Supporting Information

"Rapid Molten-salt Syntheses of Sr_2FeReO_6, Ba_2FeReO_6 and Sr_2CrReO_6 : Particle Sizes, B/B'-Site Disorder, and Magnetic Properties"

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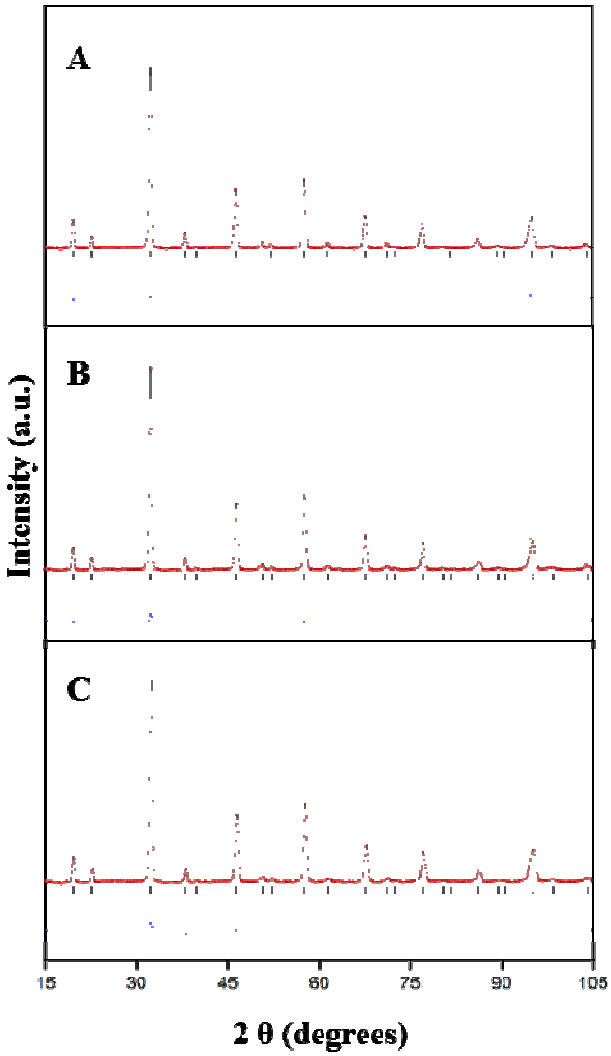

Figure S1. PXRD Rietveld refinement results for Sr_2CrReO_6 synthesized using a molten NaCl/KCl flux at (A) a 1:1 flux for 6h and slow cooling over 2 days, (B) a 3:1 flux for 6h and rapidly quenched and (C) a 3:1 flux for 6h radiatively cooled. The observed profile is indicated by the circles and the calculated profile by the solid line. Bragg peak positions are indicated by vertical peaks. The difference diffractogram is shown at the bottom.

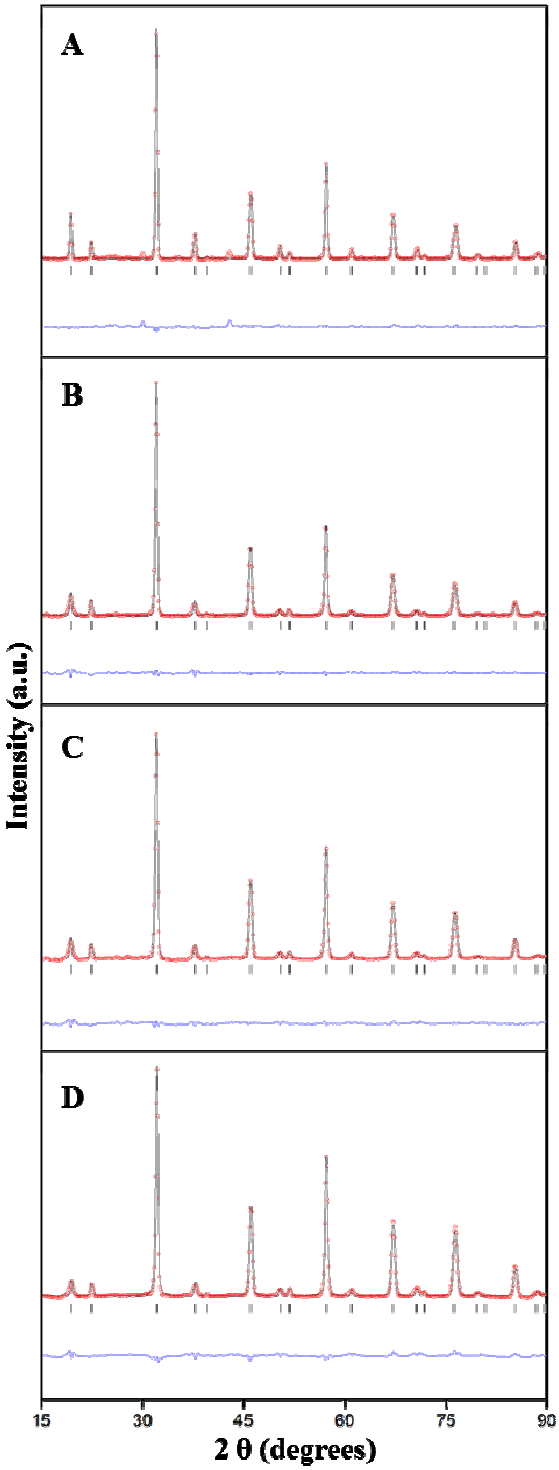

Figure S2. PXRD Rietveld refinement results for Sr_2FeReO_6 synthesized by (A) solid state method; using a molten NaCl/ KCl flux at (B) a 1:1 flux for 12h, (C) a 1:1 flux for 3h and (D) a 0.5:1 flux for 3h. The observed profile is indicated by the circles and the calculated profile by the solid line. Bragg peak positions are indicated by vertical peaks. The difference diffractogram is shown at the bottom.

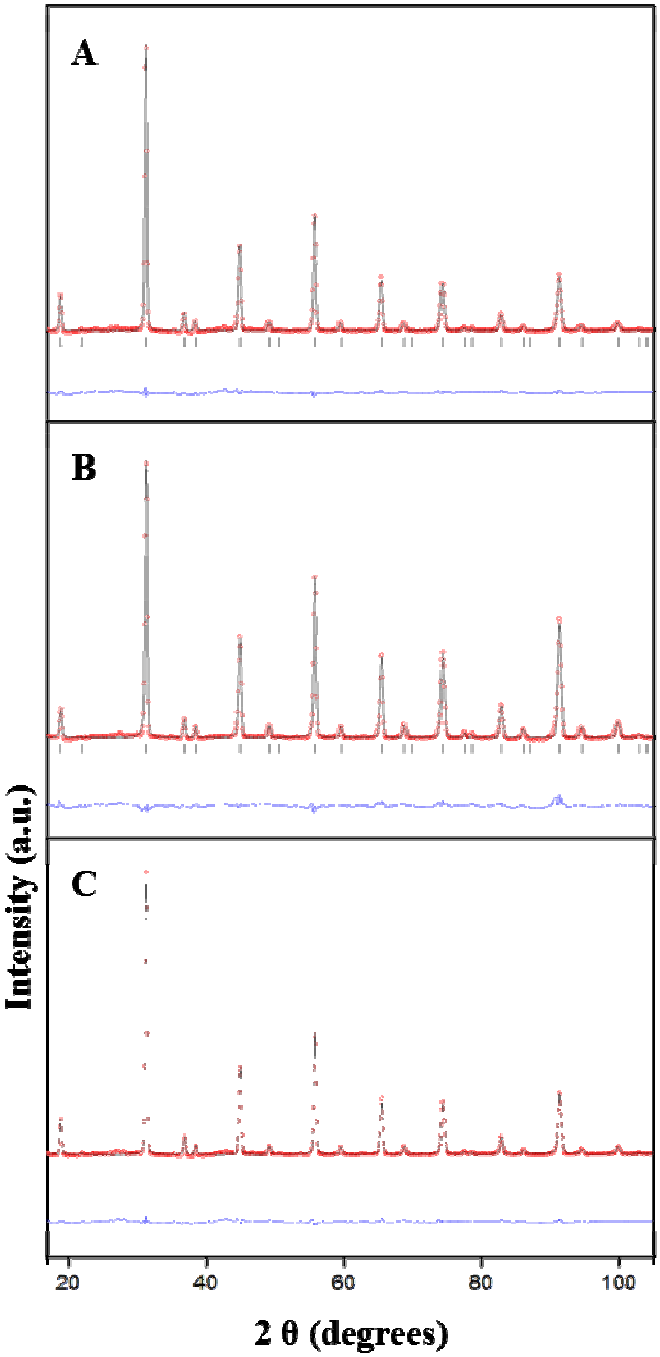

Figure S3. PXRD Rietveld refinement results for Ba_2FeReO_6 synthesized by using a molten NaCl/KCl flux at (A) a 3:1 flux for 6h and slow cooling over 24h, (B) a 3:1 flux for 6h and rapidly quenched and (C) a 3:1 flux for 6h radiatively cooled. The observed profile is indicated by the circles and the calculated profile by the solid line. Bragg peak positions are indicated by vertical peaks. The difference diffractogram is shown at the bottom.

Table S1. PXRD refinement data for Ba_2FeReO_6.

Ba_2FeReO_6				
fw	612.7			
Space group, *Z*	*F m-3m*			
Radiation	$K\alpha_1$ = 1.54059 Å, $K\alpha_1/K\alpha_2$ = 1.996			
	1:1	3:1	3:1, quenched	3:1, 24 h
Unit cell (Å), *a*	8.0540(3)	8.0533(3)	8.0536(4)	8.0548(7)
2θ range	16.5-110.0	14.0-115.0	16.5-110.0	16.5-110.0
Number of data points	936	1011	936	936
Number of variables	32	24	16	28
Background polynomial	8	8	9	8
R_{wp}	1.39%	1.71%	1.99%	1.83%
R_{exp}	2.17%	2.78%	2.24%	1.46%

Table S2. PXRD refinement data for Sr_2FeReO_6.

Sr_2FeReO_6					
fw	513.2				
Space group, *Z*	*I 4/m*				
Radiation	$K\alpha_1$ = 1.54059 Å, $K\alpha_1/K\alpha_2$ = 1.996				
	0.5:1, 3 h	0.5:1, 12 h	1:1, 3 h	1:1, 12 h	Solid state
Unit cell (Å), *a*	5.5672(3)	5.5644(4)	5.5649(4)	5.5655(2)	5.5585(3)
c	7.9003(8)	7.8962(8)	7.8986(9)	7.8990(7)	7.8969(5)
2θ range	14.0-110.0	12.9-92.0	10.2-95.0	120.0-90.0	10.2-95.0
Number of data points	961	792	849	781	849
Number of variables	24	30	27	16	27
Background polynomial	9	6	8	7	8
R_{wp}	2.19%	1.8%	2.64%	2.5%	2.37%
R_{exp}	1.68%	1.41%	3.47%	1.37%	3.1%

Table S3. PXRD refinement data for Sr_2CrReO_6.

Sr_2CrReO_6				
fw	509.4			
Space group, *Z*	*F m-3m*			
Radiation	$K\alpha_1$ = 1.54059 Å, $K\alpha_1/K\alpha_2$ = 1.996			
	1:1	3:1	3:1, quenched	1:1, 48 h
Unit cell (Å), *a*	7.8077(5)	7.8080(3)	7.8075(5)	7.8085(5)
2θ range	12.0-105.0	13.0-110.0	14.0-115.9	13.0-115.0
Number of data points	931	971	1021	1021
Number of variables	28	9	12	23
Background polynomial	9	7	8	8
R_{wp}	2.57%	2.72%	2.95%	2.85%
R_{exp}	1.66%	1.96%	1.23%	1.77%

Table S4. PXRD refinement results including thermal parameters for Sr_2FeReO_6 synthesized using a 0.5:1 flux for 12h, Ba_2FeReO_6 at a 1:1 flux for 6h radiatively cooled and Sr_2CrReO_6 at a 1:1 flux for 6h radiatively cooled.

Compound	Atoms	x	y	z	Occupancy	B (Å^2)
Sr_2FeReO_6	Sr	0	0.5	0.25	1	0.51(6)
I4/m	Fe1	0	0	0	0.8440(3)	0.3(1)
a (Å)= 5.5644(4)	Re1	0	0	0	0.1559(3)	0.3(1)
c (Å)= 7.8962(8)	Re2	0	0	0.5	0.8440(3)	0.36(7)
	Fe2	0	0	0.5	0.1559(3)	0.36(7)
	O1	0	0	0.250(3)	1	1.1(1)
	O2	0.266(5)	0.230(4)	0	1	1.1(1)
Ba_2FeReO_6	Ba	0.25	0.25	0.25	1	0.67(9)
Fm-3m	Fe1	0	0	0	0.90627(6)	0.3(1)
A= 8.0540(3)	Re1	0	0	0	0.09373(6)	0.3(1)
	Re2	0.5	0.5	0.5	0.90627(6)	0.37(7)
	Fe2	0.5	0.5	0.5	0.09373(6)	0.37(7)
	O	0.2590(7)	0	0	1	1.4(1)
Sr_2CrReO_6	Sr	0.25	0.25	0.25	1	0.50(5)
Fm-3m	Cr1	0	0	0	0.87343(5)	1.2(1)
A= 7.8077(5)	Re1	0	0	0	0.12657(5)	1.2(1)
	Re2	0.5	0.5	0.5	0.87343(5)	0.72(7)
	Cr2	0.5	0.5	0.5	0.12657(5)	0.72(7)
	O	0.2479(6)	0	0	1	0.84(9)

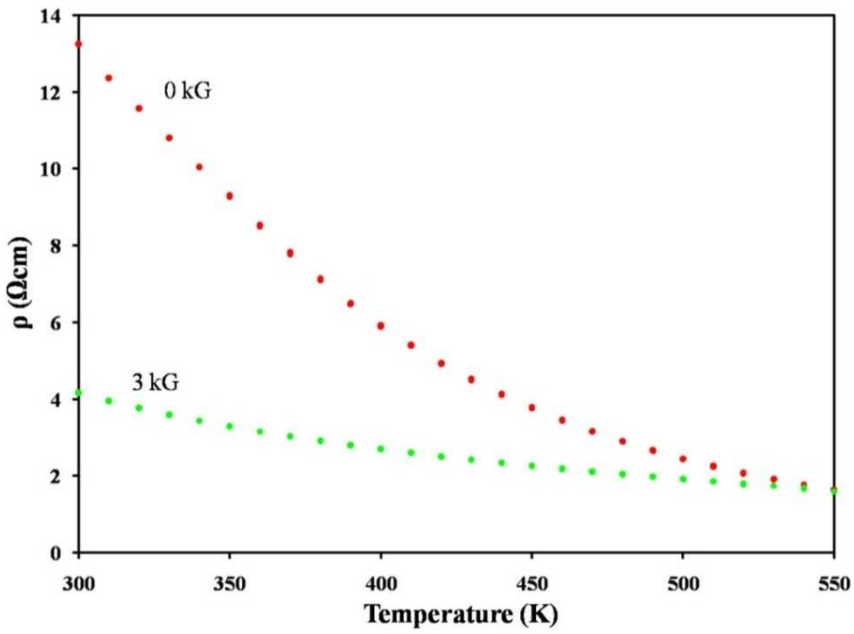

Figure S4. Temperature-dependent resistivity measurements at 0 kG and 3 kG for Sr_2CrReO_6 particles prepared by a NaCl/KCl flux synthesis at 800°C for 6 h using a 1:1 flux:product molar ratio radiatively cooled.

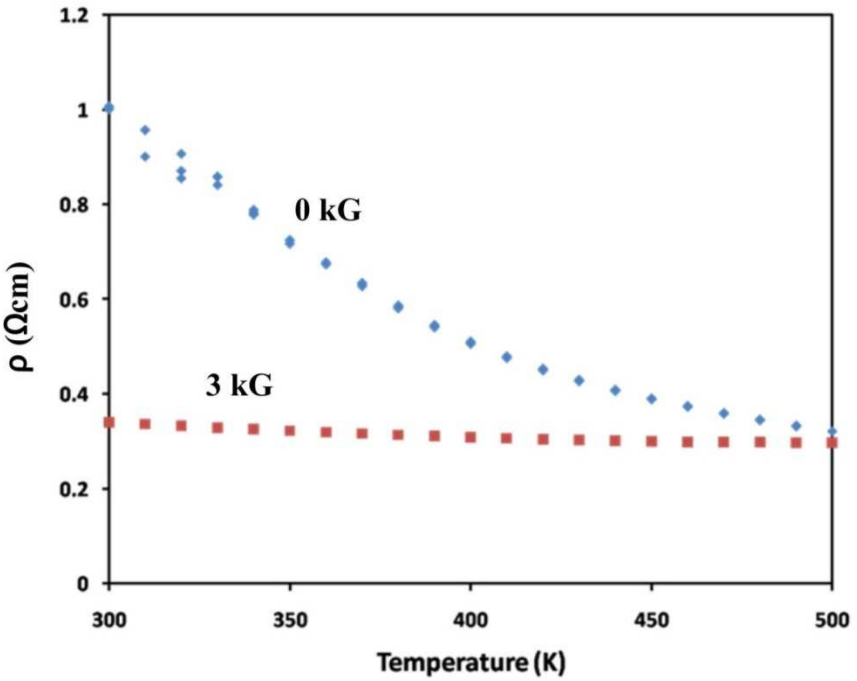

Figure S5. Temperature-dependent resistivity measurements at 0 kG and 3 kG for Ba_2FeReO_6 particles prepared by a NaCl/KCl flux synthesis at 800°C for 6 h using a 1:1 flux:product molar ratio radiatively cooled.