	0.9	Fe($8j_2$)	0.3188(4)	0.3188(4)	0.2464(4)	1	3.146(101)
Fe(4e)	0	0	0.6164(2)	0.9	Fe(4e)	0	0	0.6198(8)	0.880(16)	2.519(149)
Fe(4c)	0	0.5	0	0.9	Fe(4c)	0	0.5	0	0.996(8)	3.243(125)
Co($16k_1$)	0.2235(1)	0.5665(1)	0.1259(1)	0.1	Co($16k_1$)	0.2214(6)	0.5646(5)	0.1271(4)	0.137(12)	2.469(94)
Co($16k_2$)	0.0380(1)	0.3573(1)	0.1737(1)	0.1	Co($16k_2$)	0.0394(5)	0.3589(5)	0.1750(3)	0.173(10)	2.499(88)
Co($8j_1$)	0.0981(1)	0.0981(1)	0.1995(1)	0.1	Co($8j_1$)	0.0964(4)	0.0964(4)	0.1997(4)	0.168(10)	2.689(94)
Co($8j_2$)	0.3177(1)	0.3177(1)	0.2458(1)	0.1	Co($8j_2$)	0.3188(4)	0.3188(4)	0.2464(4)	0	3.146(101)
Co(4e)	0	0	0.6164(2)	0.1	Co(4e)	0	0	0.6198(8)	0.120(16)	2.519(149)
Co(4c)	0	0.5	0	0.1	Co(4c)	0	0.5	0	0.004(8)	3.243(125)
B(4g)	0.3619(13)	0.6381(13)	0		B(4g)	0.3674(11)	0.6325(11)	0		
a		8.7315(2)			*a*		8.7317(5)			
c		11.9240(2)			*c*		11.9231(7)			
Rp		5.36			Rp		5.61			
Rexp		1.12			Rexp		2.3			