Supporting Information

for

Crystal structure and ferrimagnetism of $AgCo_3Cr(MoO_4)_5$ with mixed occupation of the transition metal sites

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Table 1S. Preparation conditions of simple molybdates and silver dimolybdate

Composition	Reaction mixture	Annealing temperature, K
Ag_2MoO_4	$2AgNO_3 + MoO_3$	623−723
$Ag_2Mo_2O_7$	$Ag_2MoO_4 + MoO_3$	573−663
$NiMoO_4$	$NiO + MoO_3$	723−1023
$CoMoO_4$	$Co(NO_3)_3{\cdot}6H_2O + MoO_3$	573−1023
$Cr_2(MoO_4)_3$	$2Cr(NO_3)_3{\cdot}9H_2O + 3MoO_3$	573−1023
$Sc_2(MoO_4)_3$	$Sc_2O_3 + 3MoO_3$	723−1023
$In_2(MoO_4)_3$	$In_2O_3 + 3MoO_3$	723−1073

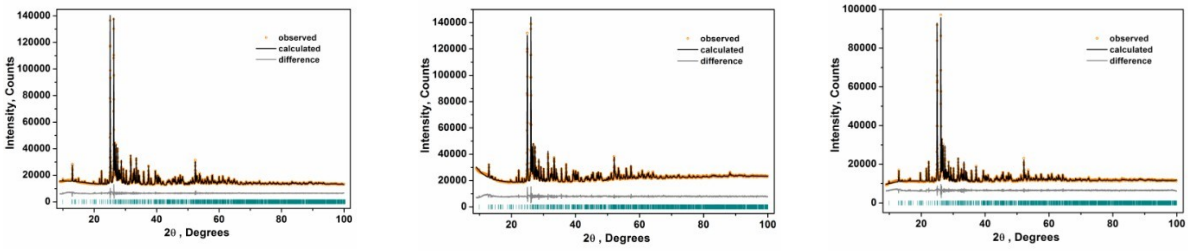


Fig. S1. Experimental, calculated and difference powder XRD patterns of $AgNi_3In(MoO_4)_5$ (left), $AgCo_3In(MoO_4)_5$ (center) and $AgCo_3Sc(MoO_4)_5$ (right). Bragg reflection positions (sp. gr. $P\bar{1}$) are marked with green vertical lines.

Table S2. Atomic coordinates and equivalent isotropic displacement parameters for $Ag_{0.92}Co_{2.93}Cr_{1.07}(MoO_4)_5$.

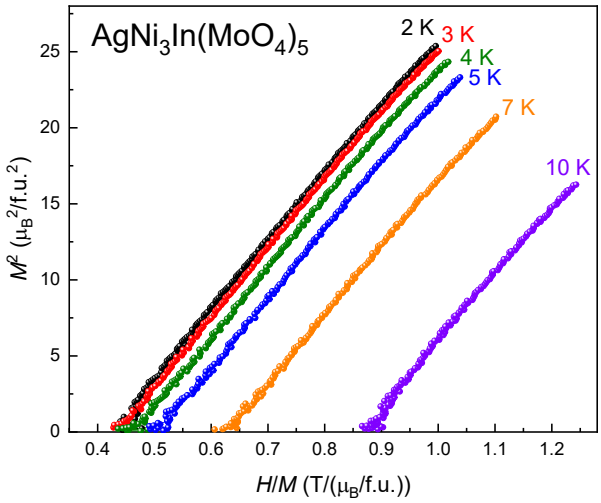
Atom	Occupancy	*x/a*	*y/b*	*z/c*	U_{eq} (Å^2)*
Mo1	1	0.27451(4)	0.30799(4)	0.52669(2)	0.00745(5)
Mo2	1	0.21304(4)	0.82551(4)	0.28461(2)	0.00795(6)
Mo3	1	0.68746(4)	0.21936(4)	0.31020(2)	0.00952(6)
Mo4	1	0.27479(4)	0.05996(3)	0.90598(2)	0.00727(5)
Mo5	1	0.24698(4)	0.54549(4)	0.08640(2)	0.00805(6)
*M*1	0.719(3)Co+0.281(3)Cr	0.18163(7)	0.82750(6)	0.49274(2)	0.00761(9)
*M*2	0.946(3)Co+0.054(3)Cr	0.16823(7)	0.08268(6)	0.11591(2)	0.00832(9)
*M*3	0.789(3)Co+0.211(3)Cr	0.77820(7)	0.42397(6)	0.12572(2)	0.00770(9)
*M*4	0.469(3)Co+0.531(3)Cr	0.24974(7)	0.30574(6)	0.73573(2)	0.00756(9)
Ag1	0.295(3)	0.1457(5)	0.3429(4)	0.2789(3)	0.0379(7)
Ag2	0.306(3)	0.1126(6)	0.3362(4)	0.3185(3)	0.0293(10)
Ag3	0.322(3)	0.1131(6)	0.3425(6)	0.3415(2)	0.0298(7)
O1	1	0.5233(4)	0.2098(3)	0.50514(14)	0.0175(5)
O2	1	0.2498(4)	0.3512(4)	0.62410(13)	0.0209(6)
O3	1	0.2034(4)	0.5318(3)	0.47672(13)	0.0160(5)
O4	1	0.1257(4)	0.1321(3)	0.50369(13)	0.0126(4)
O5	1	0.1906(4)	0.8770(3)	0.38041(12)	0.0177(5)
O6	1	0.4573(4)	0.7161(3)	0.26217(13)	0.0163(5)
O7	1	0.1533(4)	0.0516(3)	0.23283(13)	0.0150(5)
O8	1	0.0498(4)	0.6616(3)	0.26674(13)	0.0153(5)
O9	1	0.4417(4)	0.2915(4)	0.33654(14)	0.0242(6)
O10	1	0.7180(4)	–0.0127(3)	0.27067(14)	0.0209(6)
O11	1	0.8280(4)	0.2045(3)	0.39180(12)	0.0158(5)
O12	1	0.7686(4)	0.3997(3)	0.24385(12)	0.0124(4)
O13	1	0.2067(4)	0.1138(3)	0.99918(12)	0.0173(5)
O14	1	0.5253(4)	–0.0368(4)	0.89493(14)	0.0192(5)
O15	1	0.1446(3)	–0.1262(3)	0.88103(12)	0.0104(4)
O16	1	0.2328(3)	0.2875(3)	0.85023(12)	0.0100(4)
O17	1	0.4802(4)	0.4570(4)	0.12224(14)	0.0196(5)
O18	1	0.2461(4)	0.5360(4)	–0.01202(13)	0.0196(5)
O19	1	0.1673(4)	0.7906(3)	0.11048(14)	0.0201(5)
O20	1	0.0860(3)	0.3863(3)	0.12475(12)	0.0114(4)

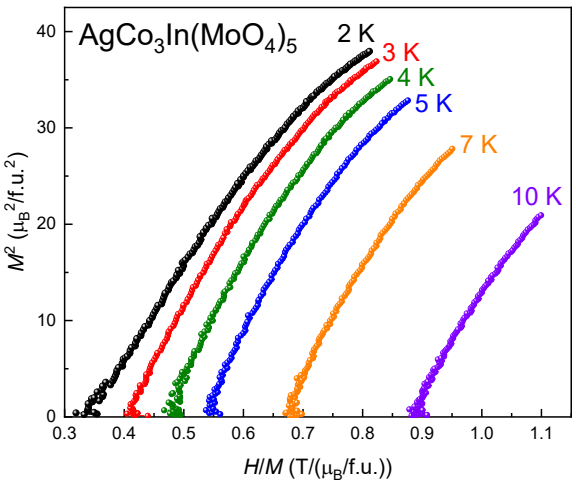
*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S3. Selected interatomic distances (Å) in $Ag_{0.92}Co_{2.93}Cr_{1.07}(MoO_4)_5$ structure.

Mo1-tetrahedron		Mo2-tetrahedron		Mo3-tetrahedron	
Mo1–O1	1.745(2)	Mo2–O5	1.737(2)	Mo3–O9	1.714(3)
–O2	1.753(2)	–O6	1.739(2)	–O10	1.756(2)
–O3	1.759(2)	–O7#1	1.779(2)	–O11	1.762(2)
–O4	1.810(2)	–O8	1.794(2)	–O12	1.834(2)
<Mo1–O>	1.767	<Mo2–O>	1.762	<Mo3–O>	1.767
Mo4-tetrahedron		Mo5-tetrahedron		*M*1-octahedron	
Mo4–O13	1.725(2)	Mo5–O17	1.743(3)	*M*1–O1#2	1.997(2)
–O14	1.729(3)	–O18	1.743(2)	–O5	2.002(2)
–O15	1.790(2)	–O19	1.751(2)	–O11#2	2.043(2)
–O16	1.817(2)	–O20	1.806(2)	–O3	2.065(2)
<Mo4–O>	1.765	<Mo5–O>	1.761	–O4#3	2.076(1)
				–O4#1	2.096(1)
				<*M*(1)–O>	2.046
*M*2-octahedron		*M*3-octahedron		*M*4-octahedron	
*M*2–O19#4	2.042(2)	*M*3–O17	2.021(3)	*M*4–O2	1.986(2)
–O7	2.069(2)	–O18#8	2.028(2)	–O6#2	1.993(2)
–O14#5	2.070(3)	–O15#5	2.046(2)	–O10#5	2.017(2)
–O13#6	2.076(2)	–O16#2	2.056(2)	–O16	2.022(2)
–O20	2.091(2)	–O20#9	2.081(2)	–O8#3	2.031(2)
–O15#7	2.112(2)	–O12	2.087(2)	–O12#2	2.075(2)
<*M*2–O>	2.077	<*M*3–O>	2.053	<*M*4–O>	2.012
Ag1-polyhedron		Ag2-polyhedron		Ag3-polyhedron	
Ag1–O8	2.207(3)	Ag2–O9	2.260(5)	Ag3–O9	2.217(5)
–O9	2.230(4)	–O8	2.380(4)	–O11#10	2.461(5)
–O7	2.249(3)	–O7	2.503(5)	–O8	2.518(4)
–O12#10	2.677(4)	–O11#10	2.592(5)	–O7	2.809(5)
–O20	2.875(4)	–O12#10	2.716(4)	–O3	2.919(4)
<Ag1–O>	2.448	<Ag2–O>	2.490	–O12#10	2.953(4)
Ag1–Ag2	0.627(4)	Ag1–Ag3	1.014(5)	–O2#3	3.007(5)
Ag2–Ag3	0.412(6)			<Ag3–O>	2.694

Symmetry transformations used to generate equivalent atoms:
#1 *x*, *y*+1, *z*; #2 1–*x*, 1–*y*, 1–*z*; #3 –*x*, 1–*y*, 1–*z* ; #4 *x*, *y*–1, *z*; #5 1–*x*, –*y*, 1–*z*; #6 *x*, *y*, *z*–1; #7 –*x*, –*y*, 1–*z*; #8 1–*x*, 1–*y*, –*z*; #9 *x*+1, *y*, *z* ; #10 *x*–1, *y*, *z*.





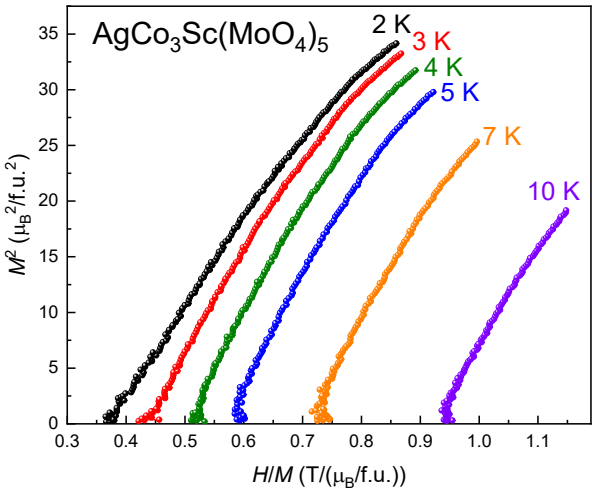


Fig. S2. The Arrott plots for $AgNi_3In(MoO_4)_5$, $AgCo_3In(MoO_4)_5$ and $AgCo_3Sc(MoO_4)_5$ compounds.