Supplementary Information for

"Ternary borides $Nb_7Fe_3B_8$ and $Ta_7Fe_3B_8$ with Kagome-type iron framework"

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Table S1. Anisotropic displacement parameters (in Å^2) for $Nb_7Fe_3B_8$ and $Ta_7Fe_3B_8$

atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
$Nb_7Fe_3B_8$						
Nb1	0.26(2)	B_{11}	0.29(3)	$1/2B_{11}$	0	0
Nb2	0.24(1)	0.29(1)	0.32(1)	$1/2B_{22}$	0	0
Fe	0.27(2)	0.35(2)	0.50(3)	$1/2B_{22}$	0	0
B1	0.4(1)	B_{11}	0.4(2)	$1/2B_{11}$	0	0
B2	0.5(1)	0.6(1)	0.4(1)	$1/2B_{22}$	0	0
$Ta_7Fe_3B_8$						
Ta1	0.07(2)	B_{11}	0.41(4)	$1/2B_{11}$	0	0
Ta2	0.12(2)	0.17(2)	0.44(2)	$1/2B_{22}$	0	0
Fe	0.14(5)	0.24(7)	0.58(7)	$1/2B_{22}$	0	0

Table S2. Crystallographic data for NbFeB and TaFeB

Composition	NbFeB	TaFeB
Crystal system	hexagonal	
Space group	$P\bar{6}2m$	
Lattice parameters*		
a /Å	6.0082(1)	5.9837(1)
c /Å	3.2109(1)	3.2041(1)
V /Å^3	100.380(7)	99.352(7)
Formula unit/cell, Z	3	3
Calculated density/(g cm^{-3})	7.9184(5)	12.4144(8)
Diffraction system	Huber Image Plate Guinier Camera G670	
Radiation; wavelength	Cu-$K_{\alpha 1}$; 1.54056 Å	
Profile range / ° 2θ	3.0-100.3	
Step size / ° 2θ	0.005	
R_I, R_P	0.036, 0.108	0.034, 0.091

* From Powder XRD data with LaB6 as an internal standard

Table S3. Atomic coordinates and isotropic displacement parameters for NbFeB and TaFeB

atom	*site*	*x*	*y*	*z*	B_{iso}/B_{eq}
NbFeB					
Nb	3*g*	0.58651(5)	0	1/2	0.22(1)
Fe	3*f*	0.2427(2)	0	0	1.05(2)
B1	1*b*	0	0	1/2	0.9(2)
B2	2*c*	1/3	2/3	0	1.7(2)
TaFeB					
Ta1	3*g*	0.58745(5)	0	1/2	0.21(1)
Fe	3*f*	0.2396(3)	0	0	1.09(3)
B1	1*b*	0	0	1/2	1.0*
B2	2*c*	1/3	2/3	0	1.0*

* Fixed to be 1.0

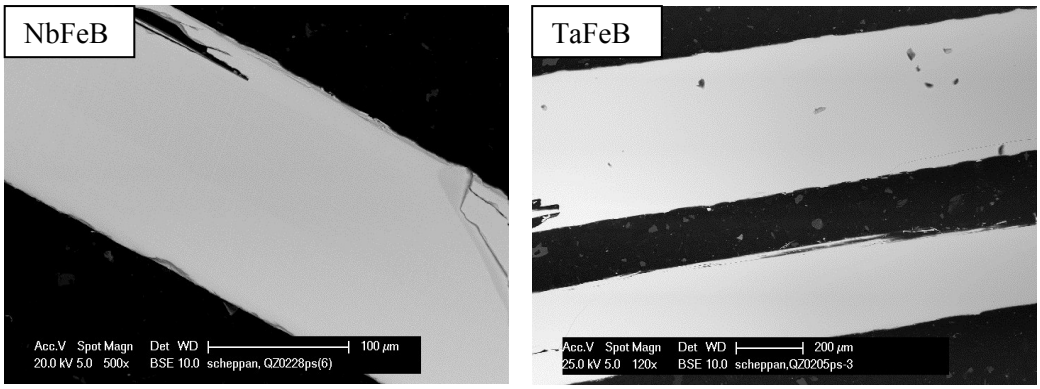

Fig. S1 SEM images for NbFeB and TaFeB single crystals

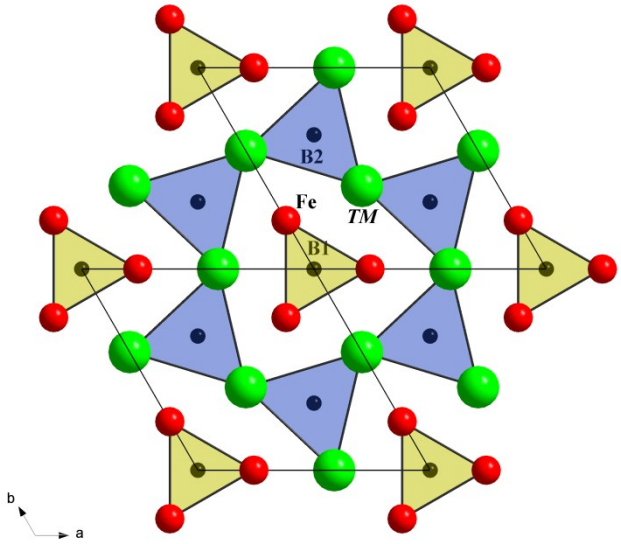

Fig. S2 Crystal structure of *TM*FeB, which is constructed by [BFe$_6$] and [B*TM*$_6$] trigonal prisms

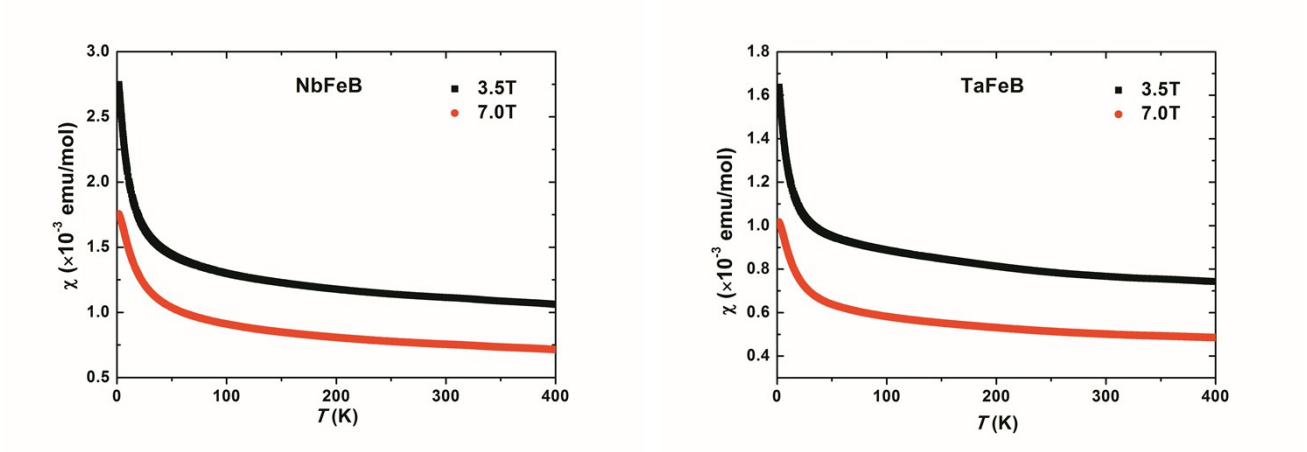

Fig. S3 Magnetic data for NbFeB and TaFeB.