TG analysis

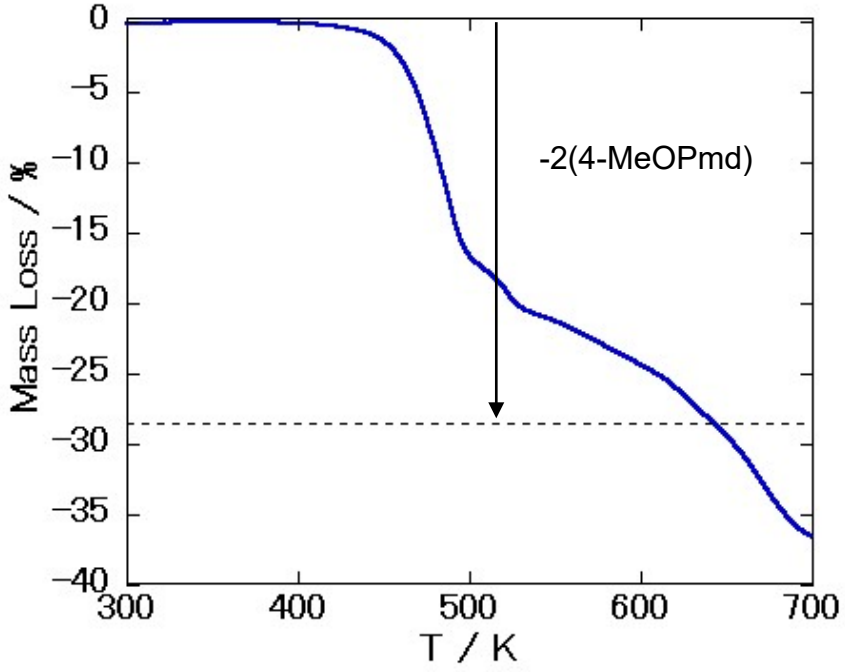

Fig. S1 TG analysis of 1Au

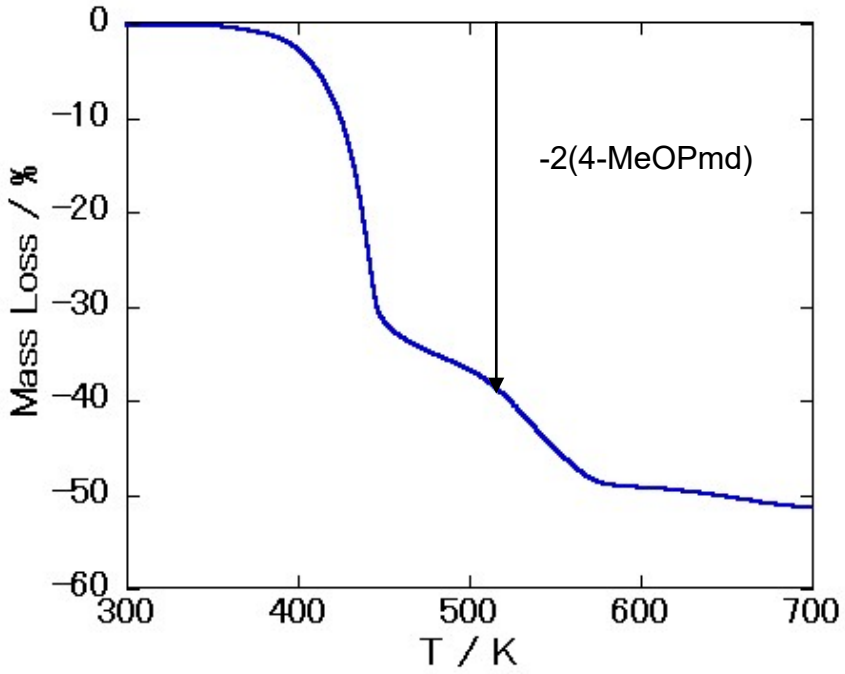

Fig. S2 TG analysis of 1Ag and 1Ag·0.25G

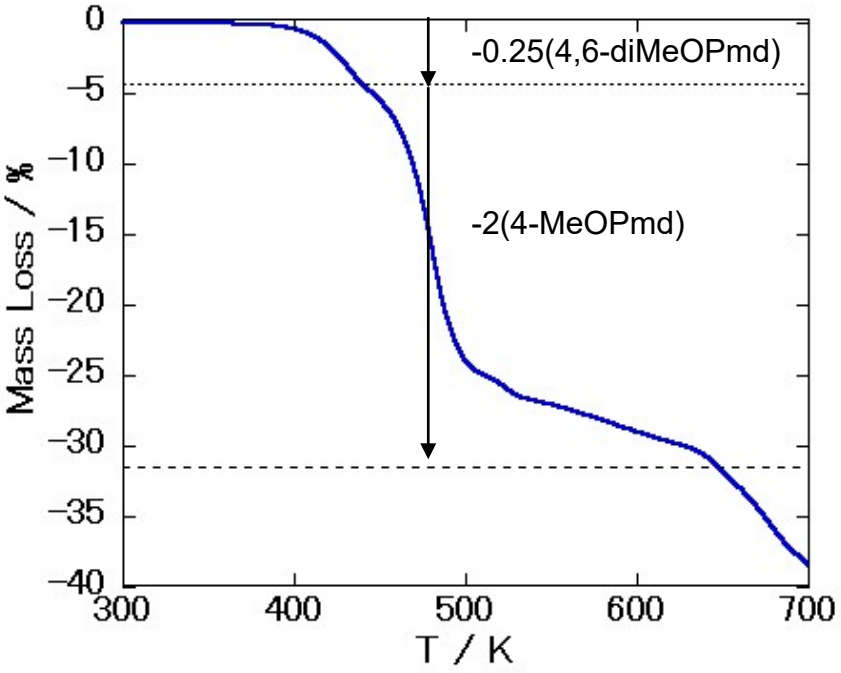

Fig. S3 TG analysis of 2Au·0.25G

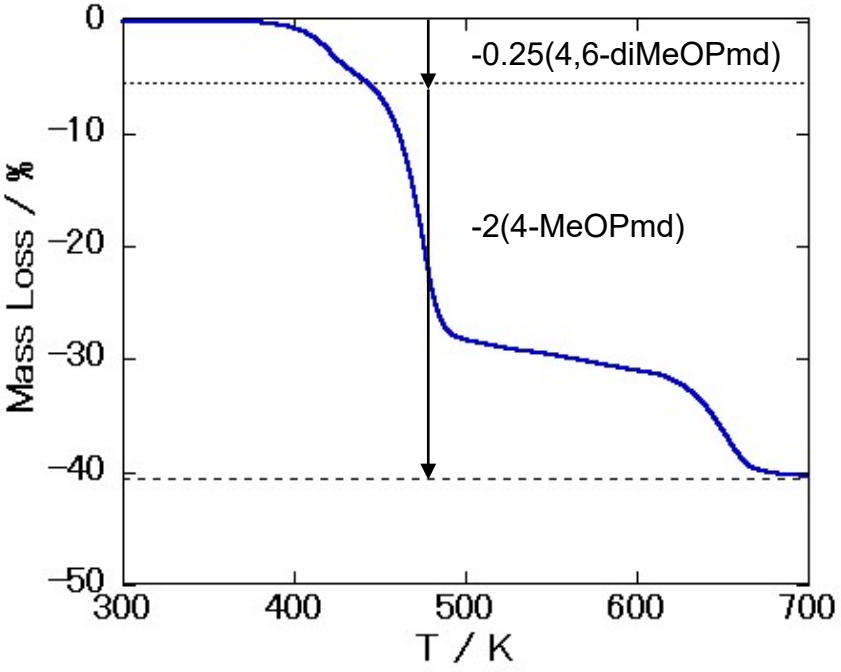

Fig. S4 TG analysis of 2Ag·0.25G

IR spectra (Nujol method)

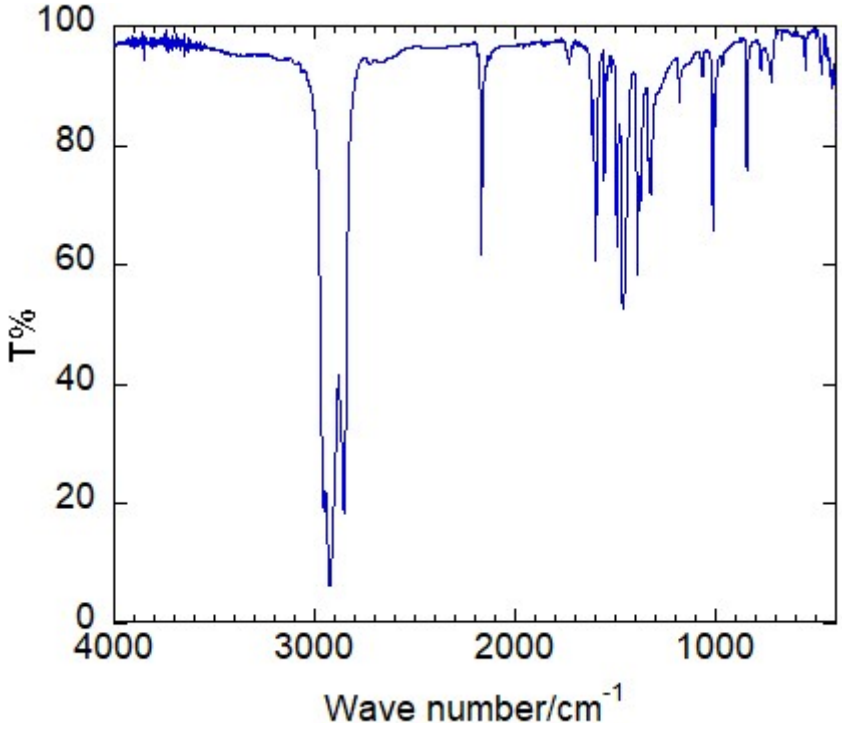

Fig. S5 IR spectrum of 1Au

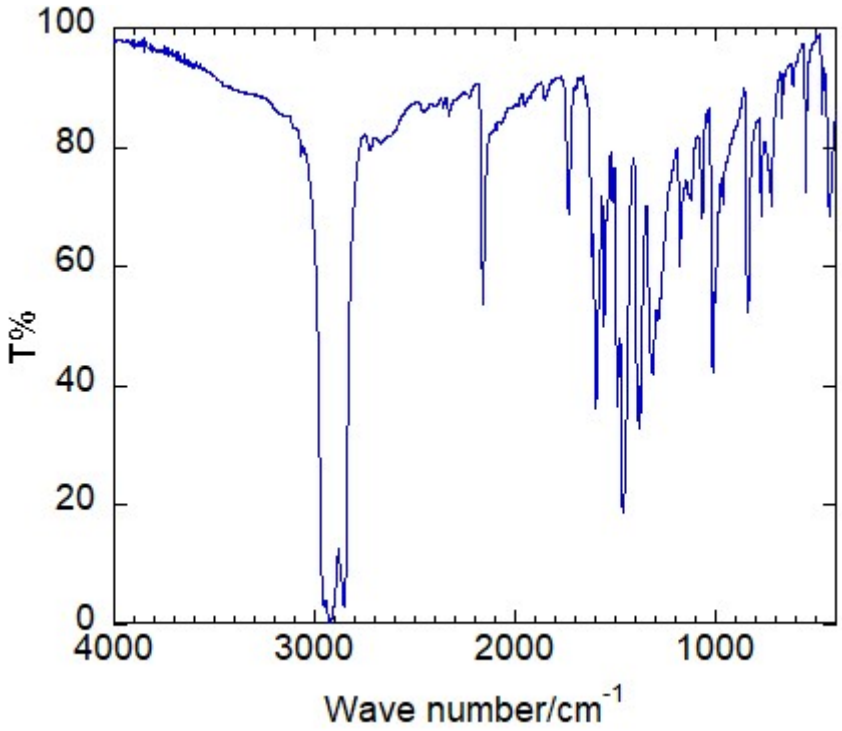

Fig. S6 IR spectrum of 1Ag and 1Ag·0.25G

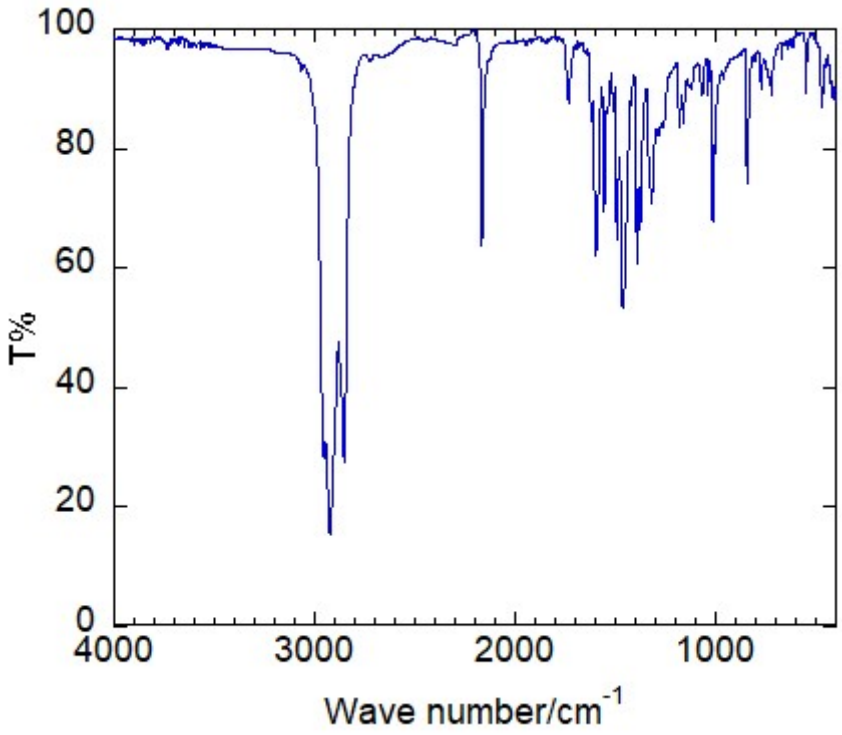

Fig. S7 IR spectrum of 2Au·0.25G

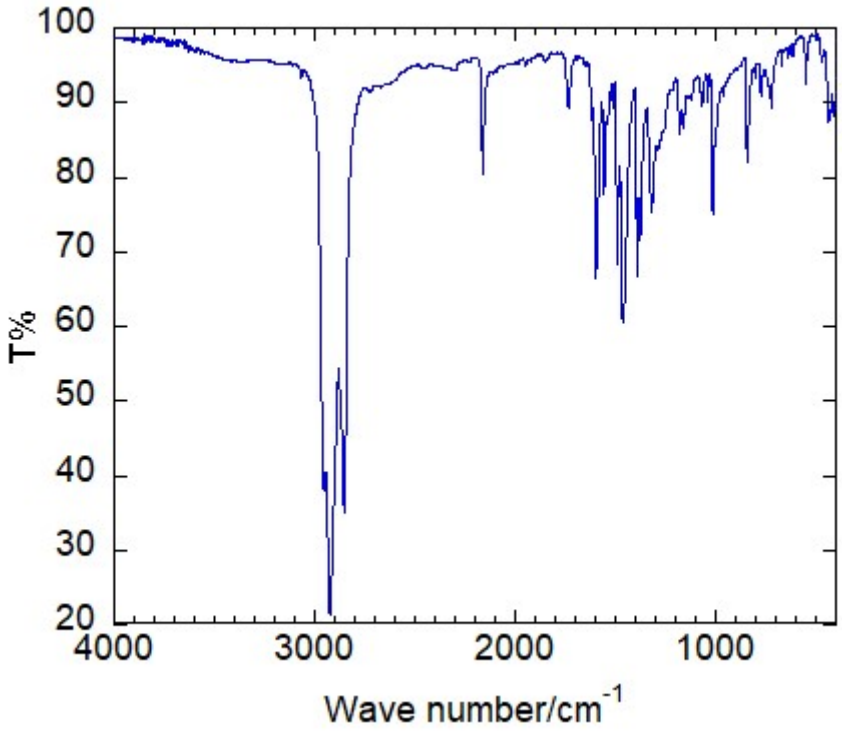

Fig. S8 IR spectrum of 2Ag·0.25G

Powder X-ray Pattern

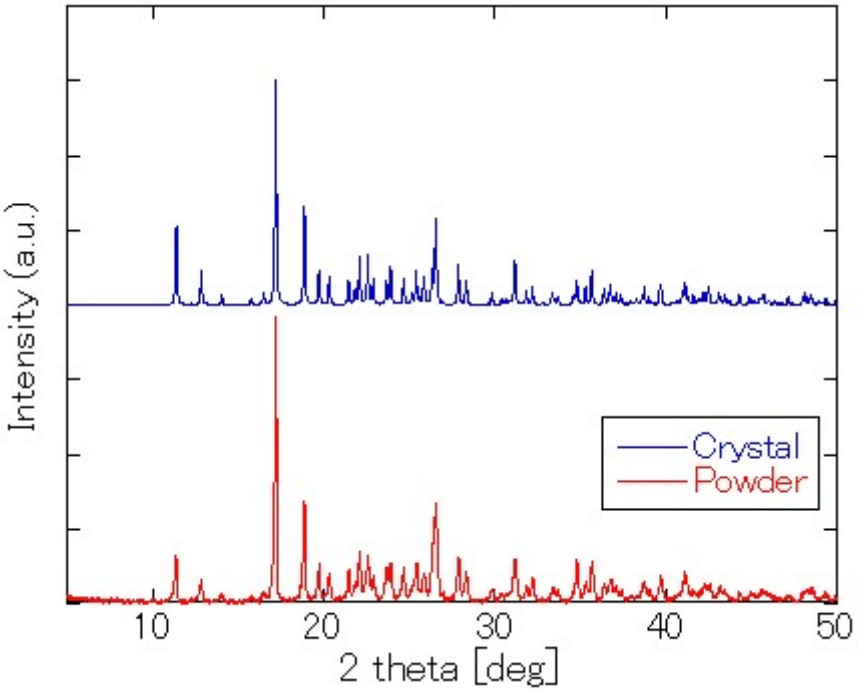

Fig. S9 Powder X-ray diffraction of 1Au

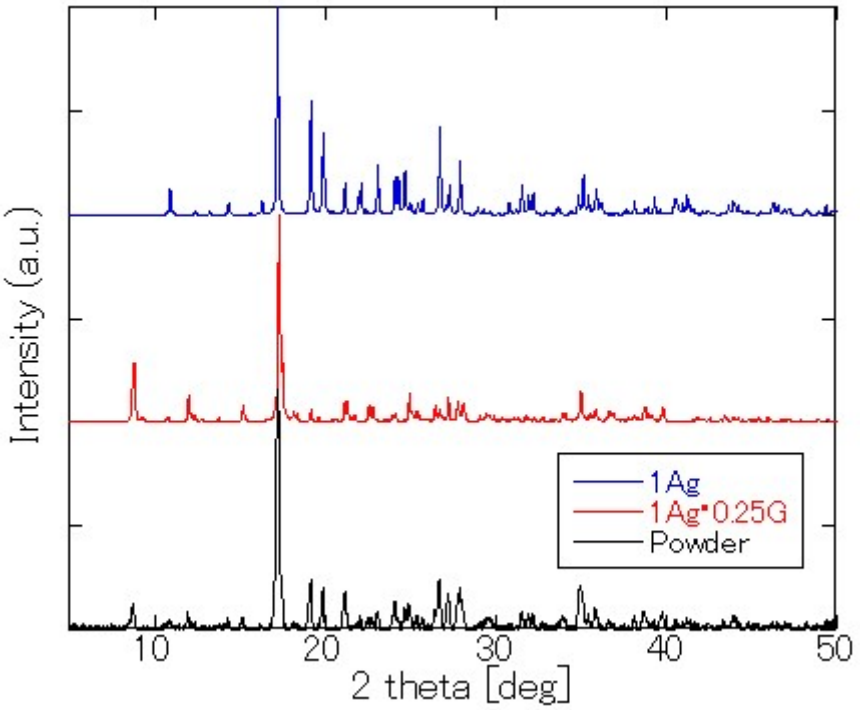

Fig. S10 Powder X-ray diffraction of 1Ag·0.25G

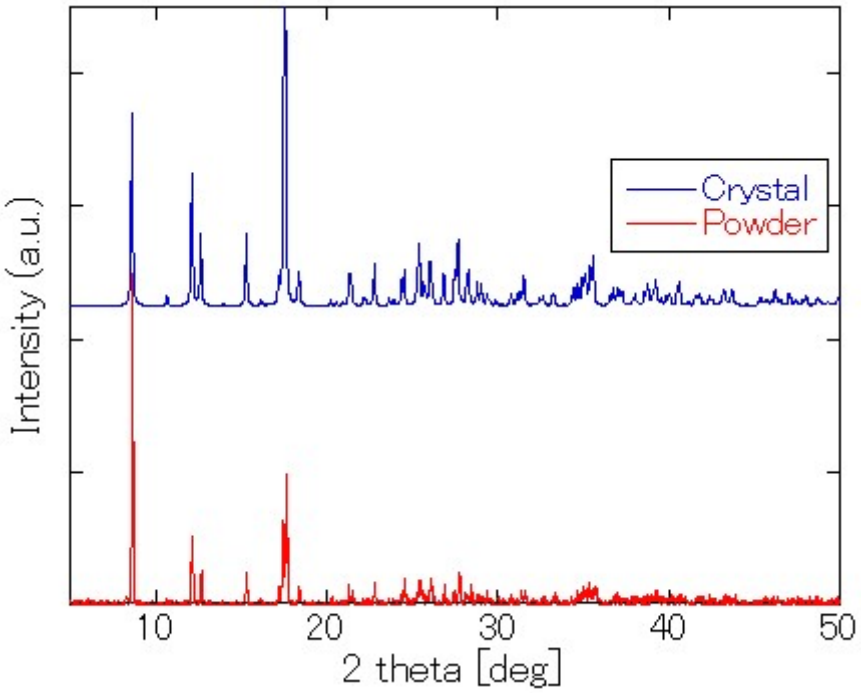

Fig. S11 Powder X-ray diffraction of 2Au·0.25G

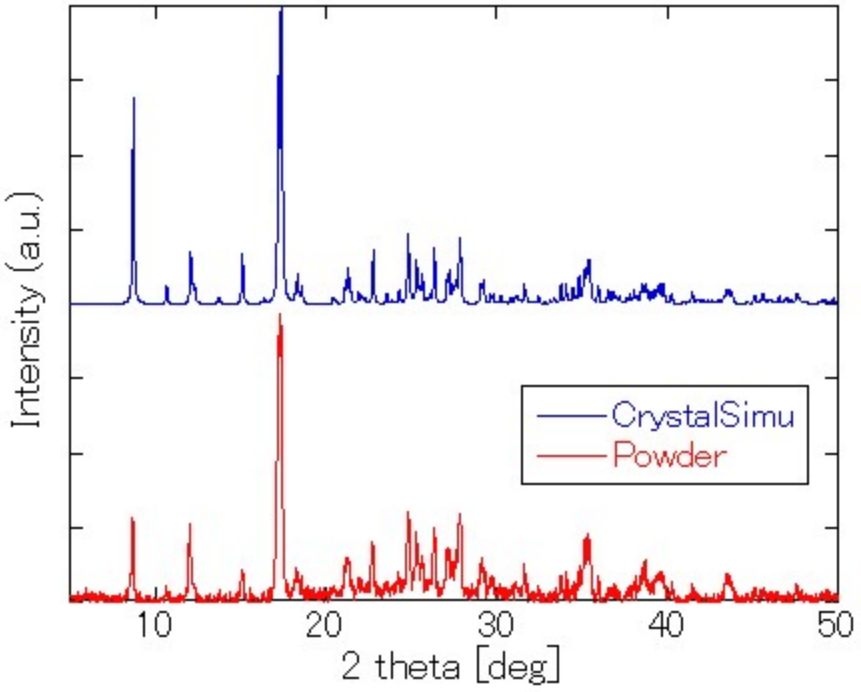

Fig. S12 Powder X-ray diffraction of 2Ag·0.25G

Remeasurement of magnetic susceptibility

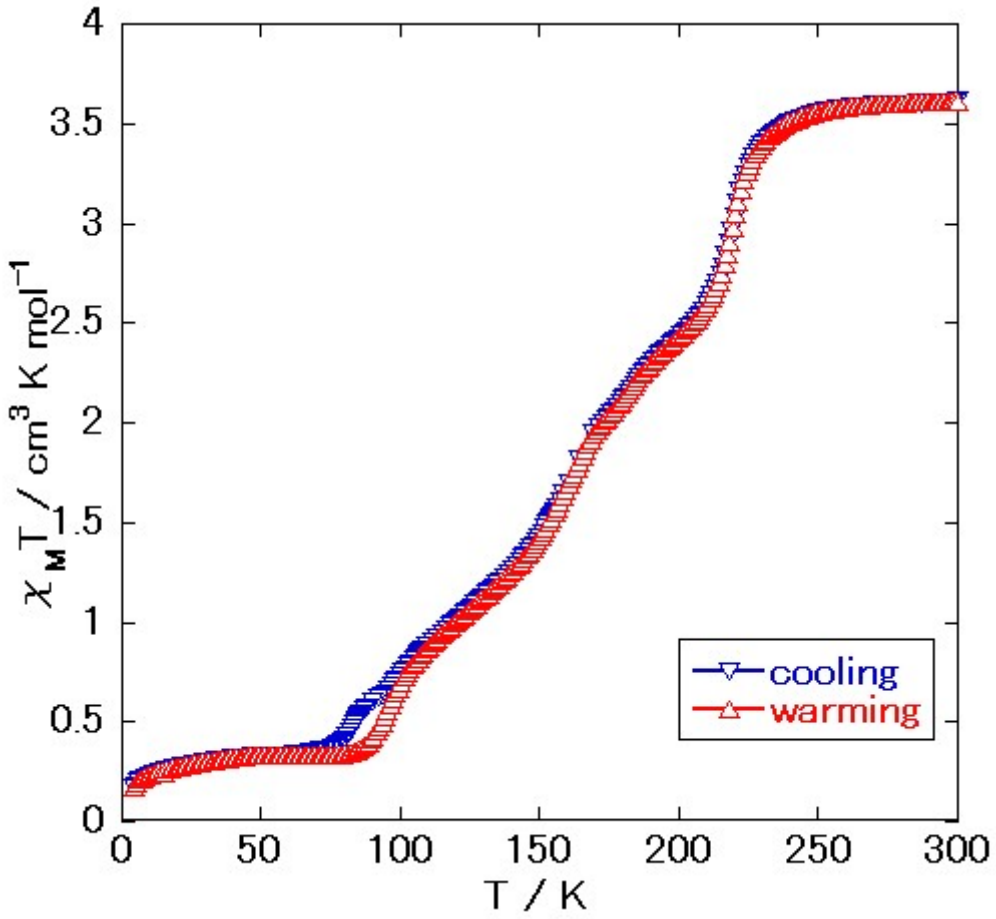

Fig. S13 Remeasurement of magnetic susceptibility of 1Ag·0.25G (Powder)

Additional crystallographic data

Table S1. Crystal data and structure refinement for 1Au at 296 K

Identification code	test_0_APEX3_a	
Empirical formula	C14 H12 Au2 Fe N8 O2	
Formula weight	774.10	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.9892(5) Å	α = 90°.
	b = 15.5225(9) Å	β = 111.4960(10)°.
	c = 8.7466(5) Å	γ = 90°.
Volume	1009.24(10) $Å^3$	
Z	2	
Density (calculated)	2.547 Mg/m^3	
Absorption coefficient	15.235 mm^{-1}	
F(000)	704	
Crystal size	0.407 x 0.210 x 0.142 mm^3	
Theta range for data collection	2.624 to 31.376°.	
Index ranges	-8<=h<=11, -19<=k<=22, -11<=l<=12	
Reflections collected	7753	
Independent reflections	3051 [R(int) = 0.0252]	
Completeness to theta = 25.000°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.22 and 0.15	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3051 / 0 / 125	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R1 = 0.0263, wR2 = 0.0586	
R indices (all data)	R1 = 0.0372, wR2 = 0.0621	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.925 and -1.935 $e.Å^{-3}$	

Table S2. Crystal data and structure refinement for 1Au at 100 K

Identification code	test_0_APEX3_a	
Empirical formula	C14 H12 Au2 Fe N8 O2	
Formula weight	774.10	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.9046(8) Å	α = 90°.
	b = 15.6559(15) Å	β = 112.5380(10)°.
	c = 8.5964(8) Å	γ = 90°.
Volume	982.59(16) $Å^3$	
Z	2	
Density (calculated)	2.616 Mg/m^3	
Absorption coefficient	15.649 mm^{-1}	
F(000)	704	
Crystal size	0.407 x 0.210 x 0.142 mm^3	
Theta range for data collection	2.602 to 31.276°.	
Index ranges	-11<=h<=8, -20<=k<=22, -12<=l<=11	
Reflections collected	7372	
Independent reflections	2971 [R(int) = 0.0201]	
Completeness to theta = 25.000°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.21 and 0.15	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2971 / 0 / 125	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0194, wR2 = 0.0406	
R indices (all data)	R1 = 0.0238, wR2 = 0.0420	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.093 and -1.092 $e.Å^{-3}$	

Table S3. Crystal data and structure refinement for 1Ag at 298 K

Identification code	test_0_APEX3_a	
Empirical formula	C14 H12 Ag2 Fe N8 O2	
Formula weight	595.91	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.8105(4) Å	α = 90°.
	b = 16.1809(8) Å	β = 110.5400(10)°.
	c = 8.4579(4) Å	γ = 90°.
Volume	1000.96(9) $Å^3$	
Z	2	
Density (calculated)	1.977 Mg/m^3	
Absorption coefficient	2.677 mm^{-1}	
F(000)	576	
Crystal size	0.300 x 0.270 x 0.200 mm^3	
Theta range for data collection	2.517 to 27.511°.	
Index ranges	-9<=h<=10, -21<=k<=13, -10<=l<=9	
Reflections collected	6225	
Independent reflections	2294 [R(int) = 0.0216]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.62 and 0.48	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2294 / 0 / 126	
Goodness-of-fit on F^2	1.064	
Final R indices [I>2sigma(I)]	R1 = 0.0230, wR2 = 0.0560	
R indices (all data)	R1 = 0.0260, wR2 = 0.0575	
Extinction coefficient	0.0192(8)	
Largest diff. peak and hole	0.950 and -0.903 $e.Å^{-3}$	

Table S4. Crystal data and structure refinement for 1Ag at 90 K

Identification code	test_0_APEX3_a	
Empirical formula	C14 H12 Ag2 Fe N8 O2	
Formula weight	595.91	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.6006(3) Å	α = 90°.
	b = 16.5407(7) Å	β = 110.2280(10)°.
	c = 8.1805(3) Å	γ = 90°.
Volume	965.02(7) $Å^3$	
Z	2	
Density (calculated)	2.051 Mg/m^3	
Absorption coefficient	2.777 mm^{-1}	
F(000)	576	
Crystal size	0.300 x 0.270 x 0.200 mm^3	
Theta range for data collection	2.463 to 27.527°.	
Index ranges	-9<=h<=6, -21<=k<=21, -6<=l<=10	
Reflections collected	5998	
Independent reflections	2223 [R(int) = 0.0129]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.61 and 0.50	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2223 / 0 / 125	
Goodness-of-fit on F^2	1.155	
Final R indices [I>2sigma(I)]	R1 = 0.0158, wR2 = 0.0391	
R indices (all data)	R1 = 0.0164, wR2 = 0.0394	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.372 and -0.604 $e.Å^{-3}$	

Table S5. Crystal data and structure refinement for 1Ag·0.25G at 296 K

Identification code	test_1_a	
Empirical formula	C61 H54 Ag8 Fe4 N34 O9	
Formula weight	2493.74	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 15.7353(17) Å	α = 90°.
	b = 28.498(3) Å	β = 110.685(2)°.
	c = 21.353(2) Å	γ = 90°.
Volume	8957.8(17) $Å^3$	
Z	4	
Density (calculated)	1.849 Mg/m^3	
Absorption coefficient	2.399 mm^{-1}	
F(000)	4840	
Crystal size	0.400 x 0.290 x 0.280 mm^3	
Theta range for data collection	1.245 to 25.438°.	
Index ranges	-19<=h<=17, 0<=k<=34, 0<=l<=25	
Reflections collected	16355	
Independent reflections	16355 [R(int) = ?]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.55 and 0.39	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16355 / 0 / 1058	
Goodness-of-fit on F^2	0.998	
Final R indices [I>2sigma(I)]	R1 = 0.0491, wR2 = 0.1320	
R indices (all data)	R1 = 0.0966, wR2 = 0.1667	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.782 and -0.819 $e.Å^{-3}$	

Table S6. Crystal data and structure refinement for 1Ag·0.25G at 190 K.

Identification code	test_1_a	
Empirical formula	C61 H54 Ag8 Fe4 N34 O9	
Formula weight	2493.74	
Temperature	190(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 15.588(3) Å	α = 90°.
	b = 28.221(5) Å	β = 111.301(3)°.
	c = 21.120(4) Å	γ = 90°.
Volume	8656(3) $Å^3$	
Z	4	
Density (calculated)	1.914 Mg/m^3	
Absorption coefficient	2.483 mm^{-1}	
F(000)	4840	
Crystal size	0.400 x 0.290 x 0.280 mm^3	
Theta range for data collection	1.262 to 30.822°.	
Index ranges	-22<=h<=22, 0<=k<=39, -30<=l<=29	
Reflections collected	34874	
Independent reflections	34874 [R(int) = ?]	
Completeness to theta = 25.242°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.54 and 0.40	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	34874 / 0 / 1058	
Goodness-of-fit on F^2	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0602, wR2 = 0.1513	
R indices (all data)	R1 = 0.1113, wR2 = 0.1856	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.545 and -1.506 $e.Å^{-3}$	

Table S7. Crystal data and structure refinement for 1Ag·0.25G at 130 K

Identification code	test_1_a	
Empirical formula	C61 H54 Ag8 Fe4 N34 O9	
Formula weight	2493.74	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 15.575(5) Å	α = 90°.
	b = 27.881(9) Å	β = 112.615(5)°.
	c = 21.080(9) Å	γ = 90°.
Volume	8450(5) $Å^3$	
Z	4	
Density (calculated)	1.960 Mg/m^3	
Absorption coefficient	2.544 mm^{-1}	
F(000)	4840	
Crystal size	0.400 x 0.290 x 0.280 mm^3	
Theta range for data collection	1.276 to 31.099°.	
Index ranges	-19<=h<=21, -38<=k<=0, -19<=l<=28	
Reflections collected	20006	
Independent reflections	20006 [R(int) = ?]	
Completeness to theta = 25.000°	96.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.54 and 0.36	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	20006 / 21 / 1059	
Goodness-of-fit on F^2	1.134	
Final R indices [I>2sigma(I)]	R1 = 0.0629, wR2 = 0.1609	
R indices (all data)	R1 = 0.0972, wR2 = 0.1905	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.545 and -1.845 $e.Å^{-3}$	

Table S8. Crystal data and structure refinement for 1Ag·0.25G at 87 K

Identification code	test_1_a	
Empirical formula	C61 H54 Ag8 Fe4 N34 O9	
Formula weight	2493.74	
Temperature	87(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 15.4985(18) Å	α = 90°.
	b = 27.743(3) Å	β = 112.563(2)°.
	c = 20.928(3) Å	γ = 90°.
Volume	8310.0(18) $Å^3$	
Z	4	
Density (calculated)	1.993 Mg/m^3	
Absorption coefficient	2.586 mm^{-1}	
F(000)	4840	
Crystal size	0.400 x 0.290 x 0.280 mm^3	
Theta range for data collection	1.284 to 28.992°.	
Index ranges	-19<=h<=21, -37<=k<=0, -18<=l<=28	
Reflections collected	20724	
Independent reflections	20724 [R(int) = ?]	
Completeness to theta = 25.242°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.53 and 0.28	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	20724 / 12 / 1058	
Goodness-of-fit on F^2	1.098	
Final R indices [I>2sigma(I)]	R1 = 0.0564, wR2 = 0.1456	
R indices (all data)	R1 = 0.0994, wR2 = 0.1792	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.305 and -2.891 $e.Å^{-3}$	

Table S9. Crystal data and structure refinement for 2Au·0.25G at 296 K

Identification code	test_1_a	
Empirical formula	C31 H28 Au4 Fe2 N17 O5	
Formula weight	1618.27	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 29.201(4) Å	α = 90°.
	b = 10.9601(14) Å	β = 90.275(2)°.
	c = 14.0059(17) Å	γ = 90°.
Volume	4482.4(10) $Å^3$	
Z	4	
Density (calculated)	2.398 Mg/m^3	
Absorption coefficient	13.729 mm^{-1}	
F(000)	2964	
Crystal size	0.230 x 0.200 x 0.180 mm^3	
Theta range for data collection	1.395 to 30.298°.	
Index ranges	-41<=h<=41, 0<=k<=15, 0<=l<=19	
Reflections collected	6408	
Independent reflections	6408 [R(int) = ?]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.746011 and 0.468132	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6408 / 22 / 368	
Goodness-of-fit on F^2	0.873	
Final R indices [I>2sigma(I)]	R1 = 0.0460, wR2 = 0.1218	
R indices (all data)	R1 = 0.0649, wR2 = 0.1337	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.361 and -2.380 $e.Å^{-3}$	

Table S10. Crystal data and structure refinement for 2Au·0.25G at 90 K

Identification code	test_1_a	
Empirical formula	C31 H28 Au4 Fe2 N17 O5	
Formula weight	1618.27	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 28.654(7) Å	α = 90°.
	b = 10.772(3) Å	β = 90.172(4)°.
	c = 13.756(3) Å	γ = 90°.
Volume	4246.1(17) $Å^3$	
Z	4	
Density (calculated)	2.531 Mg/m^3	
Absorption coefficient	14.493 mm^{-1}	
F(000)	2964	
Crystal size	0.230 x 0.200 x 0.180 mm^3	
Theta range for data collection	1.421 to 28.203°.	
Index ranges	-37<=h<=15, -14<=k<=13, -18<=l<=17	
Reflections collected	13759	
Independent reflections	5162 [R(int) = 0.0426]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Numerical Mu From Formula	
Max. and min. transmission	0.18 and 0.09	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5162 / 12 / 321	
Goodness-of-fit on F^2	1.154	
Final R indices [I>2sigma(I)]	R1 = 0.0467, wR2 = 0.1370	
R indices (all data)	R1 = 0.0477, wR2 = 0.1380	
Extinction coefficient	n/a	
Largest diff. peak and hole	6.074 and -4.791 $e.Å^{-3}$	

Table S11. Crystal data and structure refinement for 2Ag·0.25G at 296 K

Identification code	test_1_a	
Empirical formula	C31 H28 Ag4 Fe2 N17 O5	
Formula weight	1261.88	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 29.288(6) Å	α = 90°.
	b = 10.788(2) Å	β = 90.039(4)°.
	c = 14.325(3) Å	γ = 90°.
Volume	4526.1(17) $Å^3$	
Z	4	
Density (calculated)	1.852 Mg/m^3	
Absorption coefficient	2.376 mm^{-1}	
F(000)	2452	
Crystal size	0.218 x 0.204 x 0.088 mm^3	
Theta range for data collection	1.391 to 28.422°.	
Index ranges	-37<=h<=39, -14<=k<=11, -18<=l<=19	
Reflections collected	15585	
Independent reflections	5665 [R(int) = 0.0363]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Numerical Mu From Formula	
Max. and min. transmission	0.82 and 0.62	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5665 / 26 / 347	
Goodness-of-fit on F^2	0.836	
Final R indices [I>2sigma(I)]	R1 = 0.0410, wR2 = 0.1140	
R indices (all data)	R1 = 0.0617, wR2 = 0.1314	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.818 and -0.921 $e.Å^{-3}$	

Table S12. Crystal data and structure refinement for 2Ag·0.25G at 150 K

Identification code	test_1_a	
Empirical formula	C31 H28 Ag4 Fe2 N17 O5	
Formula weight	1261.88	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 28.896(6) Å	α = 90°.
	b = 10.623(3) Å	β = 90.033(4)°.
	c = 14.044(3) Å	γ = 90°.
Volume	4310.9(17) $Å^3$	
Z	4	
Density (calculated)	1.944 Mg/m^3	
Absorption coefficient	2.495 mm^{-1}	
F(000)	2452	
Crystal size	0.218 x 0.204 x 0.088 mm^3	
Theta range for data collection	1.409 to 28.785°.	
Index ranges	-38<=h<=37, -14<=k<=13, -18<=l<=11	
Reflections collected	15149	
Independent reflections	5581 [R(int) = 0.0374]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Numerical Mu From Formula	
Max. and min. transmission	0.81 and 0.62	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5581 / 9 / 305	
Goodness-of-fit on F^2	0.817	
Final R indices [I>2sigma(I)]	R1 = 0.0363, wR2 = 0.1008	
R indices (all data)	R1 = 0.0449, wR2 = 0.1138	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.661 and -1.453 $e.Å^{-3}$	

Table S13. Crystal data and structure refinement for 2Ag·0.25G at 90 K

Identification code	test_1_a	
Empirical formula	C33 H30 Ag4 Fe2 N18 O5	
Formula weight	1301.93	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 28.882(5) Å	α = 90°.
	b = 10.5619(19) Å	β = 90.020(3)°.
	c = 13.999(3) Å	γ = 90°.
Volume	4270.6(13) $Å^3$	
Z	4	
Density (calculated)	2.025 Mg/m^3	
Absorption coefficient	2.523 mm^{-1}	
F(000)	2536	
Crystal size	0.218 x 0.204 x 0.084 mm^3	
Theta range for data collection	1.410 to 29.713°.	
Index ranges	-17<=h<=40, -14<=k<=14, -18<=l<=19	
Reflections collected	13470	
Independent reflections	5289 [R(int) = 0.0458]	
Completeness to theta = 25.242°	99.4 %	
Absorption correction	Numerical Mu From Formula	
Max. and min. transmission	0.87 and 0.66	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5289 / 52 / 305	
Goodness-of-fit on F^2	1.665	
Final R indices [I>2sigma(I)]	R1 = 0.0643, wR2 = 0.2263	
R indices (all data)	R1 = 0.0761, wR2 = 0.2357	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.080 and -2.701 $e.Å^{-3}$	