Supporting Information for:

Fragile magnetic ordering between robust 2D-ferrimagnets in the AFe$_3$(SeO$_3$)$_2$F$_6$ (A=K, Rb, Cs) series

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Figure S12. (a) The temperature dependence of C_p/T under 0 Oe in $AFe_3(SeO_3)_2F_6$ (A= K,Rb), (b) The temperature dependence of C_p under 10 Oe in $AFe_3(SeO_3)_2F_6$ (A= K,Rb).

Figure S13. (a) The isothermal initial magnetization around T_c for $RbFe_3F_6(SeO_3)_2$, (b) the Arrott plot of M^2 vs. H/M.

Figure S14. The isotherms of $M^{1/\beta}$ vs. $(H/M)^{1/\gamma}$ with parameters of (a)3D-XY model, (b) 3D-Heisenberg model, (c)3D-tricritical mean field model, (d) 3D-Ising model.

Table S1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters of $KFe_3(SeO_3)_2F_6$.

Table S2. Harmonic displacement parameters obtained for the compound $KFe_3(SeO_3)_2F_6$.

Table S3.Bond lengths (Å) and Band angles (degrees) of $KFe_3(SeO_3)_2F_6$.

Table S4. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters of $RbFe_3(SeO_3)_2F_6$.

Table S5. Harmonic displacement parameters obtained for the compound $RbFe_3(SeO_3)_2F_6$.

Table S6. Bond lengths (Å) and Band angles (degrees) of $RbFe_3(SeO_3)_2F_6$.
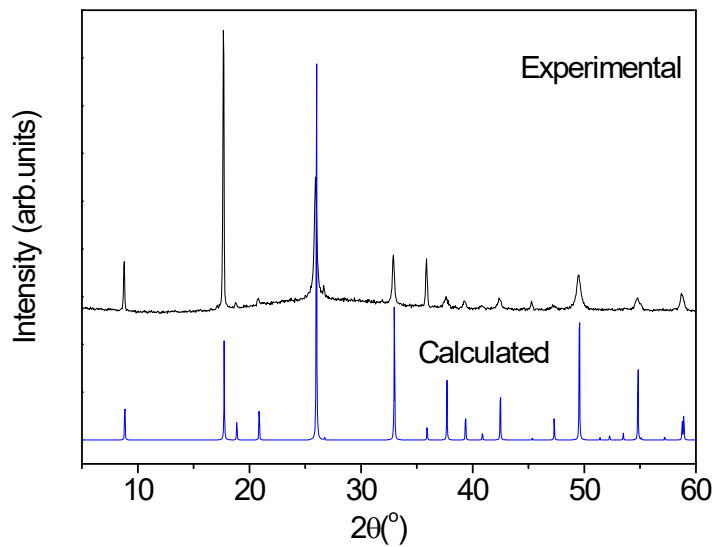
Table S7. BVS of $AFe_3(SeO_3)_2F_6$ (A=K, and Rb).

Figure S1. Calculated and observed powder X-ray diffraction patterns for $KFe_3(SeO_3)_2F_6$.

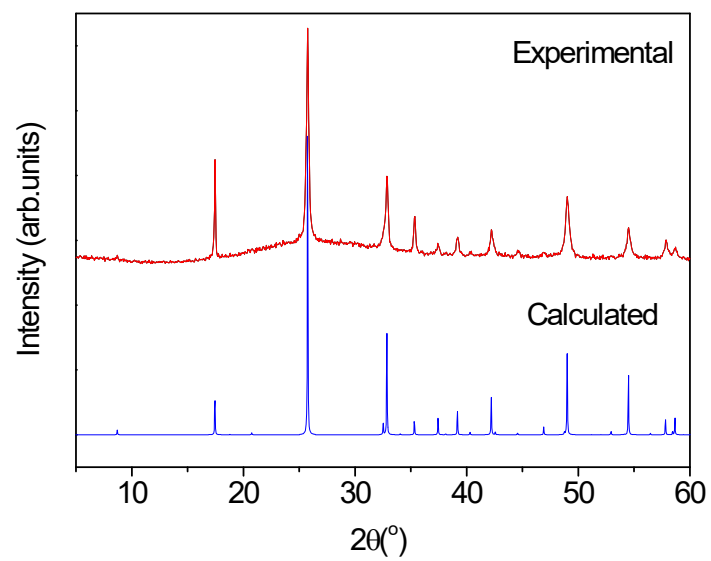Figure S2. Calculated and observed powder X-ray diffraction patterns for $RbFe_3(SeO_3)_2F_6$.

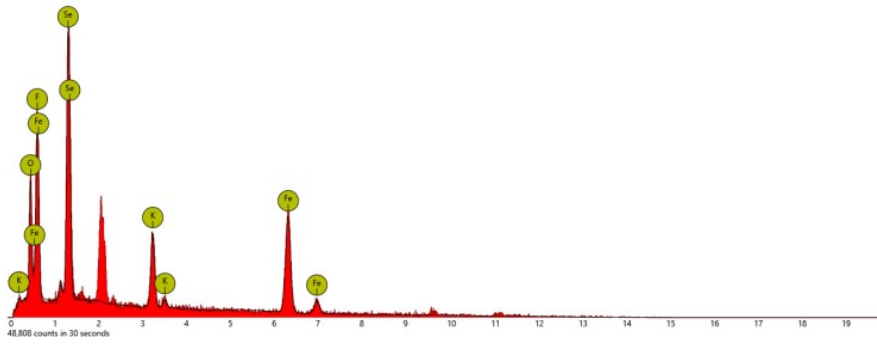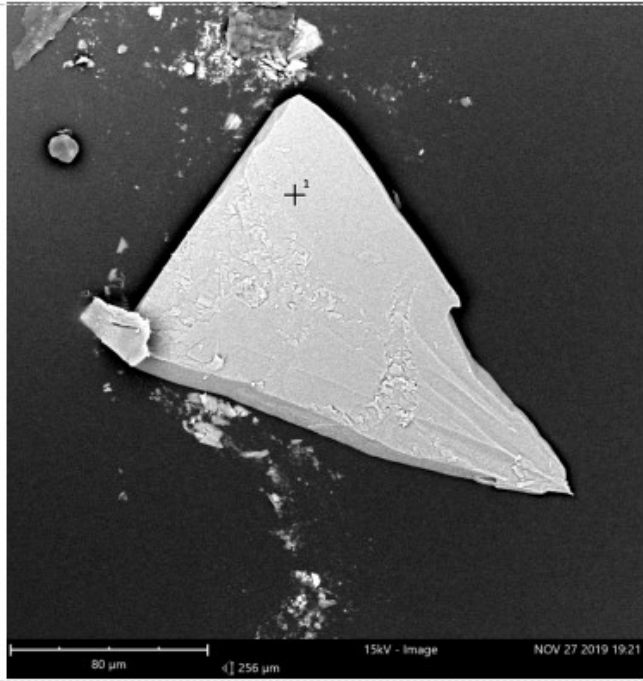Figure S3. The corresponding EDX spectra for $KFe_3(SeO_3)_2F_6$.
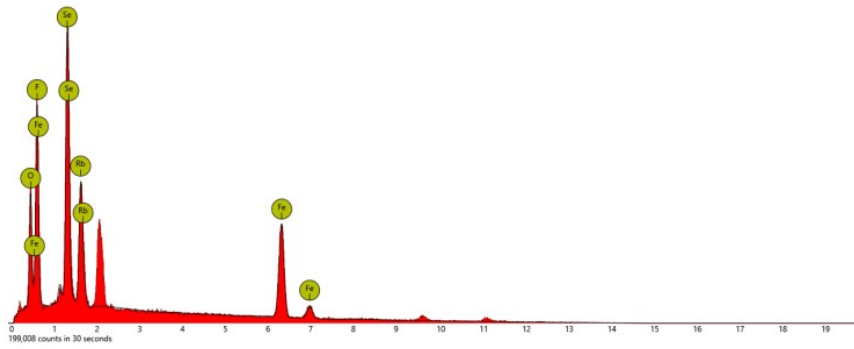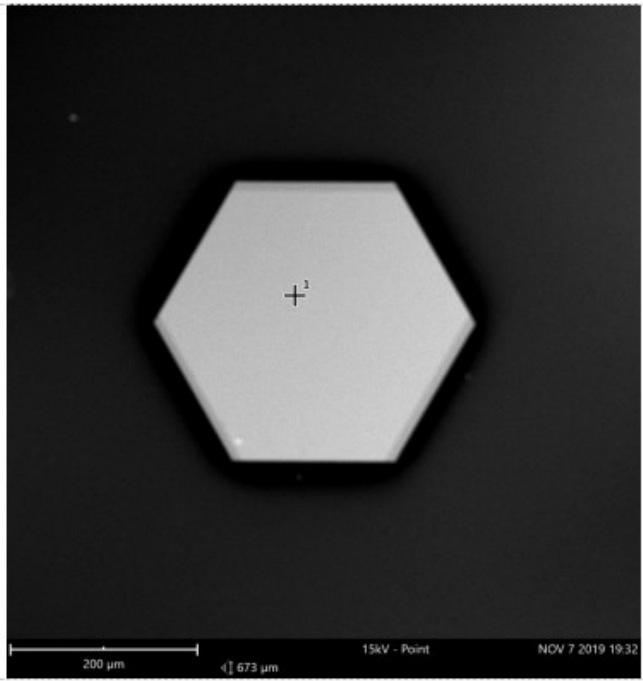
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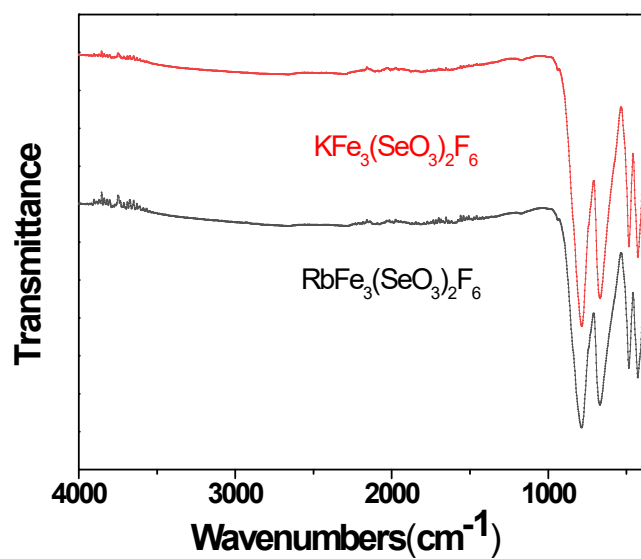
Figure S5. Infrared spectra of $AFe_3(SeO_3)_2F_6$ (A=K, and Rb).
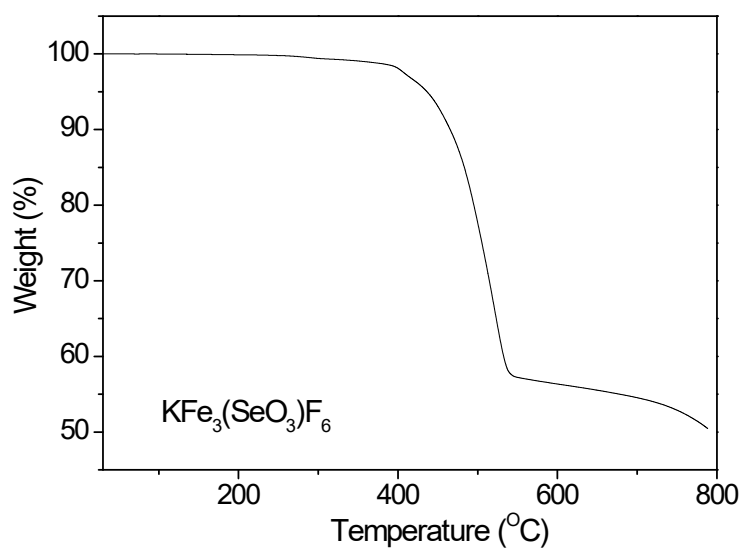
Figure S6. TGA diagram for $KFe_3(SeO_3)_2F_6$.
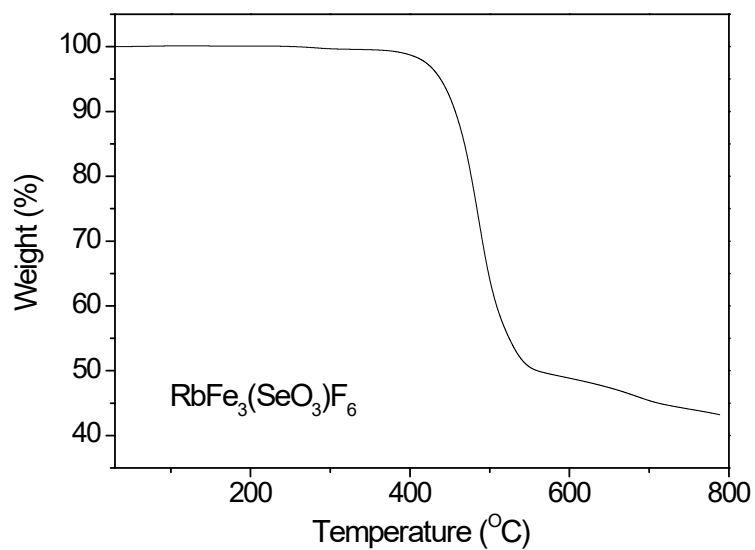
Figure S7. TGA diagram for $RbFe_3(SeO_3)_2F_6$.

FM : $E = E0 + (12 J_{intra} + 6 J_{inter})n^2/4$

AFM1: $E = E0 + (- 12 J_{intra} + 6 J_{inter})n^2/4$

AFM2 : $E = E0 + (12 J_{intra} - 6 J_{inter})n^2/4$
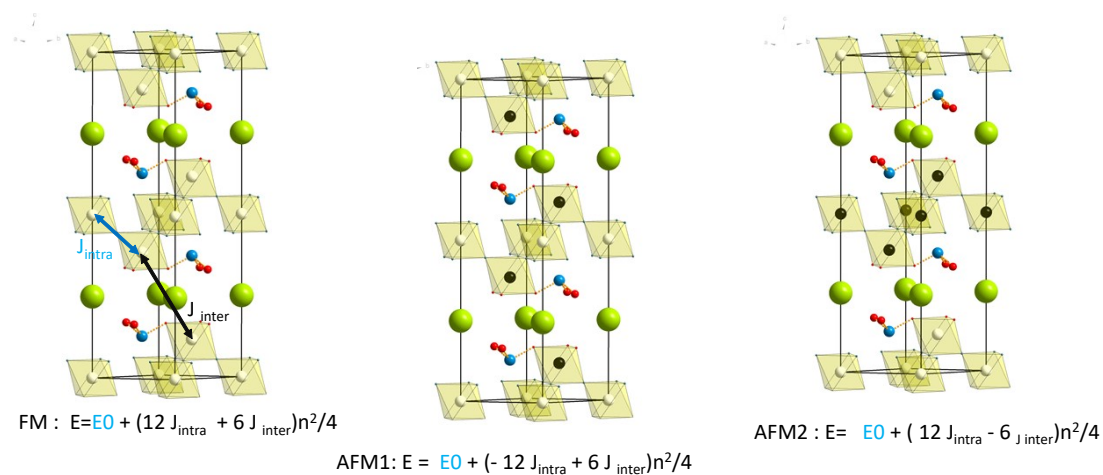
Figure S8. the three configurations and their energy used by DFT +U with polarized spins (white and black Fe atoms represent up and down spins). n=5 electron per site for Fe^{3+}, E0 is the energy of the system besides magnetic perturbations.
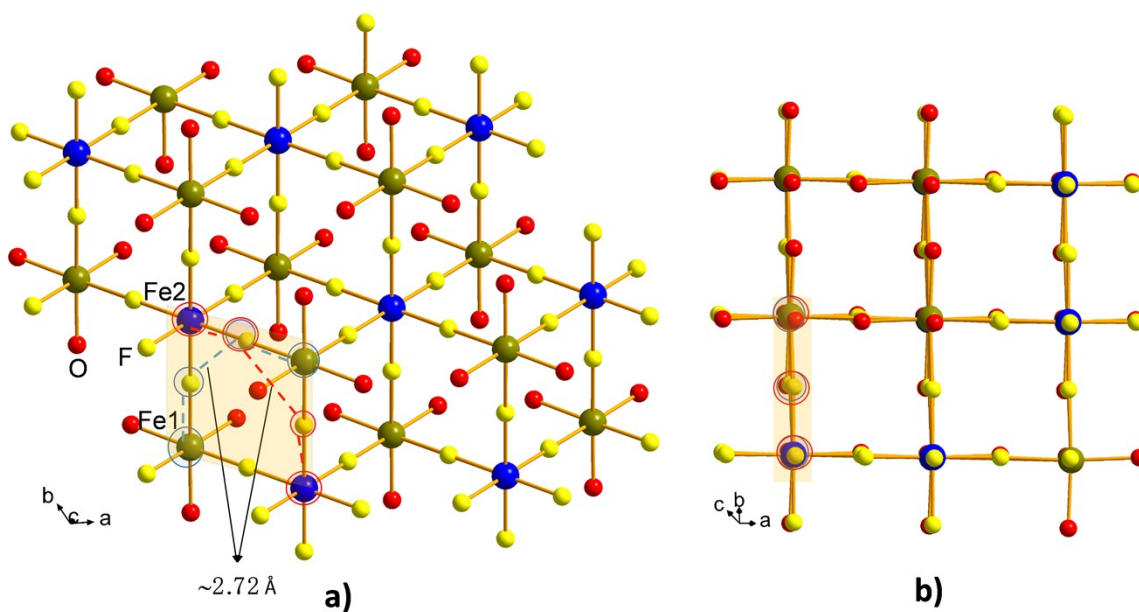
Figure S9. 2D $[Fe_3(SeO_3)_2F_6]^-$ block along different axis, where Fe-F-F-Fe super-exchange paths (a) and Fe-F-F-Fe dihedral angles (b) are highlighted respectively.
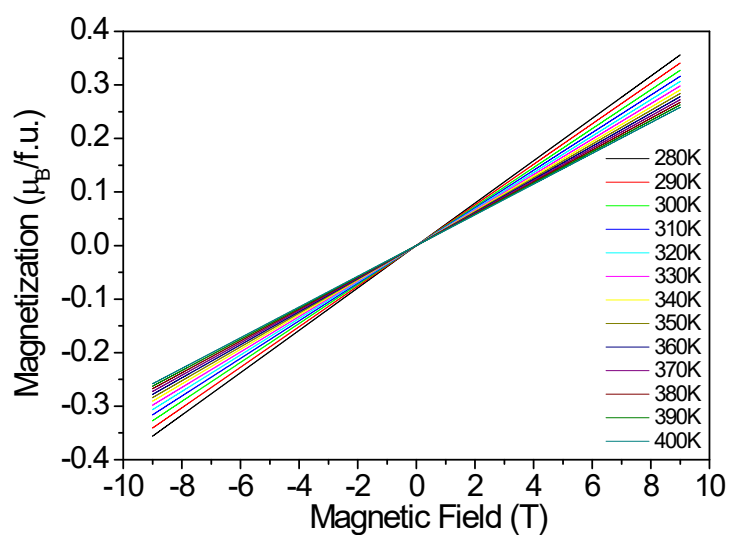
Figure S10. Field dependence of Magnetization for $KFe_3(SeO_3)_2F_6$ between 280K and 400K.
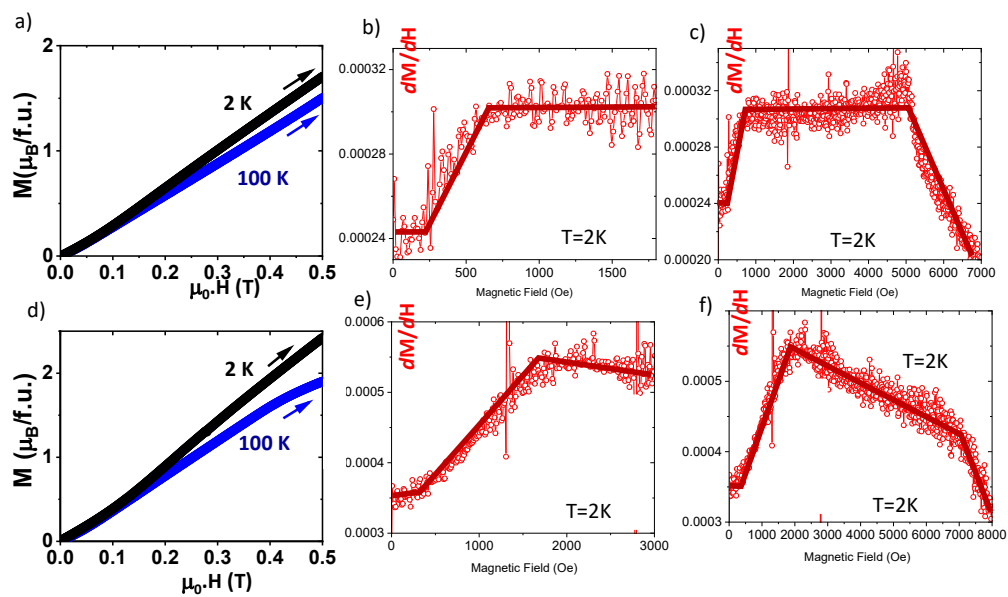
Figure S11. M(H) and dM/dH curves at different low Field for $AFe_3(SeO_3)_2F_6$ (A=K(a,b,c,) Rb (d,e,f))
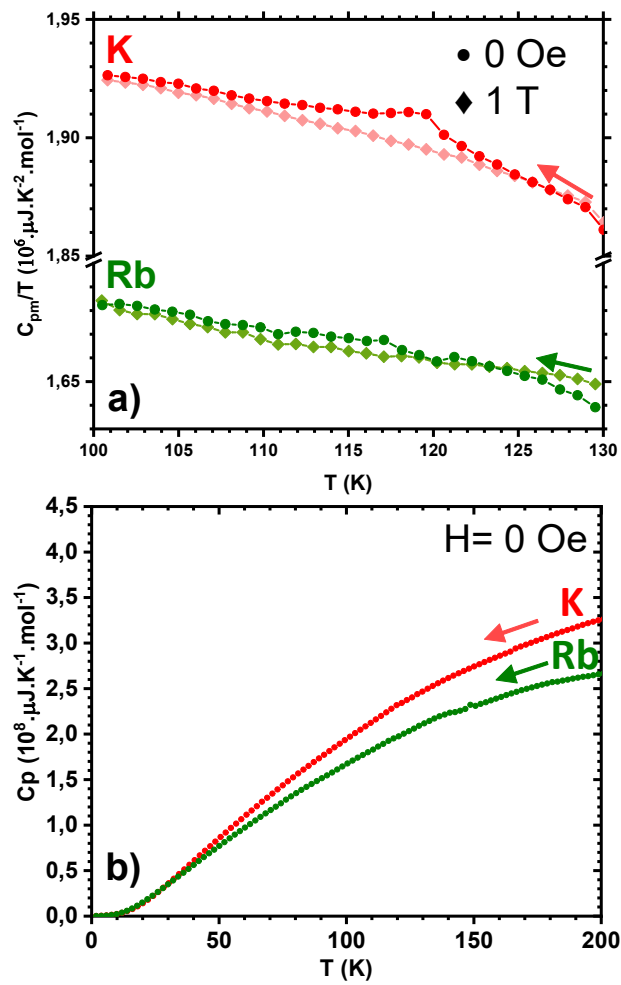
Figure S12. (a) The temperature dependence of C_p/T under 0 Oe and 1T in $AFe_3(SeO_3)_2F_6$ (A= K,Rb), (b) The temperature dependence of C_p under 0 Oe in $AFe_3(SeO_3)_2F_6$ (A= K,Rb).
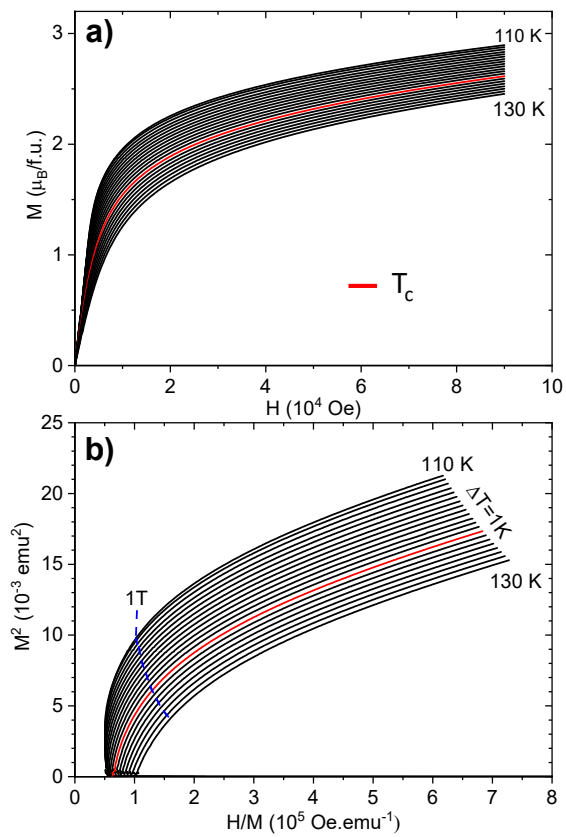
Figure S13 (a) The isothermal initial magnetization around T_c for $RbFe_3F_6(SeO_3)_2$, (b) the Arrott plot of M^2 vs. H/M.
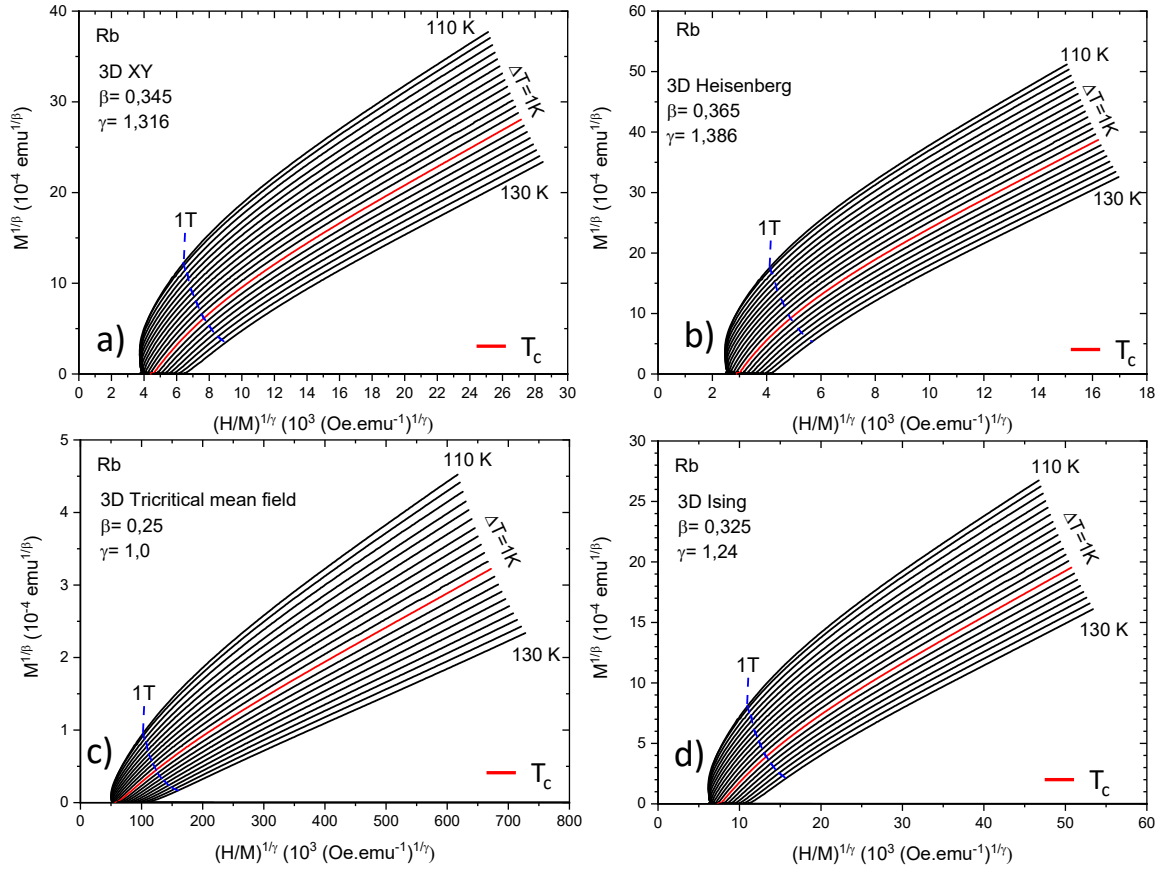
Figure S14 The isotherms of $M^{1/\beta}$ vs. $(H/M)^{1/\gamma}$ with parameters of (a)3D-XY model, (b) 3D-Heisenberg model, (c)3D-tricritical mean field model, (d) 3D-Ising model.

Table S1: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters of $KFe_3(SeO_3)_2F_6$.

	Wyck.	x	y	z	Uiso*/Ueq	Occ.(<1)
K1	1b	0	0	0.5	0.0360(12)	1
Fe1	2d	0.3333	0.6667	0.23621(13)	0.0075(4)	1
Fe2	1a	0	0	0	0.0052(5)	1
Se1	2d	0.6667	0.3333	0.25824(9)	0.0083(3)	1
F1	6i	0.1663(3)	0.3327(7)	0.1113(3)	0.0190(8)	1
O1	6i	0.5077(5)	0.4923(5)	0.3387(4)	0.0182(9)	1

Table S2. Harmonic displacement parameters obtained for the compound $KFe_3(SeO_3)_2F_6$.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
K1	0.0418(15)	0.0418(15)	0.025(2)	0.0209(8)	0	0
Fe1	0.0067(5)	0.0067(5)	0.0093(7)	0.0033(2)	0	0
Fe2	0.0052(6)	0.0052(6)	0.0053(9)	0.0026(3)	0	0
Se1	0.0080(4)	0.0080(4)	0.0091(5)	0.00398(18)	0	0

Table S3. Bond lengths (Å) and Band angles (degrees) of $KFe_3(SeO_3)_2F_6$.

Atom1	Atom2	distances	Band angles	degrees
K1	O1×12	3.156(3)	F1-Fe1-F1×3	85.35(12)
Fe1	F1×3	2.005(3)	F1-Fe1-O1×6	89.89(14)
	O1×3	1.933(3)	F1-Fe1-O1×3	173.52(16)
Fe2	F1×6	1.919(3)	O1-Fe1-O1×3	94.50(15)
Se1	O1×3	1.697(3)	F1-Fe2-F1×6	89.76(12)
			F1-Fe2-F1×6	90.24(10)
			F1-Fe2-F1×3	180.0(5)
			O1-Se1-O1×3	99.37(16)
			Fe1-F1-Fe2	176.95(19)

Table S4: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters of $RbFe_3(SeO_3)_2F_6$.

	Wyck.	x	y	z	Uiso*/Ueq	Occ.(<1)
Rb1	1a	0	0	0.5	0.0236(5)	1
Fe1	2d	0.3333	0.6667	0.23188(11)	0.0082(4)	1
Fe2	1b	0	0	0	0.0070(5)	1
Se1	2d	0.6667	0.3333	0.25402(8)	0.0099(3)	1
F1	6i	0.1664(4)	0.3329(7)	0.1088(3)	0.0183(8)	1
O1	6i	0.5074(5)	0.4926(5)	0.3329(3)	0.0130(9)	1

Table S5. Harmonic displacement parameters obtained for the compound $RbFe_3(SeO_3)_2F_6$.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rb1	0.0247(6)	0.0247(6)	0.0215(7)	0.0123(3)	0.00000	0.00000
Fe1	0.0072(5)	0.0072(5)	0.0100(7)	0.0036(2)	0.00000	0.00000
Fe2	0.0069(6)	0.0069(6)	0.0069(8)	0.0034(3)	0.00000	0.00000
Se1	0.0092(4)	0.0092(4)	0.0113(5)	0.00459(18)	0.00000	0.00000

Table S6. Bond lengths (Å) and Band angles (degrees) of $RbFe_3(SeO_3)_2F_6$.

Atom1	Atom2	distances	Band angles	degrees
Rb1	O1×12	3.210(2)	F1-Fe1-F1×3	85.42(12)
Fe1	F1×3	2.011(3)	F1-Fe1-O1×6	89.85(13)
	O1×3	1.937(3)	F1-Fe1-O1×3	173.56(14)
Fe2	F1×6	1.920(3)	O1-Fe1-O1×3	94.52(13)
Se1	O1×3	1.703(3)	F1-Fe2-F1×6	90.18(12)
			F1-Fe2-F1×6	89.82(9)
			F1-Fe2-F1×3	180.0(5)
			O1-Se1-O1×3	99.65(15)
			Fe1-F1-Fe2	176.69(18)

Table S7. BVS of $AFe_3(SeO_3)_2F_6$ (A=K, and Rb).

	$KFe_3(SeO_3)_2F_6$				$RbFe_3(SeO_3)_2F_6$		
Atom	V_{K*}	V_{Fe*}	V_{Se*}	**Atom**	V_{Rb*}	V_{Fe*}	V_{Se*}
K(1)	0.753(2)			Rb(1)	0.928(2)		
Fe(1)		3.12(1)		Fe(1)		3.08(1)	
Fe(2)		3.14(1)		Fe(2)		3.12(1)	
Se(1)			4.08(2)	Se(1)			4.02(2)
Atom	V_{F*}	V_{O*}		**Atom**	V_{F*}	V_{O*}	
F(1)	-0.94(1)			F(1)	-0.93(1)		
O(1)		-2.11(1)		O(1)		-2.11(2)	

* (R, b) parameters being for K^+-O (2.132, 0.37), K^+-F (1.992, 0.37), Rb^+-O (2.263, 0.37), Rb^+-F (2.16, 0.37), Fe^{3+}-O (1.759, 0.37), Fe^{3+}-F (1.679, 0.37), and Se^{6+}-O (1.788, 0.37)