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Electronic Supplementary Information

Photoluminescence of Self-assembled Ag(I) and Au(I) N-heterocyclic Carbene Complexes. Interplay the aurophilic, hydrogen bonding and hydrophobic interactions.

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Experimental Section.

NMR spectra were recorded on Avance^{II} spectrometer spectrometer (^{1}H, 400 MHz; ^{13}C, 100 MHz). The solvents and regents were purchased from Aldrich Acros and used as received. Elemental microanalyses were performed by the Taiwan Instrumentation Center. IR spectra were recorded with a Perkin-Elmer Spectrum One. Raman spectra were measured using a Jobin Yvon 64000 Raman microscope (HORIBA, Minami-ku, Kyoto, Japan) equipped with a Linkam optical DSC system (THMS600; Linkam Scientific Instruments, Surrey, UK). Optical characterization was performed on an Olympus BH-2 polarizing microscope equipped with a Mettler FP 82 hot stageand a Mettler FP 90 central processor. Differential scanning calorimetry (DSC) was performed by using a Perkin-Elmer DSC-10 calorimeter under flowing N_2. The powder X-ray diffraction data was collected by National Dong Hwa University with Cu Kα radiation (XRD D8 Advanced, Bruker). Emission spectra were recorded on an Edinburgh FLSP-920 fluorescence spectrophotometer. Emission lifetime measurements were performed by a time-correlated single-photon counting method (TCSPC) with an Edinburgh FLSP-920 fluorescence spectrophotometer. The decay signal was recorded by a R955 PMT (Hamamatsu). Single crystal X-ray diffraction data were collected on a Bruker SMART diffractometer equipped with a CCD array detector with graphite monochromatized Mo-K_α radiation (λ = 0.71073 Å) in ϕ and ω scan modes.

[C_{16},C_{16}(2-OH)-imH][BF_4] and **[C_{16},C_{16}(2-OH)-imH][PF_6]**

[C_{16},C_{16}(2-OH)-imH][BF_4] and [C_{16},C_{16}(2-OH)-imH][PF_6] were prepared by anion metathesis of [C_{16},C_{16}(2-OH)-imH][Cl] salts (200 mg, 0.35 mmol) in 10 mL EtOH-H_2O (80:20 v/v) solvent

system using corresponding ammonium salts (0.35 mmol). After 2 hours the precipitate was filtered and washed with 10 mL EtOH-H_2O (20 : 80 v/v) to afford the white solid product.

[C_{16},C_{16}(2-OH)-imH][BF_4]

White solid, 207 mg, 0.33 mmol, 94 % yield.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 0.88 (t, ^3J = 7 Hz, 6H), 1.24-1.46 (m, 52H), 1.86 (m, 2H), 3.35 (b, 1H), 3.87 (m, 1H), 4.07 (m, 1H), 4.16 (m, 2H), 4.28 (m, 1H), 7.24 (s, 1H), 7.37 (s, 1H), 8.78 (s, 1H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 14.15, 22.72, 25.50, 26.28, 29.58, 31.95, 34.24, 50.15, 55.54, 69.81, 121.41, 123.27, 136.21. ^{19}F-NMR (376.5 MHz, $CDCl_3$): δ = -150.80 ($^{10}BF_4$) and -150.85 ($^{11}BF_4$). Anal. Calcd. for $C_{35}H_{69}N_2OBF_4$: C 67.72, H 11.20, N 4.51. Found: C 67.72, H 11.05, N 4.50 %.

[C_{16},C_{16}(2-OH)-imH][PF_6]

White solid, 224 mg, 0.33 mmol, 94 % yield.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 0.88 (t, ^3J = 7 Hz, 6H), 1.26-1.67 (m, 52H), 1.87 (m, 2H), 2.57 (b, 1H), 3.92 (m, 1H), 4.02 (m, 1H), 4.14 (m, 2H), 4.26 (m, 1H), 7.24 (s, 1H), 7.37 (s, 1H), 8.78 (s, 1H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 14.03, 22.64, 25.29, 26.21, 29.52, 31.90, 34.28, 50.20, 55.47, 69.98, 121.49, 123.37, 135.75. ^{19}F-NMR (376.5 MHz, $CDCl_3$): δ = -72.08 (d, $^1J_{PF}$ = 760 Hz). ^{31}P-NMR (162 MHz, $CDCl_3$): δ = -144.35 (septet, $^1J_{PF}$ = 760 Hz). Anal. Calcd. for $C_{35}H_{69}N_2OPF_6$: C 61.92, H 10.24, N 4.13. Found: C 61.52, H 9.89, N 3.77 %.

[Ag(C_{16},C_{16}(2-OH)-imy)$_2$][Ag_2Cl_4] (1)

[C_{16},C_{16}(2-OH)-im][Cl] (200 mg, 0.35 mmol) was reacted with silver(I) oxide (0.17 mg, 40 mmol) in CH_2Cl_2 at room temperature for 24 h and the reaction was performed in the dark. Added activated carbon when the reaction is finished. Filtration over celite followed by removal of the solvent from the filtrate gave the crude product. The product as a white solid powder is obtained followed by recrystallization with CH_2Cl_2/ hexane (95 mg, 0.14 mmol, 40 % yield). ^{1}H-NMR (400 MHz, d^6-DMSO): δ = 0.84 (t, ^3J = 7 Hz, 6H), 1.22 (m, 52H), 1.76 (m, 2H), 3.76 (m, 1H), 4.00 (m, 1H), 4.07 (m, 2H), 4.89 (m, 1H), 7.38 (s, 1H), 7.42 (s, 1H). ^{13}C-NMR (100 MHz, d^6-DMSO): δ = 14.33, 22.51, 25.44, 26.24, 29.14, 29.50, 31.30, 31.74, 34.67, 51.35, 57.42, 70.24, 121.73, 123.23, 178.87. Anal. Calcd. for $C_{35}H_{69}N_2OAgCl$: C 62.07, H 10.27, N 4.14. Found: C 62.53, H 10.00, N

3.78 %.

[Au(C_{16},C_{16}(2-OH)-imy)Cl] (2)

[Au(SMe_2)Cl] (55 mg, 0.19 mmol) in CH_2Cl_2 (20 mL) was added to a CH_2Cl_2 (20 mL) solution of [Ag(C_{16},C_{16}(2-OH)-imy)$_2$][Ag_2Cl_4] (120 mg, 0.18 mmol) and stir for 2 h. Filtration over celite followed by removal of the solvent from the filtrate gave the crude product. The white solid product were obtained by recrystallized with CH_2Cl_2/hexane (102 mg, 0.13 mmol, 74 % yield). ^{1}H-NMR (400 MHz, *d*^{6}-DMSO): δ = 0.84 (t, ^3J = 7 Hz, 6H), 1.22-1.38 (m, 52H), 1.78 (m, 2H), 3.84 (m, 1H), 4.01 (m, 1H), 4.08 (m, 2H), 4.96 (m, 1H), 7.37 (s, 1H), 7.43 (s, 1H). ^{13}C-NMR (100 MHz, *d*^{6}-DMSO): δ = 14.38, 22.55, 25.36, 26.02, 29.28, 30.75, 31.76, 34.54, 50.71, 56.64, 69.86, 121.39, 123.08, 168.91. Anal. Calcd. for $C_{35}H_{69}N_2OAuCl$: C 54.85, H 9.08, N 3.66. Found: C 54.87, H 8.88, N 3.52 %.

Preparation of **2** as thin film

[Au(C_{16},C_{16}(2-OH)-imy)Cl] (20 mg) was dissolved in 5 mL CH_2Cl_2. This solution was used to prepare the thin film sample via drop casting method.

[Au(C_{16},C_{16}(2-OH)-imy)$_2$][BF_4] (3)

K_2CO_3 (13 mg, 0.9 mmol) was added to the mixture of [C_{16},C_{16}(2-OH)-im][BF_4] (43 mg, 0.07 mmol) and [Au(C_{16},C_{16}(2-OH)-imy)Cl] (50 mg, 0.07 mmol) in acetone (30 ml). The mixture was stirred for 24 h. The solvent was removed under reduced pressure. Dichloromethane (10 ml) was added to the residue and filtered through celite. The solvent was concentrated by rotary evaporator under vacuum. Ethylacetate (20 mL) was then added to the concentrated filtrate to give a white product (62 mg, 0.05 mmol, 70 % yield). ^{1}H-NMR (600 MHz, $CDCl_3$): δ = 0.87 (t, ^3J = 7 Hz, 12H), 1.24-1.52 (m, 104H), 1.87 (m, 4H), 3.98 (m, 1H), 3.99 (m, 1H), 4.21 (m, 8H), 4.88 (b, 2H), 6.98 (d, 2H), 7.23 (dd, 2H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 14.13, 22.71, 25.89, 26.73, 29.59, 31.38, 31.95, 34.56, 51.39, 57.68, 70.87, 120.62, 122.86, 184.08. ^{19}F-NMR (376.5 MHz, $CDCl_3$): δ = -152.53 ($^{10}BF_4$) and -152.58 ($^{11}BF_4$). Anal. Calcd. for $C_{70}H_{138}N_4O_2AuBF_4 \cdot H_2O$: C 61.38, H 10.30, N 4.09. Found: C 61.65, H 10.12, N 3.67 %.

[Au(C_{16},C_{16}(2-OH)-imy)$_2$][PF_6] (4)

K_2CO_3 (13 mg, 0.9 mmol) was added to the mixture of [C_{16},C_{16}(2-OH)-im][PF_6] (47 mg, 0.07 mmol) and [Au(C_{16},C_{16}(2-OH)-imy)Cl] (50 mg, 0.07 mmol) in acetone (30 ml). The mixture was stirred for 24 h. The solvent was removed under reduced pressure. Dichloromethane (10 ml) was added to the residue and filtered through celite. The solvent was concentrated by rotary evaporator under vacuum. Ethylacetate (20 mL) was then added to the concentrated filtrate to give a white product (68 mg, 0.05 mmol, 74 % yield). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 0.89 (t, ^3J = 7 Hz, 12H), 1.24-1.66 (m, 104H), 1.86 (m, 4H), 3.04 (b, 1H), 3.23 (b, 1H), 3.92 (m, 1H), 3.98 (m, 1H), 4.15 (m, 8H), 7.03 (m, 2H), 7.14 (dd, 2H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 14.16, 22.72, 25.73, 26.72, 29.51, 31.42, 31.96, 34.43, 51.41, 57.59, 71.46, 121.20, 122.46, 183.88. ^{19}F-NMR (376.5 MHz, $CDCl_3$): δ = -73.05 (d, $^1J_{PF}$ = 760 Hz). ^{31}P-NMR (162 MHz, $CDCl_3$): δ = -144.39 (septet, $^1J_{PF}$ = 760 Hz). Anal. Calcd. for $C_{70}H_{138}N_4O_2AuPF_6$: C 59.64, H 9.87, N 3.97. Found: C 59.58, H 9.85, N 3.49 %.

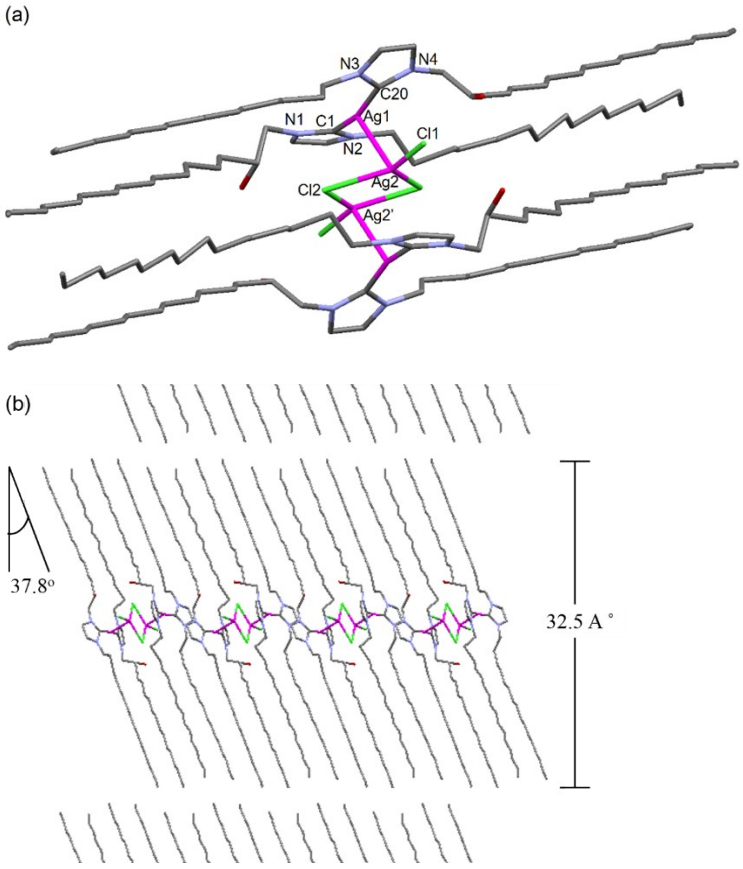

Figure S1. (a) Crystal structure of **1**. Selected bond distances [Å] and angles [°]: Ag(1)–Ag(2) 3.314(3); Ag(1)–Ag(2') 3.227(2); Ag(2)–Ag(2') 3.311(3); Ag(1)–C(1) 2.065(13); Ag(1)–C(20) 2.080(15); N(1)–C(1)–N(2) 103.9(13); N(4)-C(20)-N(3) 103.5(14); C(1)–Ag(1)–C(20) 165.3(6); Ag(2)–Ag(1)–Ag(2') 60.81(6); Ag(2) -Cl(2)-Ag(2') 80.65(16). (b) Crystal packing of **1**.

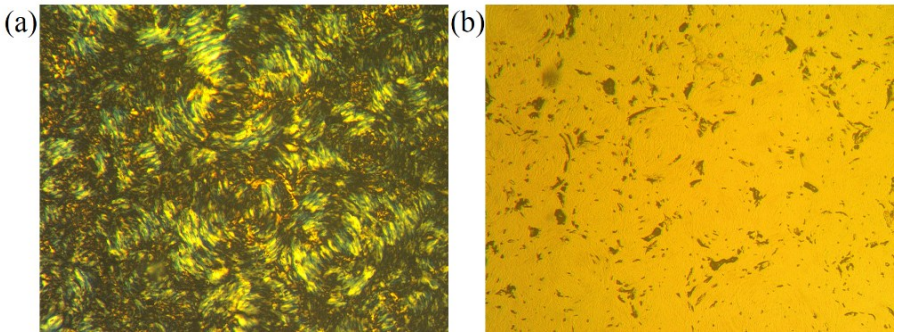

Figure S2. POM image of **2** recorded at room temperature upon cooling from isotropic liquid (a) with and (b) without cross-polarizer. (at the rate of 10 °C/min).

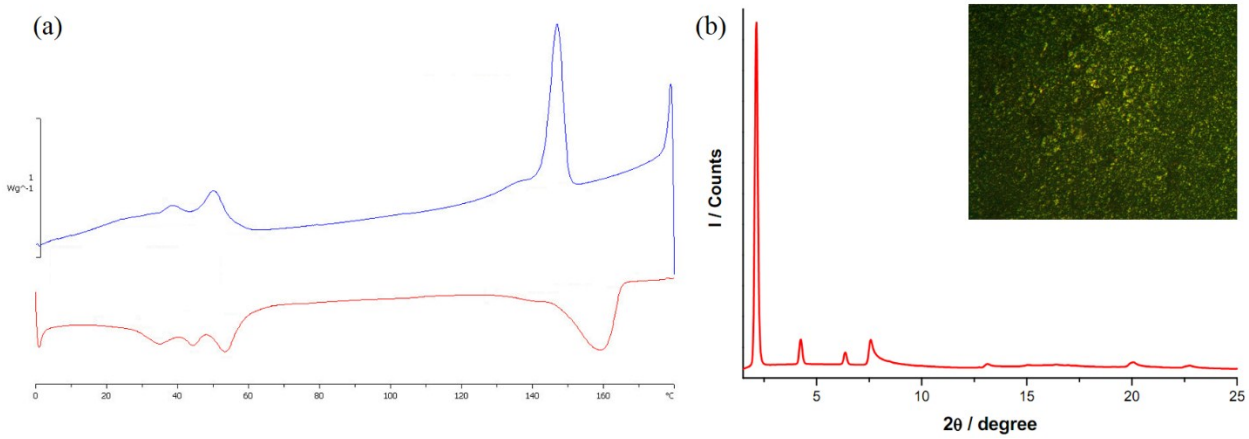

Figure S3. (a) DSC thermograms of **3**. (b) PXRD patterns and POM image of **3** at 120 °C under cooling process (at the rate of 10 °C/min).

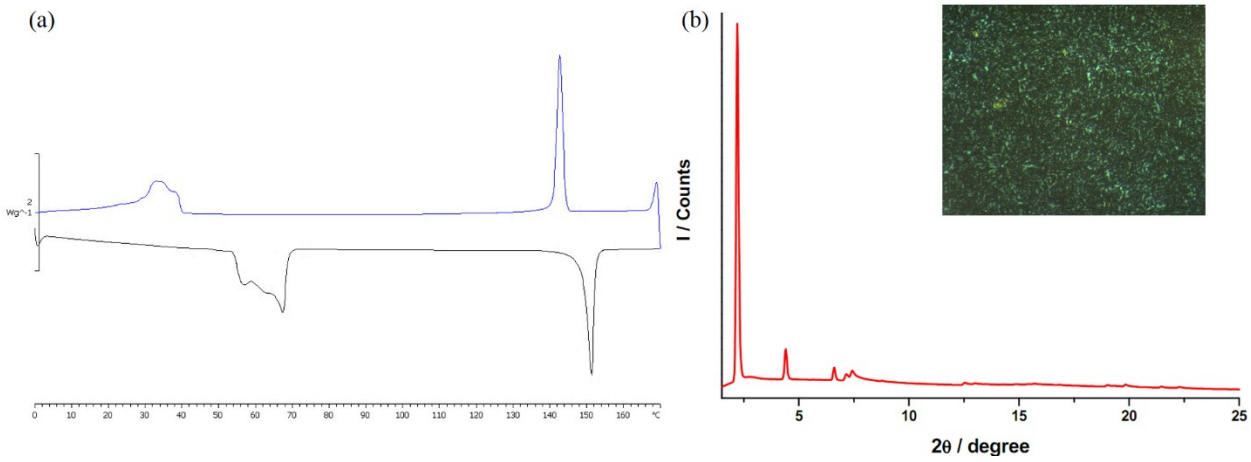

Figure S4. (a) DSC thermograms of **4**. (b) PXRD patterns and POM image of **4** at 120 °C under cooling process (at the rate of 10 °C/min).

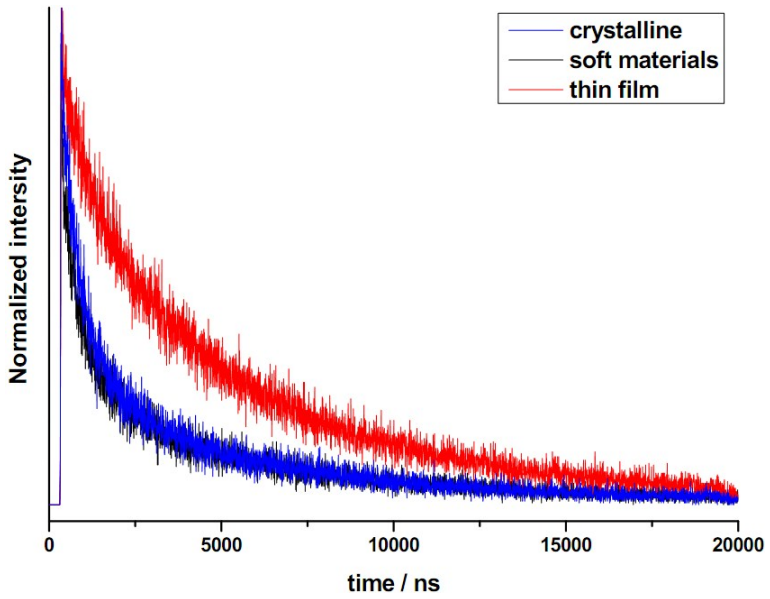

Figure S5. Emission decay profiles of **2** as crystalline at 610 nm (blue line), soft materials at 620 nm (black line) and thin film at 650 nm (red line) under excitation at 306 nm.

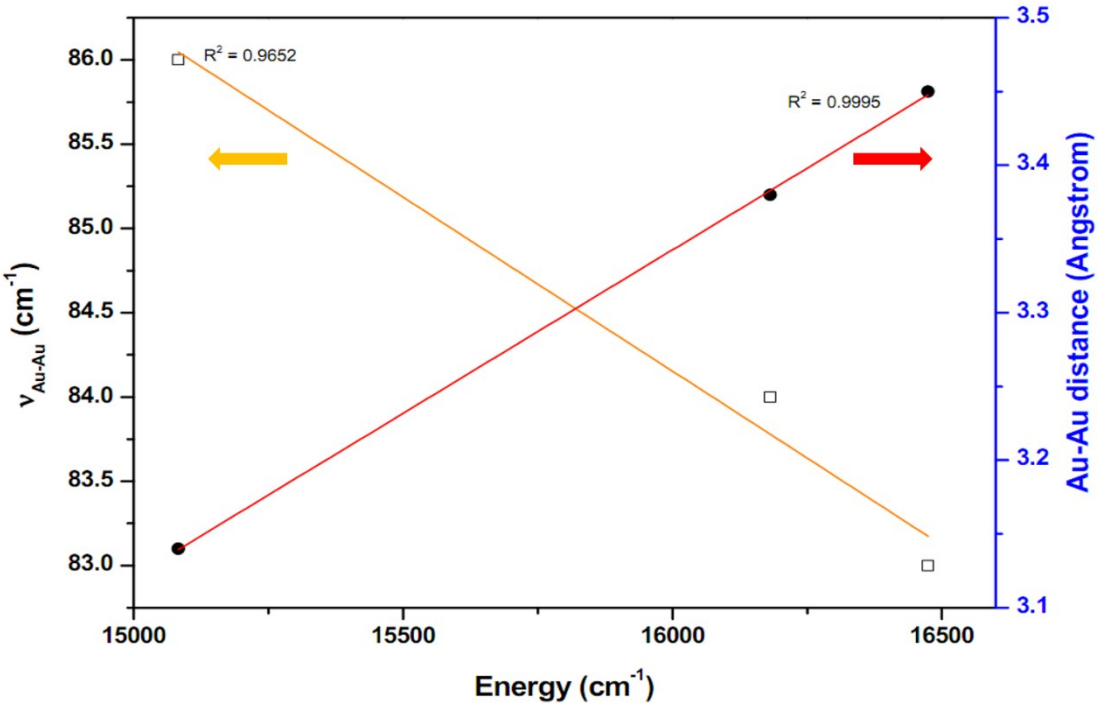

Figure S6. Plot of $\nu_{Au\text{-}Au}$ (cm^{-1}) (left) and Au-Au distance (Å) (right) versus the emission energy (cm^{-1}).

Table S1. Crystal data and structure refinement for **1**.

Identification code	1
Empirical formula	$C_{70}\ H_{136}\ Ag_2\ Cl_2\ N_4\ O_2$
Formula weight	1352.46
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P(-)1
Unit cell dimensions	a = 10.710(6) Å α = 90.210(11) °. b = 12.206(7) Å β = 92.509(12) °. c = 32.320(19) Å γ = 113.758(10) °.
Volume	3862(4) $Å^3$
Z	2
Density (calculated)	1.163 Mg/m^3
Absorption coefficient	0.617 mm^{-1}
F(000)	1456
Crystal size	0.210 x 0.110 x 0.070 mm^3
Theta range for data collection	1.823 to 25.000°.
Index ranges	-12<=h<=12, -14<=k<=14, -38<=l<=38
Reflections collected	44934
Independent reflections	13579 [R(int) = 0.3862]
Completeness to theta = 25.000°	99.9 %
Max. and min. transmission	0.7454 and 0.4403
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13579 / 528 / 722
Goodness-of-fit on F^2	0.918
Final R indices [I>2sigma(I)]	R1 = 0.0894, wR2 = 0.2044
R indices (all data)	R1 = 0.3441, wR2 = 0.3622
Largest diff. peak and hole	0.573 and -0.487 $e.Å^{-3}$

[a] $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$.

[b] $wR_2 = \{\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2\}^{1/2}$.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**.

Atom	x	y	z	U(eq)[a]
Ag(1)	7559(14)	5019(10)	258(5)	108(8)
Ag(2)	4230(15)	3537(11)	63(5)	123(8)
Cl(2)	4638(5)	5303(4)	566(16)	108(17)
Cl(1)	3188(4)	1413(3)	191(18)	128(2)
O(1)	8914(19)	8403(15)	-814(6)	214(7)
O(2)	4380(3)	1920(2)	1187(7)	271(10)
N(2)	6899(12)	2347(10)	39(5)	93(4)
N(1)	6644(15)	2587(13)	688(6)	121(5)
N(4)	9506(13)	7447(11)	-81(6)	100(4)
N(3)	8998(13)	7717(11)	540(5)	105(4)
C(1)	6937(15)	3200(11)	336(6)	96(4)
C(20)	8673(16)	6856(13)	221(6)	98(4)
C(4)	6630(3)	3130(2)	1103(7)	171(7)
C(58)	7280(2)	2643(17)	-383(7)	138(6)
C(2)	6556(16)	1288(11)	219(7)	105(5)
C(21)	10299(16)	8636(14)	37(7)	106(5)
C(42)	9602(19)	6991(15)	-475(7)	120(5)
C(43)	8900(3)	7230(2)	-812(9)	155(7)
C(22)	9953(18)	8755(15)	416(7)	118(6)
C(3)	6399(18)	1362(15)	619(7)	116(6)
C(48)	9460(3)	5390(2)	2264(8)	174(9)
C(9)	4320(3)	5670(3)	2169(8)	197(11)
C(47)	9860(3)	5160(2)	1868(8)	210(12)
C(49)	9180(3)	6430(2)	2380(8)	206(12)
C(45)	10530(3)	4010(2)	1347(8)	205(12)
C(10)	3990(3)	5940(3)	2580(8)	198(11)
C(52)	8090(3)	7800(3)	3289(9)	226(13)
C(46)	10180(3)	4190(2)	1763(8)	190(10)
C(11)	3750(3)	6960(3)	2675(9)	205(12)
C(26)	7390(3)	9580(3)	1612(9)	208(12)
C(23)	8330(2)	7506(17)	916(7)	140(6)
C(25)	7490(3)	8450(2)	1463(8)	182(9)
C(27)	6880(3)	9610(3)	2009(9)	195(10)
C(28)	6730(3)	10700(3)	2141(9)	204(11)
C(29)	6270(3)	10870(3)	2546(9)	205(11)
C(63)	7770(4)	60(3)	-1795(11)	309(18)
C(30)	6210(4)	11990(3)	2655(10)	233(14)
C(68)	9730(4)	-2580(3)	-3218(13)	310(2)
C(65)	8120(4)	-1310(2)	-2391(12)	294(17)
C(72)	10900(5)	-4910(3)	-4285(15)	380(3)

C(62)	7730(3)	1250(2)	-1679(9)	236(11)
C(64)	8460(3)	-100(2)	-2179(9)	235(11)
C(59)	6320(3)	1880(2)	-732(7)	255(12)
C(34)	5010(4)	14490(3)	3710(11)	248(14)
C(33)	5180(4)	13390(3)	3588(11)	254(15)
C(38)	3920(5)	16920(3)	4725(11)	360(3)
C(36)	4480(5)	15770(4)	4219(11)	310(2)
C(37)	3870(4)	15670(3)	4644(11)	320(2)
C(61)	7130(4)	1280(3)	-1266(10)	285(17)
C(66)	9150(3)	-1330(3)	-2698(12)	291(17)
C(73)	10530(4)	-6200(3)	-4443(12)	340(2)
C(69)	9490(4)	-3690(3)	-3389(12)	277(16)
C(71)	10030(4)	-4940(3)	-3917(12)	290(16)
C(16)	2080(4)	9590(3)	4132(10)	266(17)
C(53)	7850(3)	8820(2)	3434(9)	210(12)
C(51)	8530(3)	7590(2)	2902(9)	213(13)
C(31)	5730(4)	12080(3)	3062(10)	242(14)
C(50)	8760(3)	6620(2)	2778(8)	196(11)
C(35)	4560(4)	14730(3)	4110(12)	300(2)
C(32)	5590(3)	13200(3)	3185(10)	231(13)
C(5)	5310(4)	3050(3)	1153(8)	227(10)
C(44)	9250(3)	7040(2)	-1243(8)	177(9)
C(54)	7460(4)	9050(3)	3822(10)	244(15)
C(13)	3130(3)	8220(3)	3189(8)	211(12)
C(14)	2770(3)	8450(3)	3621(8)	218(13)
C(8)	4730(4)	4720(3)	2117(8)	231(15)
C(7)	4820(3)	4350(2)	1701(7)	192(11)
C(56)	6900(4)	10260(3)	4324(11)	272(16)
C(55)	7250(4)	10030(3)	3936(10)	252(15)
C(6)	5270(4)	3340(3)	1613(8)	259(12)
C(12)	3380(3)	7180(2)	3085(8)	193(11)
C(57)	6690(4)	11250(3)	4483(11)	350(2)
C(17)	1900(4)	10730(3)	4201(10)	246(14)
C(15)	2490(4)	9480(3)	3708(10)	236(14)
C(18)	1600(5)	10950(3)	4642(10)	310(2)
C(19)	1480(4)	12010(3)	4738(11)	320(2)
C(60)	7100(4)	2470(2)	-1121(9)	279(14)
C(70)	10250(5)	-3820(4)	-3748(15)	340(2)
C(67)	8870(4)	-2410(3)	-2876(12)	287(17)
C(24)	7870(3)	8530(2)	999(8)	179(9)

[a] U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ag(1)	85(11)	50(8)	19(18)	26(7)	2(10)	3(8)
Ag(2)	108(13)	62(9)	19(2)	28(9)	8(12)	-2(10)
Cl(2)	106(3)	70(3)	15(5)	38(3)	6(3)	-6(3)
Cl(1)	72(3)	58(2)	25(7)	27(2)	0(3)	-14(3)
O(1)	250(19)	148(11)	28(16)	118(13)	5(14)	15(11)
O(2)	300(2)	300(2)	24(19)	141(17)	78(14)	16(15)
N(2)	64(8)	55(6)	18(9)	36(6)	15(7)	17(6)
N(1)	119(11)	68(7)	18(9)	38(7)	17(8)	16(6)
N(4)	55(7)	58(6)	19(10)	28(5)	-1(6)	6(6)
N(3)	76(8)	55(6)	18(10)	23(6)	1(7)	1(6)
C(1)	61(9)	58(6)	17(10)	27(6)	12(7)	9(5)
C(20)	61(8)	49(6)	19(10)	24(5)	3(7)	1(5)
C(4)	260(2)	111(12)	17(11)	108(14)	26(10)	21(8)
C(58)	162(17)	106(12)	19(10)	97(12)	43(9)	39(8)
C(2)	82(12)	64(7)	18(11)	37(7)	7(10)	14(7)
C(21)	52(9)	62(7)	20(12)	15(6)	2(8)	7(7)
C(42)	101(12)	74(10)	19(11)	45(9)	9(8)	9(7)
C(43)	157(17)	117(12)	21(12)	76(13)	-23(11)	-1(10)
C(22)	85(11)	61(7)	20(12)	22(7)	7(9)	0(7)
C(3)	98(13)	72(7)	18(11)	36(8)	14(10)	18(7)
C(48)	210(2)	152(17)	16(16)	76(17)	-28(15)	-41(14)
C(9)	250(3)	210(2)	15(16)	120(2)	10(16)	17(15)
C(47)	340(3)	170(2)	16(17)	140(2)	2(18)	-26(15)
C(49)	320(3)	158(18)	16(17)	120(2)	23(19)	-16(15)
C(45)	290(3)	140(2)	19(2)	100(2)	0(2)	-50(16)
C(10)	270(3)	200(2)	15(16)	120(2)	21(17)	32(15)
C(52)	320(4)	210(2)	17(19)	120(2)	30(2)	-32(17)
C(46)	250(3)	158(18)	18(19)	104(19)	-19(18)	-43(15)
C(11)	280(3)	210(2)	16(16)	130(2)	14(17)	27(15)
C(26)	260(3)	207(19)	20(17)	140(2)	14(17)	-11(15)
C(23)	108(14)	93(11)	20(12)	18(10)	21(10)	-8(9)
C(25)	190(2)	179(17)	20(16)	99(17)	17(14)	-5(13)
C(27)	220(3)	207(19)	19(17)	120(19)	-6(16)	-15(15)
C(28)	240(3)	205(19)	20(18)	120(2)	12(18)	-7(16)
C(29)	230(3)	220(2)	19(18)	120(2)	-1(17)	-8(16)
C(63)	340(4)	185(19)	31(3)	0(2)	100(3)	102(17)
C(30)	310(4)	240(2)	20(19)	160(2)	10(2)	-2(18)
C(68)	260(4)	200(2)	35(3)	-40(2)	90(3)	70(2)
C(65)	240(3)	210(2)	32(3)	-30(2)	50(2)	60(19)
C(72)	410(5)	290(3)	35(4)	30(3)	100(4)	60(3)
C(62)	190(2)	178(17)	24(2)	-29(17)	12(18)	74(15)

C(64)	160(2)	204(19)	25(2)	-19(17)	-12(18)	79(16)
C(59)	320(2)	174(19)	21(13)	37(18)	-9(12)	30(11)
C(34)	260(3)	250(2)	24(2)	110(2)	10(2)	-20(2)
C(33)	310(4)	260(3)	22(2)	140(3)	10(2)	-10(2)
C(38)	540(7)	320(3)	29(3)	240(4)	70(4)	10(3)
C(36)	430(6)	270(3)	27(3)	180(3)	60(3)	10(2)
C(37)	440(5)	300(3)	27(3)	200(4)	60(3)	10(2)
C(61)	320(4)	180(2)	27(2)	10(2)	70(2)	74(16)
C(66)	220(3)	220(2)	32(3)	-30(2)	40(2)	60(2)
C(73)	350(5)	290(3)	31(3)	50(3)	20(3)	40(3)
C(69)	260(3)	200(2)	26(3)	-10(2)	20(3)	90(2)
C(71)	280(4)	230(3)	26(3)	10(2)	10(3)	70(2)
C(16)	360(5)	250(2)	22(2)	150(3)	30(2)	10(2)
C(53)	280(3)	200(2)	17(19)	100(2)	9(19)	-39(16)
C(51)	310(3)	190(2)	17(18)	120(2)	20(19)	-24(16)
C(31)	320(4)	250(2)	20(2)	160(3)	10(2)	-1(18)
C(50)	270(3)	179(19)	15(17)	100(2)	-1(17)	-30(15)
C(35)	400(5)	270(3)	26(2)	180(3)	60(3)	10(2)
C(32)	290(4)	230(2)	21(2)	140(2)	10(2)	3(19)
C(5)	280(2)	270(2)	18(15)	165(16)	35(13)	16(14)
C(44)	210(2)	143(17)	21(13)	103(18)	-9(12)	14(11)
C(54)	330(4)	240(3)	18(2)	130(3)	20(2)	-50(18)
C(13)	280(3)	220(2)	16(17)	140(2)	-1(18)	28(16)
C(14)	290(3)	210(2)	18(17)	120(2)	23(19)	27(17)
C(8)	370(4)	270(3)	12(15)	210(3)	15(17)	26(15)
C(7)	270(3)	230(2)	12(14)	150(2)	3(16)	24(14)
C(56)	330(4)	310(3)	20(2)	160(3)	0(2)	-90(2)
C(55)	340(4)	250(3)	19(2)	150(3)	10(2)	-68(19)
C(6)	390(3)	290(2)	19(15)	230(2)	33(15)	26(14)
C(12)	250(3)	210(2)	15(16)	120(2)	7(16)	34(15)
C(57)	480(7)	350(4)	27(3)	230(4)	30(4)	-110(3)
C(17)	290(4)	220(2)	24(2)	110(3)	20(2)	10(2)
C(15)	300(4)	230(2)	20(2)	140(3)	0(2)	8(18)
C(18)	480(7)	260(3)	25(2)	200(4)	70(3)	30(2)
C(19)	470(7)	250(3)	28(3)	190(4)	70(3)	20(2)
C(60)	350(3)	200(2)	24(15)	50(2)	22(15)	58(13)
C(70)	350(5)	230(3)	33(4)	-10(3)	90(4)	70(2)
C(67)	220(3)	210(2)	30(3)	-50(2)	50(3)	70(2)
C(24)	190(2)	143(15)	22(16)	76(16)	40(15)	-22(13)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1**.

Atom	x	y	z	U(eq)
H(1A)	885	861	-58	32
H(2A)	429	155	97	41
H(4A)	689	270	132	21
H(4B)	728	396	112	21
H(58A)	816	262	-41	17
H(58B)	739	347	-42	17
H(2B)	644	58	8	13
H(8)	1094	922	-12	13
H(7)	1056	730	-54	14
H(21B)	928	613	-46	14
H(43A)	794	669	-79	19
H(22A)	1032	946	58	14
H(3A)	618	76	81	14
H(48A)	1016	538	246	21
H(48B)	863	470	232	21
H(9A)	353	551	199	24
H(9B)	504	639	207	24
H(47A)	914	513	167	25
H(47B)	1066	588	181	25
H(49A)	1001	713	233	25
H(49B)	849	646	218	25
H(45A)	980	402	116	25
H(45B)	1134	470	129	25
H(10A)	318	526	265	24
H(10B)	473	596	277	24
H(52A)	874	772	349	27
H(52B)	724	711	333	27
H(46A)	941	347	183	23
H(46B)	1095	424	195	23
H(11A)	304	696	248	25
H(11B)	457	765	261	25
H(26A)	830	1022	161	25
H(26B)	682	977	141	25
H(23A)	894	747	114	17
H(23B)	754	675	90	17
H(25A)	663	777	149	22
H(25B)	818	831	163	22
H(27A)	749	946	221	23
H(27B)	600	895	202	23
H(28A)	762	1136	212	25
H(28B)	612	1083	194	25

H(29A)	536	1025	257	25
H(29B)	685	1072	276	25
H(63A)	684	-52	-182	37
H(63B)	821	-16	-156	37
H(30A)	562	1215	245	28
H(30B)	712	1262	264	28
H(68A)	966	-209	-345	37
H(68B)	1067	-224	-311	37
H(65A)	723	-156	-254	35
H(65B)	804	-189	-218	35
H(72A)	1074	-444	-450	46
H(72B)	1187	-455	-420	46
H(62A)	865	187	-167	28
H(62B)	720	145	-189	28
H(64A)	832	41	-239	28
H(64B)	944	23	-211	28
H(59A)	544	192	-73	31
H(59B)	620	105	-71	31
H(34A)	589	1514	367	30
H(34B)	438	1458	350	30
H(33A)	583	1331	379	31
H(33B)	431	1273	363	31
H(38A)	355	1695	499	53
H(38B)	484	1750	473	53
H(38C)	338	1710	451	53
H(6)	391	1596	401	37
H(4)	538	1642	423	37
H(5)	294	1507	464	38
H(3)	441	1547	485	38
H(61A)	763	104	-106	34
H(61B)	619	68	-128	34
H(66A)	920	-77	-292	35
H(66B)	1005	-105	-256	35
H(73A)	1107	-619	-467	51
H(73B)	1070	-666	-423	51
H(73C)	958	-655	-453	51
H(69A)	853	-408	-347	33
H(69B)	966	-416	-317	33
H(71A)	908	-535	-401	35
H(71B)	1022	-541	-370	35
H(16A)	277	956	433	32
H(16B)	123	892	418	32
H(53A)	869	951	339	25
H(53B)	717	888	324	25
H(51A)	787	765	270	26
H(51B)	937	828	286	26

H(31A)	635	1196	327	29
H(31B)	485	1142	308	29
H(50A)	792	593	282	24
H(50B)	944	657	298	24
H(35A)	366	1410	414	36
H(35B)	516	1460	432	36
H(32A)	646	1385	315	28
H(32B)	494	1330	299	28
H(5A)	502	354	96	27
H(44A)	852	704	-143	21
H(44B)	1006	773	-131	21
H(54A)	662	837	387	29
H(54B)	815	901	402	29
H(13A)	240	821	300	25
H(13B)	394	891	312	25
H(14A)	197	775	369	26
H(14B)	351	848	381	26
H(8A)	409	403	226	28
H(8B)	562	495	226	28
H(7A)	544	505	156	23
H(7B)	393	414	156	23
H(56A)	758	1018	451	33
H(56B)	605	958	437	33
H(55A)	655	1006	374	30
H(55B)	808	1071	388	30
H(2)	465	262	174	31
H(1)	617	355	174	31
H(12A)	256	649	315	23
H(12B)	410	717	328	23
H(57A)	645	1112	477	52
H(57B)	752	1196	447	52
H(57C)	597	1135	432	52
H(17A)	116	1073	402	30
H(17B)	273	1140	413	30
H(15A)	177	947	351	28
H(15B)	331	1019	366	28
H(18A)	76	1029	471	37
H(18B)	233	1090	482	37
H(19A)	130	1203	503	48
H(19B)	232	1268	469	48
H(19C)	75	1207	457	48
H(60A)	659	276	-131	34
H(60B)	801	309	-106	34
H(70A)	1007	-336	-397	41
H(70B)	1122	-342	-367	41
H(67A)	794	-272	-299	34

H(67B)	890	-294	-266	34
H(24A)	709	844	82	21
H(24B)	860	930	95	21

Table S5. Bond lengths [Å] and angles [°] for **1**.

Bond lengths			
Ag(1)-C(1)	2.065(13)	C(36)-C(37)	1.531(10)
C(23)-C(24)	1.54(3)	N(3)-C(20)	1.40(2)
Ag(1)-C(20)	2.080(15)	C(61)-C(60)	1.530(10)
C(25)-C(24)	1.56(3)	N(3)-C(23)	1.41(2)
Ag(1)-Ag(2)^{i}	3.227(2)	C(66)-C(67)	1.36(4)
C(27)-C(28)	1.47(3)	C(4)-C(5)	1.40(4)
Ag(1)-Ag(2)	3.314(3)	C(69)-C(70)	1.48(5)
C(28)-C(29)	1.47(3)	C(58)-C(59)	1.519(10)
Ag(2)-Cl(1)	2.420(5)	C(71)-C(70)	1.40(5)
C(29)-C(30)	1.44(3)	C(2)-C(3)	1.32(2)
Ag(2)-Cl(2)^{i}	2.540(5)	C(16)-C(15)	1.48(3)
C(63)-C(62)	1.522(10)	C(21)-C(22)	1.32(2)
Ag(2)-Cl(2)	2.577(5)	C(16)-C(17)	1.49(4)
C(63)-C(64)	1.526(10)	C(42)-C(43)	1.40(3)
Ag(2)-Ag(1)^{i}	3.227(2)	C(53)-C(54)	1.40(3)
C(30)-C(31)	1.45(3)	C(43)-C(44)	1.50(3)
Ag(2)-Ag(2)^{i}	3.311(3)	C(51)-C(50)	1.37(3)
C(68)-C(69)	1.38(4)	C(48)-C(47)	1.43(3)
Cl(2)-Ag(2)^{i}	2.540(5)	C(31)-C(32)	1.48(3)
C(68)-C(67)	1.529(10)	C(48)-C(49)	1.47(3)
O(1)-C(43)	1.42(2)	C(5)-C(6)	1.535(10)
C(65)-C(64)	1.518(10)	C(9)-C(8)	1.40(3)
O(2)-C(5)	1.35(4)	C(44)-C(45)^{ii}	1.43(3)
C(65)-C(66)	1.525(10)	C(9)-C(10)	1.46(3)
N(2)-C(2)	1.336(17)	C(54)-C(55)	1.35(3)
C(72)-C(73)	1.533(10)	C(47)-C(46)	1.41(3)
N(2)-C(1)	1.400(19)	C(13)-C(12)	1.44(3)
C(72)-C(71)	1.534(10)	C(49)-C(50)	1.43(3)
N(2)-C(58)	1.45(2)	C(13)-C(14)	1.519(10)
C(62)-C(61)	1.514(10)	C(45)-C(44)^{ii}	1.43(3)
N(1)-C(1)	1.34(2)	C(14)-C(15)	1.43(3)
C(59)-C(60)	1.551(10)	C(45)-C(46)	1.45(3)
N(1)-C(3)	1.43(2)	C(8)-C(7)	1.44(3)
C(34)-C(35)	1.47(4)	C(10)-C(11)	1.40(3)
N(1)-C(4)	1.49(2)	C(7)-C(6)	1.523(10)
C(34)-C(33)	1.47(4)	C(52)-C(51)	1.41(3)
N(4)-C(20)	1.353(19)	C(56)-C(55)	1.39(3)
C(33)-C(32)	1.44(3)	C(52)-C(53)	1.45(3)
N(4)-C(21)	1.396(18)	C(56)-C(57)	1.41(4)
C(38)-C(37)	1.527(10)	C(11)-C(12)	1.45(3)
N(4)-C(42)	1.41(2)	C(17)-C(18)	1.520(10)
C(36)-C(35)	1.36(4)	C(26)-C(27)	1.42(3)
N(3)-C(22)	1.344(19)	C(18)-C(19)	1.39(4)

C(26)-C(25)	1.51(3)		

Angles

C(1)-Ag(1)-C(20)	165.3(6)	C(2)-N(2)-C(1)	109.1(15)
C(44)^{ii}-C(45)-C(46)	120(3)	C(38)-C(37)-C(36)	103(3)
C(1)-Ag(1)-Ag(2)^{i}	128.6(4)	C(2)-N(2)-C(58)	127.8(16)
C(11)-C(10)-C(9)	124(3)	C(62)-C(61)-C(60)	118(2)
C(20)-Ag(1)-Ag(2)^{i}	66.0(4)	C(1)-N(2)-C(58)	123.0(14)
C(51)-C(52)-C(53)	129(3)	C(67)-C(66)-C(65)	115(3)
C(1)-Ag(1)-Ag(2)	67.9(4)	C(1)-N(1)-C(3)	111.2(18)
C(47)-C(46)-C(45)	122(3)	C(68)-C(69)-C(70)	121(4)
C(20)-Ag(1)-Ag(2)	126.8(4)	C(1)-N(1)-C(4)	124.4(16)
C(10)-C(11)-C(12)	122(3)	C(70)-C(71)-C(72)	115(4)
Ag(2)^{i}-Ag(1)-Ag(2)	60.81(6)	C(3)-N(1)-C(4)	124.3(18)
C(27)-C(26)-C(25)	119(3)	C(15)-C(16)-C(17)	113(3)
Cl(1)-Ag(2)-Cl(2)^{i}	131.94(18)	C(20)-N(4)-C(21)	111.4(17)
N(3)-C(23)-C(24)	108.6(18)	C(54)-C(53)-C(52)	130(3)
Cl(1)-Ag(2)-Cl(2)	128.61(19)	C(20)-N(4)-C(42)	127.3(15)
C(26)-C(25)-C(24)	111(2)	C(50)-C(51)-C(52)	128(3)
Cl(2)^{i}-Ag(2)-Cl(2)	99.35(16)	C(21)-N(4)-C(42)	121.3(17)
C(26)-C(27)-C(28)	118(3)	C(30)-C(31)-C(32)	119(3)
Cl(1)-Ag(2)-Ag(1)^{i}	121.66(12)	C(22)-N(3)-C(20)	109.2(18)
C(29)-C(28)-C(27)	124(3)	C(51)-C(50)-C(49)	126(3)
Cl(2)^{i}-Ag(2)-Ag(1)^{i}	72.90(11)	C(22)-N(3)-C(23)	127.3(18)
C(30)-C(29)-C(28)	120(3)	C(36)-C(35)-C(34)	125(4)
Cl(2)-Ag(2)-Ag(1)^{i}	70.42(12)	C(20)-N(3)-C(23)	123.3(15)
C(62)-C(63)-C(64)	122(3)	C(33)-C(32)-C(31)	123(3)
Cl(1)-Ag(2)-Ag(2)^{i}	176.59(16)	N(1)-C(1)-N(2)	103.9(13)
C(29)-C(30)-C(31)	117(3)	O(2)-C(5)-C(4)	113(3)
Cl(2)^{i}-Ag(2)-Ag(2)^{i}	50.16(11)	N(1)-C(1)-Ag(1)	128.4(13)
C(69)-C(68)-C(67)	123(3)	O(2)-C(5)-C(6)	93(2)
Cl(2)-Ag(2)-Ag(2)^{i}	49.19(12)	N(2)-C(1)-Ag(1)	127.2(14)
C(64)-C(65)-C(66)	115(3)	C(4)-C(5)-C(6)	105(3)
Ag(1)^{i}-Ag(2)-Ag(2)^{i}	60.90(6)	N(4)-C(20)-N(3)	103.5(14)
C(73)-C(72)-C(71)	109(4)	C(45)^{ii}-C(44)-C(43)	121(2)
Cl(1)-Ag(2)-Ag(1)	119.09(12)	N(4)-C(20)-Ag(1)	127.4(13)
C(61)-C(62)-C(63)	115(2)	C(55)-C(54)-C(53)	127(4)
Cl(2)^{i}-Ag(2)-Ag(1)	69.29(12)	N(3)-C(20)-Ag(1)	127.4(14)
C(65)-C(64)-C(63)	123(3)	C(12)-C(13)-C(14)	122(3)
Cl(2)-Ag(2)-Ag(1)	70.93(11)	C(5)-C(4)-N(1)	108(2)
C(58)-C(59)-C(60)	102(2)	C(15)-C(14)-C(13)	120(3)
Ag(1)^{i}-Ag(2)-Ag(1)	119.19(6)	N(2)-C(58)-C(59)	118.4(19)
C(35)-C(34)-C(33)	126(4)	C(9)-C(8)-C(7)	118(3)
Ag(2)^{i}-Ag(2)-Ag(1)	58.29(5)	C(3)-C(2)-N(2)	111.8(15)
C(32)-C(33)-C(34)	124(4)	C(8)-C(7)-C(6)	122(2)
Ag(2)^{i}-Cl(2)-Ag(2)	80.65(16)	C(22)-C(21)-N(4)	105.2(18)
C(35)-C(36)-C(37)	110(4)	C(55)-C(56)-C(57)	131(4)

C(43)-C(42)-N(4)	117.9(19)	C(2)-C(3)-N(1)	103.9(17)
C(54)-C(55)-C(56)	126(4)	C(19)-C(18)-C(17)	119(3)
C(42)-C(43)-O(1)	116(2)	C(47)-C(48)-C(49)	126(3)
C(7)-C(6)-C(5)	115(3)	C(61)-C(60)-C(59)	92(2)
C(42)-C(43)-C(44)	119(2)	C(8)-C(9)-C(10)	119(3)
C(13)-C(12)-C(11)	123(3)	C(71)-C(70)-C(69)	121(4)
O(1)-C(43)-C(44)	105(2)	C(46)-C(47)-C(48)	126(3)
C(16)-C(17)-C(18)	115(3)	C(66)-C(67)-C(68)	122(3)
C(21)-C(22)-N(3)	110.6(19)	C(50)-C(49)-C(48)	124(3)
C(14)-C(15)-C(16)	117(3)	C(23)-C(24)-C(25)	107(2)

Symmetry transformations used to generate equivalent atoms: (i) −x+1, −y+1, −z; (ii) −x+2, −y+1, −z.

Table S6. Crystal data and structure refinement for **2**.

Identification code	1
Empirical formula	C_{35} H_{68} Au Cl N_2 O
Formula weight	765.33
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 24.165(7) Å α = 90 °. b = 8.609(3) Å β = 92.647(7) °. c = 18.260(5) Å γ = 90 °.
Volume	3794.9(19) $Å^3$
Z	4
Density (calculated)	1.340 Mg/m^3
Absorption coefficient	3.973 mm^{-1}
F(000)	1584
Crystal size	0.240 x 0.150 x 0.095 mm^3
Theta range for data collection	0.843 to 25.390°.
Index ranges	-29<=h<=28, -10<=k<=10, -21<=l<=21
Reflections collected	28778
Independent reflections	6914 [R(int) = 0.0799]
Completeness to theta = 25.242°	99.9 %
Max. and min. transmission	0.7036 and 0.4484
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6914 / 1 / 361
Goodness-of-fit on F^2	1.055
Final R indices [I>2sigma(I)]	R1 = 0.0431, wR2 = 0.0962
R indices (all data)	R1 = 0.0998, wR2 = 0.1230
Largest diff. peak and hole	1.117 and -0.774 $e.Å^{-3}$

[a] $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$.

[b] $wR_2 = \{\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2\}^{1/2}$.

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**.

Atom	x	y	z	U(eq)[a]
Au(1)	4860(1)	8436(1)	4431(1)	58(1)
Cl(1)	4826(1)	9619(3)	3309(1)	81(1)
O(1)	6170(4)	8765(10)	5776(6)	159(4)
N(1)	5253(2)	6491(8)	5715(4)	60(2)
N(2)	4453(2)	7445(8)	5872(4)	58(2)
C(1)	4861(3)	7404(9)	5391(4)	50(2)
C(2)	5099(4)	5952(11)	6387(5)	76(3)
C(3)	4599(3)	6566(10)	6488(5)	68(2)
C(4)	5805(3)	6215(10)	5448(5)	66(2)
C(5)	6239(3)	7207(11)	5851(6)	86(3)
C(6)	6825(3)	6794(10)	5612(5)	73(2)
C(7)	7280(3)	7584(13)	6062(6)	90(3)
C(8)	7857(3)	7112(12)	5905(6)	89(3)
C(9)	8314(4)	7775(13)	6373(6)	94(3)
C(10)	8881(4)	7253(14)	6276(7)	105(4)
C(11)	9340(4)	7852(14)	6741(6)	105(4)
C(12)	9907(4)	7307(14)	6658(7)	112(4)
C(13)	10365(4)	7869(15)	7125(7)	111(4)
C(14)	10927(4)	7336(15)	7040(7)	118(4)
C(15)	11397(4)	7866(16)	7490(7)	117(4)
C(16)	11952(4)	7353(15)	7414(7)	116(4)
C(17)	12422(4)	7820(17)	7841(7)	125(5)
C(18)	12989(5)	7297(16)	7763(8)	126(4)
C(19)	13459(5)	7820(20)	8180(8)	164(7)
C(20)	3944(3)	8344(9)	5777(5)	63(2)
C(21)	3462(3)	7369(11)	5523(5)	73(2)
C(22)	2925(3)	8290(10)	5415(6)	78(3)
C(23)	2429(3)	7269(11)	5180(6)	81(3)
C(24)	1896(3)	8176(11)	5047(6)	90(3)
C(25)	1402(3)	7157(11)	4820(6)	84(3)
C(26)	869(4)	8065(11)	4666(6)	91(3)
C(27)	374(3)	7056(10)	4441(6)	82(3)

C(28)	-161(3)	7962(11)	4293(6)	94(3)
C(29)	-653(3)	6996(10)	4070(6)	79(3)
C(30)	-1181(4)	7905(11)	3913(6)	91(3)
C(31)	-1682(3)	6930(11)	3707(6)	82(3)
C(32)	-2206(4)	7880(11)	3570(6)	86(3)
C(33)	-2718(4)	6914(10)	3389(5)	76(3)
C(34)	-3247(4)	7848(11)	3293(6)	85(3)
C(35)	-3752(4)	6865(13)	3127(7)	115(4)

[a] U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**.

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au(1)	48(1)	62(1)	64(1)	-4(1)	-7(1)	0(1)
Cl(1)	90(2)	86(2)	66(1)	2(1)	-7(1)	-3(1)
O(1)	111(7)	96(6)	268(12)	-15(7)	0(7)	13(5)
N(1)	36(3)	62(4)	81(5)	0(4)	-7(3)	-3(3)
N(2)	38(4)	61(4)	74(4)	-3(4)	-5(3)	-3(3)
C(1)	29(4)	56(5)	65(5)	-6(4)	0(4)	6(4)
C(2)	67(6)	76(6)	83(7)	15(5)	-6(5)	2(5)
C(3)	56(5)	69(6)	79(6)	19(5)	4(4)	3(5)
C(4)	46(5)	66(6)	87(6)	-11(4)	1(4)	18(4)
C(5)	34(5)	58(5)	164(10)	13(6)	-9(5)	1(4)
C(6)	53(5)	75(6)	91(6)	1(5)	1(4)	6(5)
C(7)	46(5)	105(8)	119(8)	-15(7)	4(5)	9(5)
C(8)	45(5)	99(8)	123(8)	-6(6)	-4(5)	1(5)
C(9)	64(7)	106(8)	113(8)	-8(7)	-4(6)	0(6)
C(10)	60(7)	104(9)	149(10)	-12(8)	0(7)	1(6)
C(11)	62(7)	124(10)	129(9)	-6(8)	-4(6)	-2(7)
C(12)	57(7)	108(9)	169(11)	-24(8)	-7(7)	-3(6)
C(13)	57(7)	139(11)	137(10)	-10(8)	-4(6)	0(7)
C(14)	65(7)	106(9)	179(12)	-21(9)	-20(7)	-4(7)
C(15)	66(7)	151(12)	132(10)	-12(8)	-14(7)	7(7)
C(16)	64(7)	108(9)	174(12)	-35(9)	-18(7)	-3(7)
C(17)	71(8)	162(13)	139(10)	-29(9)	-22(7)	15(8)
C(18)	80(9)	128(11)	168(12)	-39(9)	-7(8)	4(8)
C(19)	98(10)	209(17)	183(14)	-85(13)	-27(10)	7(10)
C(20)	40(4)	60(5)	88(6)	-16(5)	-2(4)	10(4)
C(21)	50(5)	67(6)	101(7)	-16(5)	-6(5)	-1(5)
C(22)	43(5)	72(6)	118(8)	-20(6)	-8(5)	13(5)
C(23)	47(5)	68(6)	127(8)	-10(6)	-7(5)	7(5)
C(24)	46(5)	79(7)	143(9)	-28(6)	-16(5)	6(5)
C(25)	49(5)	72(6)	128(8)	-16(6)	-16(5)	4(5)
C(26)	50(5)	74(7)	149(10)	-17(6)	-13(6)	7(5)
C(27)	45(5)	72(7)	128(8)	-14(6)	-13(5)	0(5)
C(28)	52(6)	80(7)	148(10)	-15(6)	-25(6)	11(5)

C(29)	47(5)	71(7)	118(8)	-18(5)	-14(5)	4(4)
C(30)	56(6)	66(6)	150(10)	-13(6)	-16(6)	6(5)
C(31)	53(5)	81(7)	110(8)	-9(5)	-8(5)	2(5)
C(32)	55(6)	71(6)	129(8)	-18(6)	-12(5)	3(5)
C(33)	61(6)	76(7)	91(7)	-8(5)	-6(5)	7(5)
C(34)	56(6)	78(7)	120(8)	-5(6)	-11(5)	-1(5)
C(35)	65(7)	128(11)	150(11)	1(8)	-2(7)	8(7)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **2**.

Atom	x	y	z	U(eq)
H(1A)	5864	9011	5913	238
H(2A)	5300	5297	6704	91
H(3A)	4388	6428	6896	81
H(4A)	5803	6449	4928	80
H(4B)	5899	5127	5512	80
H(5A)	6226	6963	6374	103
H(6A)	6876	5678	5648	88
H(6B)	6856	7083	5102	88
H(7A)	7247	8695	5986	108
H(7B)	7223	7383	6575	108
H(8A)	7880	5989	5942	107
H(8B)	7921	7384	5401	107
H(9A)	8307	8893	6304	113
H(9B)	8230	7580	6879	113
H(10A)	8883	6132	6328	125
H(10B)	8966	7475	5773	125
H(11A)	9250	7654	7245	126
H(11B)	9343	8970	6679	126
H(12A)	9901	6185	6710	134
H(12B)	9998	7522	6157	134
H(13A)	10370	8991	7076	133
H(13B)	10275	7647	7626	133
H(14A)	10919	6214	7088	141
H(14B)	11013	7554	6536	141
H(15A)	11404	8988	7442	140
H(15B)	11310	7650	7993	140
H(16A)	11940	6230	7454	139
H(16B)	12036	7577	6910	139
H(17A)	12338	7595	8345	150
H(17B)	12434	8943	7802	150
H(18A)	12982	6179	7826	151
H(18B)	13069	7480	7254	151

H(19A)	13783	7299	8022	246
H(19B)	13500	8923	8112	246
H(19C)	13413	7608	8689	246
H(20A)	3998	9162	5422	75
H(20B)	3863	8830	6239	75
H(21A)	3408	6555	5880	87
H(21B)	3545	6877	5063	87
H(22A)	2974	9080	5045	94
H(22B)	2848	8812	5869	94
H(23A)	2512	6720	4735	97
H(23B)	2374	6499	5558	97
H(24A)	1949	8940	4666	108
H(24B)	1814	8732	5491	108
H(25A)	1488	6581	4383	100
H(25B)	1343	6411	5207	100
H(26A)	784	8644	5103	110
H(26B)	928	8810	4279	110
H(27A)	317	6306	4827	98
H(27B)	458	6483	4003	98
H(28A)	-243	8535	4732	113
H(28B)	-101	8715	3909	113
H(29A)	-717	6253	4457	95
H(29B)	-570	6412	3634	95
H(30A)	-1259	8511	4344	110
H(30B)	-1120	8627	3517	110
H(31A)	-1741	6193	4098	98
H(31B)	-1610	6343	3268	98
H(32A)	-2268	8498	4003	103
H(32B)	-2150	8591	3168	103
H(33A)	-2663	6341	2941	92
H(33B)	-2761	6163	3779	92
H(34A)	-3300	8435	3738	102
H(34B)	-3208	8585	2897	102
H(35A)	-4072	7521	3073	172
H(35B)	-3707	6299	2681	172
H(35C)	-3799	6148	3522	172

Table S10. Bond lengths [Å] and angles [°] for **2**.

Bond lengths			
Au(1)-C(1)	1.965(8)	C(14)-C(15)	1.444(14)
Au(1)-Cl(1)	2.286(2)	C(15)-C(16)	1.426(13)
O(1)-C(5)	1.359(11)	C(16)-C(17)	1.407(13)
N(1)-C(1)	1.347(9)	C(17)-C(18)	1.455(14)
N(1)-C(2)	1.379(10)	C(18)-C(19)	1.412(15)
N(1)-C(4)	1.461(9)	C(20)-C(21)	1.492(10)
N(2)-C(1)	1.351(9)	C(21)-C(22)	1.524(11)
N(2)-C(3)	1.387(10)	C(22)-C(23)	1.533(11)
N(2)-C(20)	1.456(9)	C(23)-C(24)	1.516(11)
C(2)-C(3)	1.339(11)	C(24)-C(25)	1.524(11)
C(4)-C(5)	1.517(12)	C(25)-C(26)	1.523(11)
C(5)-C(6)	1.543(11)	C(26)-C(27)	1.518(11)
C(6)-C(7)	1.504(12)	C(27)-C(28)	1.524(11)
C(7)-C(8)	1.493(11)	C(28)-C(29)	1.494(11)
C(8)-C(9)	1.478(12)	C(29)-C(30)	1.512(11)
C(9)-C(10)	1.461(13)	C(30)-C(31)	1.506(12)
C(10)-C(11)	1.459(13)	C(31)-C(32)	1.519(11)
C(11)-C(12)	1.463(13)	C(32)-C(33)	1.515(12)
C(12)-C(13)	1.449(13)	C(33)-C(34)	1.513(11)
C(13)-C(14)	1.449(13)	C(34)-C(35)	1.504(12)
Angles			
C(1)-Au(1)-Cl(1)	178.0(2)	C(13)-C(12)-C(11)	121.8(10)
C(1)-N(1)-C(2)	111.9(7)	C(14)-C(13)-C(12)	121.8(11)
C(1)-N(1)-C(4)	125.7(7)	C(15)-C(14)-C(13)	123.7(11)
C(2)-N(1)-C(4)	122.1(7)	C(16)-C(15)-C(14)	124.4(11)
C(1)-N(2)-C(3)	110.3(7)	C(17)-C(16)-C(15)	126.6(11)
C(1)-N(2)-C(20)	125.0(7)	C(16)-C(17)-C(18)	126.6(12)
C(3)-N(2)-C(20)	124.7(7)	C(19)-C(18)-C(17)	125.8(12)
N(1)-C(1)-N(2)	104.5(7)	N(2)-C(20)-C(21)	112.4(7)
N(1)-C(1)-Au(1)	128.8(5)	C(20)-C(21)-C(22)	113.3(7)
N(2)-C(1)-Au(1)	126.7(6)	C(21)-C(22)-C(23)	112.8(7)
C(3)-C(2)-N(1)	105.8(8)	C(24)-C(23)-C(22)	113.4(7)
C(2)-C(3)-N(2)	107.5(8)	C(23)-C(24)-C(25)	113.3(8)
N(1)-C(4)-C(5)	111.6(7)	C(26)-C(25)-C(24)	113.6(8)
O(1)-C(5)-C(4)	115.3(8)	C(27)-C(26)-C(25)	113.9(7)
O(1)-C(5)-C(6)	108.0(8)	C(26)-C(27)-C(28)	113.9(8)
C(4)-C(5)-C(6)	110.9(8)	C(29)-C(28)-C(27)	115.0(8)
C(7)-C(6)-C(5)	113.5(8)	C(28)-C(29)-C(30)	114.7(7)
C(8)-C(7)-C(6)	116.0(8)	C(31)-C(30)-C(29)	114.8(8)
C(9)-C(8)-C(7)	117.6(9)	C(30)-C(31)-C(32)	113.3(8)
C(10)-C(9)-C(8)	119.4(9)	C(33)-C(32)-C(31)	114.0(8)
C(11)-C(10)-C(9)	120.9(10)	C(34)-C(33)-C(32)	114.3(8)
C(10)-C(11)-C(12)	121.1(10)	C(35)-C(34)-C(33)	113.4(8)

Symmetry transformations used to generate equivalent atoms: