Electronic Supplementary Material (ESI) for Dalton Transactions.

Synthesis method

The complex was synthesized using Mohr's salt $Fe(NH_4)_2(SO_4)_2 \cdot 6H_2O$, L-ascorbic acid, $K[Au(CN)_2]$, and quinazoline. Mohr's salt was purchased from Kanto Chemical Co., L-ascorbic acid was purchased from Nacalai Tesque Co., $K[Au(CN)_2]$ was purchased from Toyo Chemical Industrial Co., and quinazoline was purchased from TCI, all commercially sourced.

In the powder sample synthesis, 0.4 mmol Mohr's salt (0.1569 g), 0.4 mmol L-ascorbic acid (0.0705 g), and the excess quinazoline (0.1180 g, 0.9 mmol) were dissolved in 8 mL water, and a yellow solution (Solution 1) was formed. Second, 0.8 mmol $K[Au(CN)_2]$ (0.2305 g) was dissolved in 10 mL water (Solution 2). Last, Solution 2 was dropped into the solution, and a yellow powder was obtained.

In the synthesis of a single crystal by a slow diffusion method, first, 0.1 mmol $K[Au(CN)_2]$ (0.0288 g) was dissolved in 0.2 mL water (Solution 3). Second, 0.3 mL water and 0.6 mL ethanol were mixed (Solution 4). Third, 0.05 mmol Mohr's salt (0.0196 g) and 0.05 mmol L-ascorbic acid (0.0088 g) were dissolved in 0.5 mL water. Then, 0.1 mmol quinazoline (0.0140 g) and 0.5 mL ethanol were added to this solution (Solution 5). Last, we gently added Solutions 3, 4, and 5 to a tube with a 7 mm diameter, in that order. Ethanol was added to Solutions 4 and 5 to adjust the density. Consequently, Solutions 3, 4, and 5 do not mix immediately, and a yellow crystal was obtained.

In the synthesis of a single crystal by the filter method, first, 0.05 mmol Mohr's salt (0.0196 g), 0.05 mmol L-ascorbic acid (0.0078 g), and 0.1 mmol $K[Au(CN)_2]$ (0.0288 g) were dissolved in 10 mL water (Solution 6). Second, 0.14 mmol quinazoline (0.0186 g) was placed in an 8 × 50 mm microtube. Ethanol was added until the microtube was full. The microtube was sealed using a Merck Co. Omnipore^{TM} 0.2 μm membrane filter. Last, the microtube was placed in a sample bottle with Solution 6. Very small amount of yellow crystal was obtained.

TG analysis

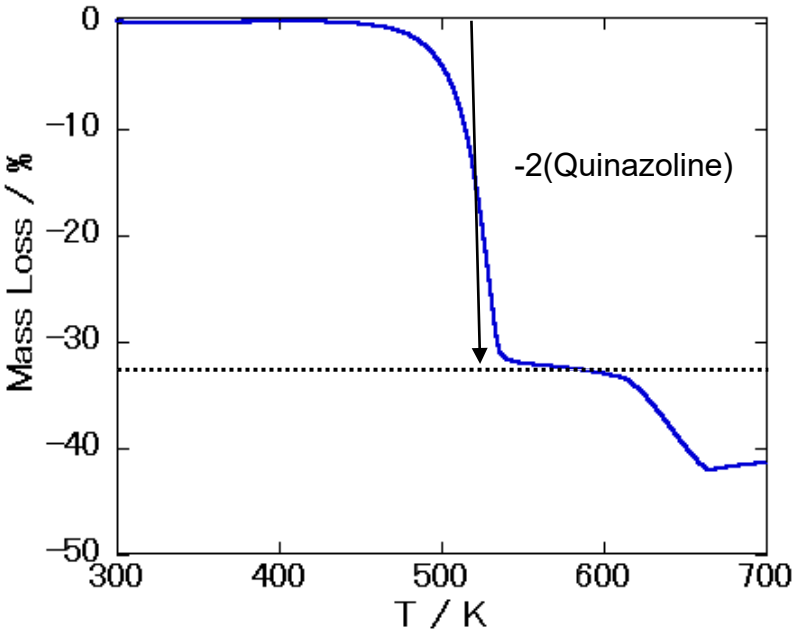

Fig. S1 TG analysis of complex 1

IR spectra (Nujol method)

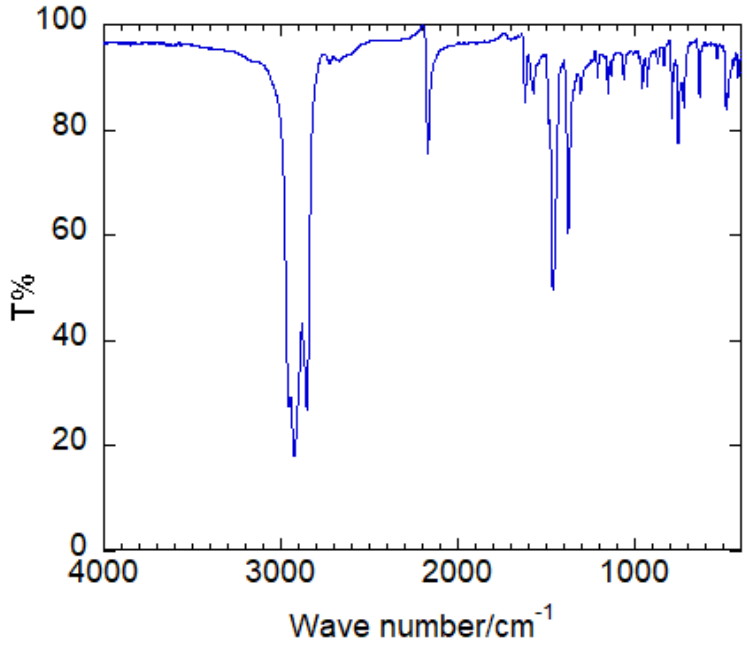

Fig. S2 IR spectrum of complex **1**

C≡N peak: 2169.53 cm^{-1}

Powder X-ray Pattern

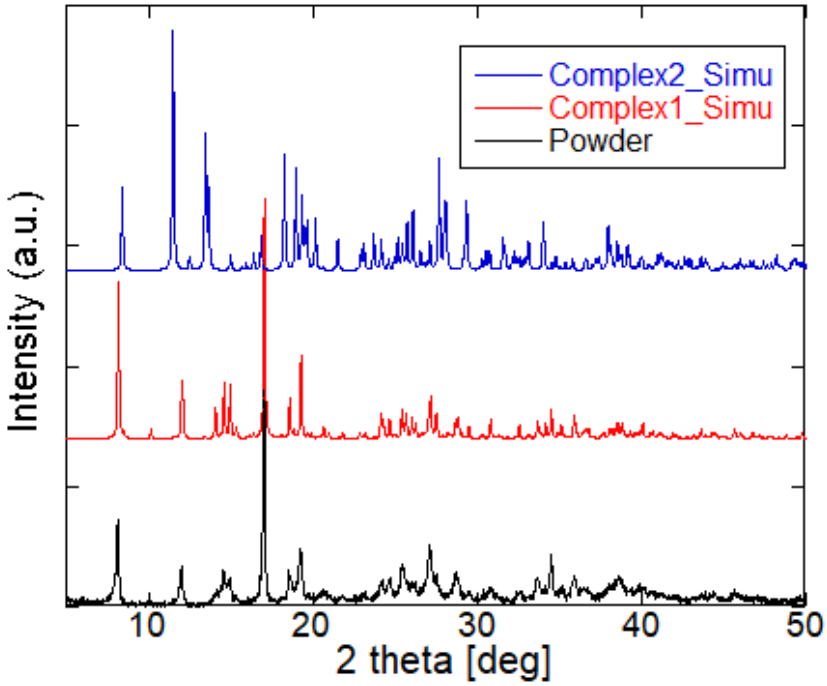

Fig. S3 Powder X-ray diffraction of synthesized complexes

Additional crystallographic data

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

Identification code	test_1_a	
Empirical formula	C20 H12 Au2 Fe N8	
Formula weight	814.16	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.8433(10) Å	α= 90°.
	b = 14.6937(14) Å	β= 93.865(2)°.
	c = 14.7279(14) Å	γ = 90°.
Volume	2341.2(4) $Å^3$	
Z	4	
Density (calculated)	2.310 Mg/m^3	
Absorption coefficient	13.136 mm^{-1}	
F(000)	1488	
Crystal size	0.244 x 0.231 x 0.102 mm^3	
Theta range for data collection	1.882 to 27.508°.	
Index ranges	-14<=h<=10, -18<=k<=19, -19<=l<=15	
Reflections collected	14851	
Independent reflections	5351 [R(int) = 0.0457]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Numerical Mu From Formula	
Max. and min. transmission	0.35 and 0.08	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5351 / 66 / 258	
Goodness-of-fit on F^2	0.951	
Final R indices [I>2sigma(I)]	R1 = 0.0438, wR2 = 0.1373	
R indices (all data)	R1 = 0.0991, wR2 = 0.1756	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.977 and -1.149 $e.Å^{-3}$	

Table S2. Crystal data and structure refinement for complex **1** at 150 K

Identification code	test_1_a	
Empirical formula	C20 H12 Au2 Fe N8	
Formula weight	814.16	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.698(3) Å	α= 90°.
	b = 14.331(4) Å	β= 94.049(4)°.
	c = 14.527(4) Å	γ = 90°.
Volume	2221.7(10) $Å^3$	
Z	4	
Density (calculated)	2.434 Mg/m^3	
Absorption coefficient	13.843 mm^{-1}	
F(000)	1488	
Crystal size	0.244 x 0.231 x 0.102 mm^3	
Theta range for data collection	1.908 to 27.220°.	
Index ranges	-13<=h<=11, -18<=k<=18, -18<=l<=14	
Reflections collected	12160	
Independent reflections	4907 [R(int) = 0.0808]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Numerical Mu From Formula	
Max. and min. transmission	0.33 and 0.08	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4907 / 66 / 258	
Goodness-of-fit on F^2	0.946	
Final R indices [I>2sigma(I)]	R1 = 0.0542, wR2 = 0.1410	
R indices (all data)	R1 = 0.1534, wR2 = 0.1944	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.148 and -1.476 $e.Å^{-3}$	

Table S3. Crystal data and structure refinement for complex **1** at 90 K

Identification code	test_1_a	
Empirical formula	C20 H12 Au2 Fe N8	
Formula weight	814.16	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.662(3) Å	α = 90°.
	b = 14.119(3) Å	β = 94.257(4)°.
	c = 14.375(4) Å	γ = 90°.
Volume	2158.0(9) $Å^3$	
Z	4	
Density (calculated)	2.506 Mg/m^3	
Absorption coefficient	14.251 mm^{-1}	
F(000)	1488	
Crystal size	0.244 x 0.231 x 0.102 mm^3	
Theta range for data collection	1.915 to 27.487°.	
Index ranges	-13<=h<=10, -17<=k<=18, -18<=l<=15	
Reflections collected	12065	
Independent reflections	4932 [R(int) = 0.0708]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Numerical Mu From Formula	
Max. and min. transmission	0.32 and 0.07	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4932 / 66 / 258	
Goodness-of-fit on F^2	0.933	
Final R indices [I>2sigma(I)]	R1 = 0.0489, wR2 = 0.1305	
R indices (all data)	R1 = 0.1282, wR2 = 0.1799	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.282 and -1.903 $e.Å^{-3}$	

Table S4. Crystal data and structure refinement for complex **2** at 296 K

Identification code	test_1	
Empirical formula	C20 H16 Au2 Fe N8 O2	
Formula weight	850.19	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.3203(8) Å	α = 81.6096(19)°.
	b = 7.8613(8) Å	β = 77.6448(18)°.
	c = 10.8262(12) Å	γ = 79.8104(18)°.
Volume	595.19(11) $Å^3$	
Z	1	
Density (calculated)	2.372 Mg/m^3	
Absorption coefficient	12.929 mm^{-1}	
F(000)	392	
Crystal size	0.220 x 0.180 x 0.090 mm^3	
Theta range for data collection	1.938 to 31.236°.	
Index ranges	-10<=h<=10, -10<=k<=11, 0<=l<=15	
Reflections collected	3361	
Independent reflections	3361 [R(int) = ?]	
Completeness to theta = 25.000°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.39 and 0.19	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3361 / 2 / 158	
Goodness-of-fit on F^2	0.985	
Final R indices [I>2sigma(I)]	R1 = 0.0380, wR2 = 0.0946	
R indices (all data)	R1 = 0.0470, wR2 = 0.0994	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.943 and -2.085 $e.Å^{-3}$	

Table S5. Crystal data and structure refinement for complex **2** at 90 K

Identification code	test_1_a	
Empirical formula	C20 H16 Au2 Fe N8 O2	
Formula weight	850.19	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.2983(11) Å	α = 80.236(4)°.
	b = 7.7651(12) Å	β = 76.919(3)°.
	c = 10.7931(17) Å	γ = 79.867(3)°.
Volume	581.11(16) $Å^3$	
Z	1	
Density (calculated)	2.429 Mg/m^3	
Absorption coefficient	13.242 mm^{-1}	
F(000)	392	
Crystal size	0.280 x 0.140 x 0.110 mm^3	
Theta range for data collection	1.955 to 27.570°.	
Index ranges	-9<=h<=9, -9<=k<=10, 0<=l<=14	
Reflections collected	2616	
Independent reflections	2616 [R(int) = ?]	
Completeness to theta = 25.000°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.32 and 0.21	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2616 / 2 / 158	
Goodness-of-fit on F^2	0.809	
Final R indices [I>2sigma(I)]	R1 = 0.0315, wR2 = 0.0875	
R indices (all data)	R1 = 0.0329, wR2 = 0.0894	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.216 and -2.607 $e.Å^{-3}$	