

## Supporting Information

# Size-Confining Growth of Atom-Precise Nanoclusters in Metal-Organic Frameworks and Catalytic Application

Lingli Liu<sup>a,b</sup>, Yongbo Song<sup>a</sup>, Hanbao Chong<sup>a</sup>, Sha Yang<sup>a</sup>, Ji Xiang<sup>a</sup>, Shan Jin<sup>a</sup>, Xi Kang<sup>a</sup>, Jun Zhang<sup>a</sup>, Haizhu Yu<sup>a</sup>, Manzhou Zhu<sup>a\*</sup>

<sup>a</sup>Department of Chemistry and Center for Atomic Engineering of Advanced Materials, Anhui University, Hefei, Anhui 230601, P. R. China

<sup>b</sup>Laboratory of Fundamental Chemistry, School of Pharmacy, Anhui Xinhua University, Hefei, Anhui, 230088, P.R. China

### 1. Preparation of $[Au_{13}Ag_{12}(PPh_3)_{10}Cl_8]^+$ NCs and $Au_{13}Ag_{12}:PPh_3 @ MIL-101(Cr)$

The composite of  $Au_{13}Ag_{12}:PPh_3 @ MIL-101(Cr)$  was synthesized as follows: HAuCl<sub>4</sub>·3H<sub>2</sub>O (78.8 mg, 0.2 mmol) was added to ethanol solution (10 mL) of evacuated MIL-101(Cr) (100 mg) and AgNO<sub>3</sub> (20 mg dissolved in 5mL ethanol) was added at room temperature, and the mixture was kept under constant, slow stirring for several hours. Then 160 mg triphenylphosphine ( $PPh_3$ ) was added to the above mixed suspension. Then an aqueous solution of NaBH<sub>4</sub> (40mg dissolved in 5mL ethanol) was quickly added to the above solution to initiate the reaction. The reaction was allowed to proceed for 2 hours. The composite of  $AuAg:PPh_3 @ MIL-101(Cr)$  was collected by centrifugation, and the precipitation and supernatant were separated. The  $[Au_{13}Ag_{12}(PPh_3)_{10}Cl_8]^+$  NCs crude product was prepared by dissolving in methylene chloride. After that, the methylene chloride solution of  $[Au_{13}Ag_{12}(PPh_3)_{10}Cl_8]^+$  NCs was dried via rotavaporation. N-hexane (~20 mL) was added to remove the redundant  $PPh_3$  and this wash/centrifugation cycle was repeated at least three times. Then 10 mL ethanol was used to extract pure  $Au_{13}Ag_{12}:PPh_3$  NCs and about 8.5% yield was synthesized.

The precipitation was washed several times with ethanol until the ethanol solution is colorless so as to remove the product on the surface,  $Au_{13}Ag_{12}:PPh_3 @ MIL-101(Cr)$  was vacuum dried overnight at 40°C.

### 2. Table S1. Physicochemical structural properties of ZIF-8-supported Au clusters.

Samples	BET surface area ( $m^2 g^{-1}$ )	Pore volume ( $cm^3 g^{-1}$ )	Pore diameter (nm)
ZIF-8	1337.82	0.80	2.39
$Au_{11}:PPh_3 @ ZIF-8$	797.56	0.39	1.41
$Au_{11} @ ZIF-8(150)$	555.40	0.38	1.97
$Au_{11} @ ZIF-8(200)$	596.52	0.21	1.52
$Au_{11} @ ZIF-8(300)$	169.5	0.11	1.93

**Table S2. Physicochemical structural properties of MIL-101(Cr)-supported AuAg clusters.**

Samples	BET surface area (m <sup>2</sup> g <sup>-1</sup> )	Pore volume (cm <sup>3</sup> g <sup>-1</sup> )	Pore diameter (nm)
MIL-101(Cr)	1301.11	0.71	2.43
Au <sub>13</sub> Ag <sub>12</sub> :PPh <sub>3</sub> @MIL-101	548.15	0.33	2.19
Au <sub>13</sub> Ag <sub>12</sub> @ MIL-101(Cr)	773.39	0.46	2.41

**3. X-ray Crystallographic Determination.****Table S2. Crystal data and structure refinement for [Au<sub>13</sub>Ag<sub>12</sub>(PPh<sub>3</sub>)<sub>10</sub>Cl<sub>8</sub>]<sup>+</sup>**

Identification code	[Au <sub>13</sub> Ag <sub>12</sub> (PPh <sub>3</sub> ) <sub>10</sub> Cl <sub>8</sub> ] <sup>+</sup>	
Empirical formula	C <sub>180</sub> H <sub>150</sub> Ag <sub>12</sub> Au <sub>13</sub> Cl <sub>8</sub> P <sub>10</sub>	
Formula weight	6761.30	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic C2/c	
Unit cell dimensions	a = 47.6239(19) Å	α = 90 deg.
	b = 16.6379(7) Å	β = 127.438(2) deg.
	c = 36.1489(13) Å	γ = 90 deg.
Volume	22742.9(16) Å <sup>3</sup>	
Z, Calculated density	4, 1.975 Mg/m <sup>3</sup>	
Absorption coefficient	9.556 mm <sup>-1</sup>	
F(000)	12428	
Crystal size	0.19 x 0.16 x 0.15 mm	
Theta range for data collection	1.34 to 25.50 deg.	
Limiting indices	-57 ≤ h ≤ 52, -20 ≤ k ≤ 20, -43 ≤ l ≤ 43	

Reflections collected / unique	<b>84995 / 21168 [R(int) = 0.0726]</b>
Completeness to theta = 25.50	<b>99.9 %</b>
Absorption correction	<b>None</b>
Max. and min. transmission	<b>0.3282 and 0.2640</b>
Refinement method	<b>Full-matrix least-squares on F<sup>2</sup></b>
Data / restraints / parameters	<b>21168 / 0 / 783</b>
Goodness-of-fit on F <sup>2</sup>	<b>0.981</b>
Final R indices [I>2sigma(I)]	<b>R1 = 0.0540, wR2 = 0.1475</b>
R indices (all data)	<b>R1 = 0.0896, wR2 = 0.1592</b>
Largest diff. peak and hole	<b>3.185 and -5.186 e. Å<sup>-3</sup></b>

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**Table S3.** Atomic coordinates (x 10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup> x 10<sup>3</sup>) for [Au<sub>13</sub>Ag<sub>12</sub>(PPh<sub>3</sub>)<sub>10</sub>Cl<sub>8</sub>]<sup>+</sup>. U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

	<b>x</b>	<b>y</b>	<b>z</b>	<b>U(eq)</b>
Ag(1)	1025(1)	2513(1)	2292(1)	50(1)
Ag(2)	85(1)	3736(1)	2141(1)	50(1)
Ag(3)	-178(1)	2263(1)	1596(1)	47(1)
Ag(4)	176(1)	913(1)	2232(1)	56(1)
Ag(5)	641(1)	1541(1)	3161(1)	55(1)
Ag(6)	600(1)	3299(1)	3131(1)	55(1)
Au(1)	812(1)	3877(1)	2588(1)	52(1)
Au(2)	331(1)	3254(1)	1637(1)	44(1)
Au(3)	389(1)	1519(1)	1693(1)	45(1)
Au(4)	915(1)	1081(1)	2660(1)	50(1)
Au(5)	1149(1)	2516(1)	3208(1)	49(1)
Au(6)	516(1)	2409(1)	2395(1)	36(1)
Au(7)	0	2325(1)	2500	70(1)
C(1)	752(2)	5948(4)	2570(2)	78(5)

C(2)	394(2)	5767(5)	2307(2)	90(5)
C(3)	151(2)	6370(6)	2192(3)	88(5)
C(4)	266(2)	7154(6)	2340(3)	91(6)
C(5)	624(2)	7336(4)	2602(3)	94(6)
C(6)	867(2)	6733(4)	2717(2)	89(5)
C(7)	1213(2)	5315(5)	2401(2)	126(8)
C(8)	1267(2)	6086(5)	2308(2)	136(9)
C(9)	1396(2)	6193(7)	2054(3)	141(9)
C(10)	1470(2)	5530(8)	1894(3)	141(9)
C(11)	1416(2)	4758(8)	1987(3)	136(9)
C(12)	1288(2)	4651(6)	2240(3)	129(8)
C(13)	1402(2)	5321(4)	3315(2)	112(7)
C(14)	1316(2)	5556(4)	3604(2)	136(9)
C(15)	1581(2)	5769(5)	4064(2)	147(10)
C(16)	1933(2)	5746(6)	4235(2)	149(10)
C(17)	2020(2)	5511(6)	3946(2)	151(10)
C(18)	1754(2)	5299(4)	3487(2)	144(9)
C(19)	300(3)	4986(5)	1080(4)	70(4)
C(20)	502(3)	5324(7)	962(4)	79(5)
C(21)	557(3)	6150(7)	995(4)	89(5)
C(22)	409(3)	6638(5)	1148(4)	93(6)
C(23)	206(3)	6300(7)	1266(4)	90(6)
C(24)	152(3)	5474(7)	1233(4)	84(5)
C(25)	-275(2)	4035(7)	532(3)	72(4)
C(26)	-399(3)	4557(6)	162(4)	77(5)
C(27)	-761(3)	4635(6)	-187(3)	90(5)
C(28)	-998(2)	4191(7)	-166(4)	93(6)
C(29)	-873(3)	3668(7)	205(4)	91(6)
C(30)	-512(3)	3591(6)	553(3)	78(5)
C(31)	375(3)	3557(6)	751(4)	68(4)
C(32)	221(2)	3571(6)	279(4)	74(5)
C(33)	407(3)	3281(7)	124(3)	83(5)
C(34)	747(3)	2978(7)	442(5)	91(6)
C(35)	901(2)	2964(7)	914(4)	93(6)
C(36)	715(3)	3253(7)	1069(3)	85(5)
C(37)	599(3)	642(7)	1051(4)	80(5)
C(38)	574(3)	132(7)	728(4)	92(6)
C(39)	859(3)	50(7)	717(4)	98(6)
C(40)	1169(3)	479(8)	1028(5)	100(6)
C(41)	1194(3)	989(7)	1351(4)	101(6)
C(42)	909(3)	1070(6)	1363(4)	93(6)
C(43)	-64(2)	1312(4)	529(2)	73(5)
C(44)	-15(3)	1555(4)	204(3)	81(5)
C(45)	-288(3)	1933(4)	-205(3)	92(6)

C(46)	-610(3)	2069(4)	-288(3)	98(6)
C(47)	-659(2)	1826(4)	37(3)	100(6)
C(48)	-386(2)	1448(3)	446(3)	89(5)
C(49)	46(2)	-160(4)	997(3)	82(5)
C(50)	-155(2)	-528(3)	562(3)	99(6)
C(51)	-321(3)	-1258(3)	501(4)	108(7)
C(52)	-285(3)	-1620(4)	874(4)	118(7)
C(53)	-84(3)	-1252(5)	1308(4)	124(8)
C(54)	82(3)	-522(5)	1370(3)	109(7)
C(55)	1293(4)	-717(10)	3261(5)	114(7)
C(56)	1479(4)	-1434(12)	3377(6)	124(8)
C(57)	1485(4)	-1976(8)	3675(6)	133(9)
C(58)	1305(5)	-1799(10)	3856(5)	138(9)
C(59)	1119(4)	-1082(12)	3740(6)	133(8)
C(60)	1113(4)	-541(8)	3442(6)	121(8)
C(61)	1733(1)	369(2)	3200(1)	96(6)
C(62)	2026(2)	-60(2)	3556(2)	111(7)
C(63)	2364(1)	184(3)	3725(2)	114(7)
C(64)	2409(2)	857(3)	3538(2)	114(7)
C(65)	2116(2)	1286(3)	3182(2)	113(7)
C(66)	1778(2)	1042(3)	3013(2)	108(7)
C(67)	1197(2)	-564(3)	2408(2)	130(8)
C(68)	912(2)	-1087(4)	2208(2)	143(9)
C(69)	822(2)	-1577(4)	1839(2)	149(10)
C(70)	1017(2)	-1544(4)	1669(2)	148(10)
C(71)	1302(2)	-1021(4)	1869(2)	145(10)
C(72)	1392(2)	-531(3)	2238(2)	144(9)
C(74)	1838(1)	1626(2)	4164(1)	81(5)
C(75)	2179(1)	1381(2)	4345(1)	86(5)
C(76)	2310(2)	659(3)	4586(1)	98(6)
C(77)	2101(2)	181(3)	4646(2)	102(6)
C(78)	1760(2)	426(3)	4465(2)	102(6)
C(79)	1629(2)	1148(3)	4224(2)	94(6)
C(80)	1690(1)	3149(3)	4349(2)	72(4)
C(81)	1912(2)	2954(3)	4820(2)	90(5)
C(82)	1902(2)	3405(3)	5135(2)	96(6)
C(83)	1671(2)	4052(4)	4980(3)	97(6)
C(84)	1450(2)	4247(3)	4509(3)	96(6)
C(85)	1459(2)	3796(3)	4194(2)	83(5)
C(86)	1995(1)	3062(2)	3889(2)	77(5)
C(87)	2306(1)	3372(2)	4286(2)	87(5)
C(88)	2557(2)	3719(3)	4256(2)	93(6)
C(89)	2498(2)	3755(3)	3830(3)	100(6)
C(90)	2187(2)	3444(3)	3433(2)	96(6)

C(91)	1936(2)	3097(2)	3463(2)	86(5)
Cl(1)	1470(1)	2605(3)	2206(2)	78(1)
Cl(2)	-428(1)	4594(2)	1703(2)	90(2)
Cl(3)	-801(1)	2374(4)	1059(2)	122(2)
Cl(4)	459(2)	400(5)	3418(3)	205(4)
P(1)	1043(1)	5141(2)	2714(2)	67(1)
P(2)	180(1)	3964(2)	992(1)	50(1)
P(3)	250(1)	797(2)	1065(1)	54(1)
P(4)	1291(1)	33(2)	2893(1)	63(1)
P(5)	1679(1)	2589(2)	3916(1)	59(1)

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Table S4. Bond lengths [Å] and angles [deg] for  $[\text{Au}_{13}\text{Ag}_{12}(\text{PPh}_3)_{10}\text{Cl}_8]^+$ .

Ag(1)-Cl(1)	2.326(4)
Ag(1)-Au(6)	2.6738(11)
Ag(1)-Au(2)	2.9216(12)
Ag(1)-Au(4)	2.9291(12)
Ag(1)-Au(3)	2.9371(11)
Ag(1)-Au(1)	2.9405(11)
Ag(1)-Au(5)	2.9920(12)
Ag(2)-Cl(2)	2.412(4)
Ag(2)-Au(6)	2.7629(11)
Ag(2)-Au(1)	2.8010(11)
Ag(2)-Au(2)	2.8171(11)
Ag(2)-Au(7)	2.8280(13)
Ag(2)-Ag(6)#1	2.8703(15)
Ag(2)-Ag(3)	2.9098(14)
Ag(2)-Ag(6)	2.9447(15)
Ag(2)-Ag(2)#1	3.154(2)
Ag(3)-Cl(3)	2.366(5)
Ag(3)-Au(6)	2.7769(10)
Ag(3)-Au(3)	2.7892(11)
Ag(3)-Au(7)	2.8368(10)
Ag(3)-Au(2)	2.8603(11)
Ag(3)-Ag(4)	2.9074(14)
Ag(3)-Ag(5)#1	3.0752(15)
Ag(3)-Ag(6)#1	3.2257(15)
Ag(4)-Cl(4)#1	2.599(7)
Ag(4)-Au(6)	2.8277(11)
Ag(4)-Au(7)	2.8557(14)
Ag(4)-Au(4)	2.8666(12)
Ag(4)-Ag(5)	2.8686(15)

Ag(4)-Au(3)	2.8687(12)
Ag(4)-Ag(4)#1	3.248(2)
Ag(5)-Cl(4)	2.490(6)
Ag(5)-Cl(3)#1	2.802(5)
Ag(5)-Au(7)	2.8049(11)
Ag(5)-Au(5)	2.8285(12)
Ag(5)-Au(6)	2.8454(11)
Ag(5)-Au(4)	2.9010(12)
Ag(5)-Ag(6)	2.9300(16)
Ag(5)-Ag(3)#1	3.0756(15)
Ag(6)-Cl(2)#1	2.504(4)
Ag(6)-Au(5)	2.7805(12)
Ag(6)-Au(7)	2.8400(11)
Ag(6)-Au(6)	2.8531(11)
Ag(6)-Au(1)	2.8652(12)
Ag(6)-Ag(2)#1	2.8705(15)
Ag(6)-Cl(3)#1	2.907(5)
Ag(6)-Ag(3)#1	3.2260(15)
Au(1)-P(1)	2.287(4)
Au(1)-Au(6)	2.6911(7)
Au(1)-Au(5)	2.8910(8)
Au(1)-Au(2)	2.9267(7)
Au(2)-P(2)	2.302(3)
Au(2)-Au(6)	2.7072(7)
Au(2)-Au(3)	2.8955(7)
Au(3)-P(3)	2.282(3)
Au(3)-Au(6)	2.6705(6)
Au(3)-Au(4)	2.8954(7)
Au(4)-P(4)	2.264(4)
Au(4)-Au(6)	2.6830(7)
Au(4)-Au(5)	2.8614(7)
Au(5)-P(5)	2.254(4)
Au(5)-Au(6)	2.6448(7)
Au(6)-Au(7)	2.7082(5)
Au(7)-Au(6)#1	2.7081(5)
Au(7)-Ag(5)#1	2.8048(11)
Au(7)-Ag(2)#1	2.8281(13)
Au(7)-Ag(3)#1	2.8370(10)
Au(7)-Ag(6)#1	2.8400(11)
Au(7)-Ag(4)#1	2.8557(14)
C(1)-C(2)	1.3900
C(1)-C(6)	1.3900
C(1)-P(1)	1.767(8)
C(2)-C(3)	1.3900

C(3)-C(4)	1.3900
C(4)-C(5)	1.3900
C(5)-C(6)	1.3900
C(7)-C(12)	1.3900
C(7)-C(8)	1.3900
C(7)-P(1)	1.769(8)
C(8)-C(9)	1.3900
C(9)-C(10)	1.3900
C(10)-C(11)	1.3900
C(11)-C(12)	1.3900
C(13)-C(14)	1.3899
C(13)-C(18)	1.3902
C(13)-P(1)	1.795(7)
C(14)-C(15)	1.3900
C(15)-C(16)	1.3899
C(16)-C(17)	1.3901
C(17)-C(18)	1.3900
C(19)-C(20)	1.3900
C(19)-C(24)	1.3900
C(19)-P(2)	1.761(8)
C(20)-C(21)	1.3900
C(21)-C(22)	1.3900
C(22)-C(23)	1.3900
C(23)-C(24)	1.3900
C(25)-C(26)	1.3900
C(25)-C(30)	1.3900
C(25)-P(2)	1.757(9)
C(26)-C(27)	1.3900
C(27)-C(28)	1.3900
C(28)-C(29)	1.3900
C(29)-C(30)	1.3900
C(31)-C(32)	1.3900
C(31)-C(36)	1.3900
C(31)-P(2)	1.752(9)
C(32)-C(33)	1.3900
C(33)-C(34)	1.3900
C(34)-C(35)	1.3900
C(35)-C(36)	1.3900
C(37)-C(38)	1.3900
C(37)-C(42)	1.3900
C(37)-P(3)	1.712(9)
C(38)-C(39)	1.3900
C(39)-C(40)	1.3900
C(40)-C(41)	1.3900

C(41)-C(42)	1.3900
C(43)-C(44)	1.3900
C(43)-C(48)	1.3900
C(43)-P(3)	1.789(8)
C(44)-C(45)	1.3900
C(45)-C(46)	1.3900
C(46)-C(47)	1.3900
C(47)-C(48)	1.3900
C(49)-C(50)	1.3900
C(49)-C(54)	1.3901
C(49)-P(3)	1.802(8)
C(50)-C(51)	1.3901
C(51)-C(52)	1.3900
C(52)-C(53)	1.3900
C(53)-C(54)	1.3900
C(55)-C(56)	1.3900
C(55)-C(60)	1.3900
C(55)-P(4)	1.819(12)
C(56)-C(57)	1.3900
C(57)-C(58)	1.3900
C(58)-C(59)	1.3900
C(59)-C(60)	1.3900
C(61)-C(62)	1.3900
C(61)-C(66)	1.3900
C(61)-P(4)	1.772(7)
C(62)-C(63)	1.3900
C(63)-C(64)	1.3900
C(64)-C(65)	1.3900
C(65)-C(66)	1.3900
C(67)-C(68)	1.3899
C(67)-C(72)	1.3901
C(67)-P(4)	1.819(6)
C(68)-C(69)	1.3900
C(69)-C(70)	1.3899
C(70)-C(71)	1.3900
C(71)-C(72)	1.3900
C(74)-C(75)	1.3899
C(74)-C(79)	1.3901
C(74)-P(5)	1.765(6)
C(75)-C(76)	1.3900
C(76)-C(77)	1.3900
C(77)-C(78)	1.3900
C(78)-C(79)	1.3900
C(80)-C(81)	1.3900

C(80)-C(85)	1.3900
C(80)-P(5)	1.793(5)
C(81)-C(82)	1.3900
C(82)-C(83)	1.3900
C(83)-C(84)	1.3900
C(84)-C(85)	1.3900
C(86)-C(87)	1.3900
C(86)-C(91)	1.3901
C(86)-P(5)	1.754(6)
C(87)-C(88)	1.3900
C(88)-C(89)	1.3899
C(89)-C(90)	1.3900
C(90)-C(91)	1.3899
Cl(2)-Ag(6)#1	2.504(4)
Cl(3)-Ag(5)#1	2.802(5)
Cl(3)-Ag(6)#1	2.907(5)
Cl(4)-Ag(4)#1	2.600(7)
Cl(1)-Ag(1)-Au(6)	179.70(12)
Cl(1)-Ag(1)-Au(2)	122.52(12)
Au(6)-Ag(1)-Au(2)	57.67(2)
Cl(1)-Ag(1)-Au(4)	122.97(12)
Au(6)-Ag(1)-Au(4)	57.00(2)
Au(2)-Ag(1)-Au(4)	106.54(3)
Cl(1)-Ag(1)-Au(3)	123.67(11)
Au(6)-Ag(1)-Au(3)	56.61(2)
Au(2)-Ag(1)-Au(3)	59.24(2)
Au(4)-Ag(1)-Au(3)	59.15(2)
Cl(1)-Ag(1)-Au(1)	122.80(11)
Au(6)-Ag(1)-Au(1)	57.04(2)
Au(2)-Ag(1)-Au(1)	59.90(2)
Au(4)-Ag(1)-Au(1)	105.38(4)
Au(3)-Ag(1)-Au(1)	105.85(4)
Cl(1)-Ag(1)-Au(5)	124.40(11)
Au(6)-Ag(1)-Au(5)	55.31(2)
Au(2)-Ag(1)-Au(5)	105.15(3)
Au(4)-Ag(1)-Au(5)	57.78(2)
Au(3)-Ag(1)-Au(5)	103.77(3)
Au(1)-Ag(1)-Au(5)	58.32(2)
Cl(2)-Ag(2)-Au(6)	160.45(13)
Cl(2)-Ag(2)-Au(1)	137.14(10)
Au(6)-Ag(2)-Au(1)	57.85(2)
Cl(2)-Ag(2)-Au(2)	113.39(13)
Au(6)-Ag(2)-Au(2)	58.04(2)

Au(1)-Ag(2)-Au(2)	62.79(3)
Cl(2)-Ag(2)-Au(7)	114.97(10)
Au(6)-Ag(2)-Au(7)	57.93(2)
Au(1)-Ag(2)-Au(7)	106.06(3)
Au(2)-Ag(2)-Au(7)	107.02(3)
Cl(2)-Ag(2)-Ag(6)#1	55.80(10)
Au(6)-Ag(2)-Ag(6)#1	111.77(4)
Au(1)-Ag(2)-Ag(6)#1	165.34(5)
Au(2)-Ag(2)-Ag(6)#1	122.62(4)
Au(7)-Ag(2)-Ag(6)#1	59.78(3)
Cl(2)-Ag(2)-Ag(3)	101.92(12)
Au(6)-Ag(2)-Ag(3)	58.55(3)
Au(1)-Ag(2)-Ag(3)	109.45(4)
Au(2)-Ag(2)-Ag(3)	59.90(3)
Au(7)-Ag(2)-Ag(3)	59.24(3)
Ag(6)#1-Ag(2)-Ag(3)	67.84(4)
Cl(2)-Ag(2)-Ag(6)	135.00(13)
Au(6)-Ag(2)-Ag(6)	59.88(3)
Au(1)-Ag(2)-Ag(6)	59.76(3)
Au(2)-Ag(2)-Ag(6)	110.48(4)
Au(7)-Ag(2)-Ag(6)	58.90(3)
Ag(6)#1-Ag(2)-Ag(6)	106.67(4)
Ag(3)-Ag(2)-Ag(6)	108.22(4)
Cl(2)-Ag(2)-Ag(2)#1	82.85(12)
Au(6)-Ag(2)-Ag(2)#1	103.74(3)
Au(1)-Ag(2)-Ag(2)#1	111.83(5)
Au(2)-Ag(2)-Ag(2)#1	161.54(3)
Au(7)-Ag(2)-Ag(2)#1	56.11(2)
Ag(6)#1-Ag(2)-Ag(2)#1	58.30(4)
Ag(3)-Ag(2)-Ag(2)#1	109.71(3)
Ag(6)-Ag(2)-Ag(2)#1	56.03(4)
Cl(3)-Ag(3)-Au(6)	162.04(14)
Cl(3)-Ag(3)-Au(3)	140.56(14)
Au(6)-Ag(3)-Au(3)	57.34(2)
Cl(3)-Ag(3)-Au(7)	106.79(12)
Au(6)-Ag(3)-Au(7)	57.68(2)
Au(3)-Ag(3)-Au(7)	106.45(3)
Cl(3)-Ag(3)-Au(2)	126.70(14)
Au(6)-Ag(3)-Au(2)	57.38(2)
Au(3)-Ag(3)-Au(2)	61.65(3)
Au(7)-Ag(3)-Au(2)	105.62(3)
Cl(3)-Ag(3)-Ag(4)	122.95(15)
Au(6)-Ag(3)-Ag(4)	59.61(3)
Au(3)-Ag(3)-Ag(4)	60.43(3)

Au(7)-Ag(3)-Ag(4)	59.61(3)
Au(2)-Ag(3)-Ag(4)	109.79(4)
Cl(3)-Ag(3)-Ag(2)	107.36(16)
Au(6)-Ag(3)-Ag(2)	58.08(3)
Au(3)-Ag(3)-Ag(2)	107.67(4)
Au(7)-Ag(3)-Ag(2)	58.94(3)
Au(2)-Ag(3)-Ag(2)	58.44(3)
Ag(4)-Ag(3)-Ag(2)	108.12(4)
Cl(3)-Ag(3)-Ag(5)#1	60.32(12)
Au(6)-Ag(3)-Ag(5)#1	110.09(4)
Au(3)-Ag(3)-Ag(5)#1	126.78(4)
Au(7)-Ag(3)-Ag(5)#1	56.47(3)
Au(2)-Ag(3)-Ag(5)#1	160.68(4)
Ag(4)-Ag(3)-Ag(5)#1	69.17(4)
Ag(2)-Ag(3)-Ag(5)#1	102.90(4)
Cl(3)-Ag(3)-Ag(6)#1	60.35(14)
Au(6)-Ag(3)-Ag(6)#1	101.71(4)
Au(3)-Ag(3)-Ag(6)#1	159.02(4)
Au(7)-Ag(3)-Ag(6)#1	55.42(3)
Au(2)-Ag(3)-Ag(6)#1	109.98(4)
Ag(4)-Ag(3)-Ag(6)#1	109.91(4)
Ag(2)-Ag(3)-Ag(6)#1	55.50(3)
Ag(5)#1-Ag(3)-Ag(6)#1	55.36(3)
Cl(4)#1-Ag(4)-Au(6)	133.0(2)
Cl(4)#1-Ag(4)-Au(7)	98.97(13)
Au(6)-Ag(4)-Au(7)	56.91(2)
Cl(4)#1-Ag(4)-Au(4)	153.08(14)
Au(6)-Ag(4)-Au(4)	56.22(2)
Au(7)-Ag(4)-Au(4)	104.72(3)
Cl(4)#1-Ag(4)-Ag(5)	145.40(17)
Au(6)-Ag(4)-Ag(5)	59.93(3)
Au(7)-Ag(4)-Ag(5)	58.68(3)
Au(4)-Ag(4)-Ag(5)	60.77(3)
Cl(4)#1-Ag(4)-Au(3)	101.5(2)
Au(6)-Ag(4)-Au(3)	55.91(2)
Au(7)-Ag(4)-Au(3)	103.86(4)
Au(4)-Ag(4)-Au(3)	60.64(3)
Ag(5)-Ag(4)-Au(3)	109.09(4)
Cl(4)#1-Ag(4)-Ag(3)	75.1(2)
Au(6)-Ag(4)-Ag(3)	57.90(3)
Au(7)-Ag(4)-Ag(3)	58.97(3)
Au(4)-Ag(4)-Ag(3)	106.47(4)
Ag(5)-Ag(4)-Ag(3)	107.97(4)
Au(3)-Ag(4)-Ag(3)	57.74(3)

Cl(4)#1-Ag(4)-Ag(4)#1	78.40(18)
Au(6)-Ag(4)-Ag(4)#1	108.25(3)
Au(7)-Ag(4)-Ag(4)#1	55.35(2)
Au(4)-Ag(4)-Ag(4)#1	125.95(5)
Ag(5)-Ag(4)-Ag(4)#1	67.19(4)
Au(3)-Ag(4)-Ag(4)#1	158.37(3)
Ag(3)-Ag(4)-Ag(4)#1	102.14(4)
Cl(4)-Ag(5)-Cl(3)#1	86.8(3)
Cl(4)-Ag(5)-Au(7)	103.06(15)
Cl(3)#1-Ag(5)-Au(7)	96.60(10)
Cl(4)-Ag(5)-Au(5)	153.31(16)
Cl(3)#1-Ag(5)-Au(5)	87.51(12)
Au(7)-Ag(5)-Au(5)	103.49(4)
Cl(4)-Ag(5)-Au(6)	146.7(2)
Cl(3)#1-Ag(5)-Au(6)	119.76(13)
Au(7)-Ag(5)-Au(6)	57.27(2)
Au(5)-Ag(5)-Au(6)	55.57(2)
Cl(4)-Ag(5)-Ag(4)	87.9(2)
Cl(3)#1-Ag(5)-Ag(4)	154.45(10)
Au(7)-Ag(5)-Ag(4)	60.43(3)
Au(5)-Ag(5)-Ag(4)	107.66(4)
Au(6)-Ag(5)-Ag(4)	59.32(3)
Cl(4)-Ag(5)-Au(4)	115.0(2)
Cl(3)#1-Ag(5)-Au(4)	143.99(11)
Au(7)-Ag(5)-Au(4)	105.13(3)
Au(5)-Ag(5)-Au(4)	59.91(3)
Au(6)-Ag(5)-Au(4)	55.66(2)
Ag(4)-Ag(5)-Au(4)	59.58(3)
Cl(4)-Ag(5)-Ag(6)	138.0(2)
Cl(3)#1-Ag(5)-Ag(6)	60.91(13)
Au(7)-Ag(5)-Ag(6)	59.32(3)
Au(5)-Ag(5)-Ag(6)	57.71(3)
Au(6)-Ag(5)-Ag(6)	59.19(3)
Ag(4)-Ag(5)-Ag(6)	109.49(4)
Au(4)-Ag(5)-Ag(6)	106.66(4)
Cl(4)-Ag(5)-Ag(3)#1	73.54(19)
Cl(3)#1-Ag(5)-Ag(3)#1	47.20(10)
Au(7)-Ag(5)-Ag(3)#1	57.47(3)
Au(5)-Ag(5)-Ag(3)#1	119.64(4)
Au(6)-Ag(5)-Ag(3)#1	108.51(4)
Ag(4)-Ag(5)-Ag(3)#1	107.43(4)
Au(4)-Ag(5)-Ag(3)#1	162.56(4)
Ag(6)-Ag(5)-Ag(3)#1	64.93(4)
Cl(2)#1-Ag(6)-Au(5)	143.50(10)

Cl(2)#1-Ag(6)-Au(7)	111.59(10)
Au(5)-Ag(6)-Au(7)	103.82(4)
Cl(2)#1-Ag(6)-Au(6)	142.14(13)
Au(5)-Ag(6)-Au(6)	55.98(2)
Au(7)-Ag(6)-Au(6)	56.81(2)
Cl(2)#1-Ag(6)-Au(1)	100.29(12)
Au(5)-Ag(6)-Au(1)	61.58(3)
Au(7)-Ag(6)-Au(1)	104.05(3)
Au(6)-Ag(6)-Au(1)	56.15(2)
Cl(2)#1-Ag(6)-Ag(2)#1	52.79(9)
Au(5)-Ag(6)-Ag(2)#1	163.17(5)
Au(7)-Ag(6)-Ag(2)#1	59.37(3)
Au(6)-Ag(6)-Ag(2)#1	109.03(4)
Au(1)-Ag(6)-Ag(2)#1	118.76(5)
Cl(2)#1-Ag(6)-Cl(3)#1	99.75(17)
Au(5)-Ag(6)-Cl(3)#1	86.38(10)
Au(7)-Ag(6)-Cl(3)#1	93.50(12)
Au(6)-Ag(6)-Cl(3)#1	115.99(12)
Au(1)-Ag(6)-Cl(3)#1	146.14(10)
Ag(2)#1-Ag(6)-Cl(3)#1	95.09(10)
Cl(2)#1-Ag(6)-Ag(5)	151.05(12)
Au(5)-Ag(6)-Ag(5)	59.31(3)
Au(7)-Ag(6)-Ag(5)	58.15(3)
Au(6)-Ag(6)-Ag(5)	58.93(3)
Au(1)-Ag(6)-Ag(5)	108.41(4)
Ag(2)#1-Ag(6)-Ag(5)	107.63(4)
Cl(3)#1-Ag(6)-Ag(5)	57.37(12)
Cl(2)#1-Ag(6)-Ag(2)	85.83(12)
Au(5)-Ag(6)-Ag(2)	105.98(4)
Au(7)-Ag(6)-Ag(2)	58.50(3)
Au(6)-Ag(6)-Ag(2)	56.89(3)
Au(1)-Ag(6)-Ag(2)	57.63(3)
Ag(2)#1-Ag(6)-Ag(2)	65.68(4)
Cl(3)#1-Ag(6)-Ag(2)	151.10(11)
Ag(5)-Ag(6)-Ag(2)	106.19(4)
Cl(2)#1-Ag(6)-Ag(3)#1	91.79(12)
Au(5)-Ag(6)-Ag(3)#1	116.22(4)
Au(7)-Ag(6)-Ag(3)#1	55.33(3)
Au(6)-Ag(6)-Ag(3)#1	104.36(4)
Au(1)-Ag(6)-Ag(3)#1	159.09(4)
Ag(2)#1-Ag(6)-Ag(3)#1	56.66(3)
Cl(3)#1-Ag(6)-Ag(3)#1	45.02(10)
Ag(5)-Ag(6)-Ag(3)#1	59.72(3)
Ag(2)-Ag(6)-Ag(3)#1	106.91(4)

P(1)-Au(1)-Au(6)	177.12(12)
P(1)-Au(1)-Ag(2)	117.89(12)
Au(6)-Au(1)-Ag(2)	60.37(2)
P(1)-Au(1)-Ag(6)	119.98(12)
Au(6)-Au(1)-Ag(6)	61.70(2)
Ag(2)-Au(1)-Ag(6)	62.61(3)
P(1)-Au(1)-Au(5)	126.36(11)
Au(6)-Au(1)-Au(5)	56.426(17)
Ag(2)-Au(1)-Au(5)	106.90(3)
Ag(6)-Au(1)-Au(5)	57.77(3)
P(1)-Au(1)-Au(2)	119.80(11)
Au(6)-Au(1)-Au(2)	57.436(16)
Ag(2)-Au(1)-Au(2)	58.87(3)
Ag(6)-Au(1)-Au(2)	109.64(3)
Au(5)-Au(1)-Au(2)	107.66(2)
P(1)-Au(1)-Ag(1)	123.44(12)
Au(6)-Au(1)-Ag(1)	56.48(2)
Ag(2)-Au(1)-Ag(1)	107.74(3)
Ag(6)-Au(1)-Ag(1)	109.53(3)
Au(5)-Au(1)-Ag(1)	61.73(3)
Au(2)-Au(1)-Ag(1)	59.73(3)
P(2)-Au(2)-Au(6)	179.23(10)
P(2)-Au(2)-Ag(2)	120.78(10)
Au(6)-Au(2)-Ag(2)	59.98(2)
P(2)-Au(2)-Ag(3)	120.61(9)
Au(6)-Au(2)-Ag(3)	59.76(2)
Ag(2)-Au(2)-Ag(3)	61.66(3)
P(2)-Au(2)-Au(3)	122.68(9)
Au(6)-Au(2)-Au(3)	56.813(16)
Ag(2)-Au(2)-Au(3)	107.31(3)
Ag(3)-Au(2)-Au(3)	57.97(2)
P(2)-Au(2)-Ag(1)	122.73(10)
Au(6)-Au(2)-Ag(1)	56.57(2)
Ag(2)-Au(2)-Ag(1)	107.82(3)
Ag(3)-Au(2)-Ag(1)	107.68(3)
Au(3)-Au(2)-Ag(1)	60.65(2)
P(2)-Au(2)-Au(1)	123.21(9)
Au(6)-Au(2)-Au(1)	56.904(17)
Ag(2)-Au(2)-Au(1)	58.33(3)
Ag(3)-Au(2)-Au(1)	107.35(3)
Au(3)-Au(2)-Au(1)	107.30(2)
Ag(1)-Au(2)-Au(1)	60.37(2)
P(3)-Au(3)-Au(6)	176.68(10)
P(3)-Au(3)-Ag(3)	115.79(10)

Au(6)-Au(3)-Ag(3)	61.10(2)
P(3)-Au(3)-Ag(4)	118.82(10)
Au(6)-Au(3)-Ag(4)	61.27(3)
Ag(3)-Au(3)-Ag(4)	61.82(3)
P(3)-Au(3)-Au(4)	125.70(10)
Au(6)-Au(3)-Au(4)	57.467(17)
Ag(3)-Au(3)-Au(4)	108.90(3)
Ag(4)-Au(3)-Au(4)	59.64(3)
P(3)-Au(3)-Au(2)	119.82(10)
Au(6)-Au(3)-Au(2)	58.038(17)
Ag(3)-Au(3)-Au(2)	60.38(2)
Ag(4)-Au(3)-Au(2)	109.89(3)
Au(4)-Au(3)-Au(2)	108.14(2)
P(3)-Au(3)-Ag(1)	125.08(11)
Au(6)-Au(3)-Ag(1)	56.72(2)
Ag(3)-Au(3)-Ag(1)	109.19(3)
Ag(4)-Au(3)-Ag(1)	109.20(3)
Au(4)-Au(3)-Ag(1)	60.28(3)
Au(2)-Au(3)-Ag(1)	60.11(2)
P(4)-Au(4)-Au(6)	174.68(11)
P(4)-Au(4)-Au(5)	119.84(10)
Au(6)-Au(4)-Au(5)	56.872(17)
P(4)-Au(4)-Ag(4)	124.03(11)
Au(6)-Au(4)-Ag(4)	61.16(3)
Au(5)-Au(4)-Ag(4)	106.82(3)
P(4)-Au(4)-Au(3)	123.46(10)
Au(6)-Au(4)-Au(3)	57.051(17)
Au(5)-Au(4)-Au(3)	108.25(2)
Ag(4)-Au(4)-Au(3)	59.71(3)
P(4)-Au(4)-Ag(5)	121.66(11)
Au(6)-Au(4)-Ag(5)	61.12(2)
Au(5)-Au(4)-Ag(5)	58.79(3)
Ag(4)-Au(4)-Ag(5)	59.65(3)
Au(3)-Au(4)-Ag(5)	107.46(3)
P(4)-Au(4)-Ag(1)	118.39(11)
Au(6)-Au(4)-Ag(1)	56.70(2)
Au(5)-Au(4)-Ag(1)	62.21(3)
Ag(4)-Au(4)-Ag(1)	109.49(3)
Au(3)-Au(4)-Ag(1)	60.56(2)
Ag(5)-Au(4)-Ag(1)	109.97(3)
P(5)-Au(5)-Au(6)	177.61(12)
P(5)-Au(5)-Ag(6)	115.13(11)
Au(6)-Au(5)-Ag(6)	63.40(3)
P(5)-Au(5)-Ag(5)	115.20(11)

Au(6)-Au(5)-Ag(5)	62.54(3)
Ag(6)-Au(5)-Ag(5)	62.98(4)
P(5)-Au(5)-Au(4)	121.85(10)
Au(6)-Au(5)-Au(4)	58.163(18)
Ag(6)-Au(5)-Au(4)	111.98(3)
Ag(5)-Au(5)-Au(4)	61.31(3)
P(5)-Au(5)-Au(1)	123.31(10)
Au(6)-Au(5)-Au(1)	57.968(17)
Ag(6)-Au(5)-Au(1)	60.65(3)
Ag(5)-Au(5)-Au(1)	110.54(3)
Au(4)-Au(5)-Au(1)	108.49(2)
P(5)-Au(5)-Ag(1)	126.07(11)
Au(6)-Au(5)-Ag(1)	56.23(2)
Ag(6)-Au(5)-Ag(1)	110.42(3)
Ag(5)-Au(5)-Ag(1)	110.21(3)
Au(4)-Au(5)-Ag(1)	60.00(2)
Au(1)-Au(5)-Ag(1)	59.95(2)
Au(5)-Au(6)-Au(3)	122.72(2)
Au(5)-Au(6)-Ag(1)	68.46(3)
Au(3)-Au(6)-Ag(1)	66.68(3)
Au(5)-Au(6)-Au(4)	64.965(19)
Au(3)-Au(6)-Au(4)	65.483(19)
Ag(1)-Au(6)-Au(4)	66.29(3)
Au(5)-Au(6)-Au(1)	65.606(19)
Au(3)-Au(6)-Au(1)	122.00(2)
Ag(1)-Au(6)-Au(1)	66.47(3)
Au(4)-Au(6)-Au(1)	120.61(2)
Au(5)-Au(6)-Au(2)	122.68(2)
Au(3)-Au(6)-Au(2)	65.149(19)
Ag(1)-Au(6)-Au(2)	65.76(3)
Au(4)-Au(6)-Au(2)	120.90(2)
Au(1)-Au(6)-Au(2)	65.660(19)
Au(5)-Au(6)-Au(7)	111.45(2)
Au(3)-Au(6)-Au(7)	113.83(2)
Ag(1)-Au(6)-Au(7)	179.26(4)
Au(4)-Au(6)-Au(7)	114.38(3)
Au(1)-Au(6)-Au(7)	112.80(3)
Au(2)-Au(6)-Au(7)	113.87(2)
Au(5)-Au(6)-Ag(2)	115.46(3)
Au(3)-Au(6)-Ag(2)	115.74(3)
Ag(1)-Au(6)-Ag(2)	117.09(3)
Au(4)-Au(6)-Ag(2)	176.60(3)
Au(1)-Au(6)-Ag(2)	61.79(3)
Au(2)-Au(6)-Ag(2)	61.99(3)

Au(7)-Au(6)-Ag(2)	62.24(3)
Au(5)-Au(6)-Ag(3)	173.64(3)
Au(3)-Au(6)-Ag(3)	61.56(3)
Ag(1)-Au(6)-Ag(3)	117.82(3)
Au(4)-Au(6)-Ag(3)	115.80(3)
Au(1)-Au(6)-Ag(3)	117.01(3)
Au(2)-Au(6)-Ag(3)	62.86(3)
Au(7)-Au(6)-Ag(3)	62.27(2)
Ag(2)-Au(6)-Ag(3)	63.37(3)
Au(5)-Au(6)-Ag(4)	114.32(3)
Au(3)-Au(6)-Ag(4)	62.82(3)
Ag(1)-Au(6)-Ag(4)	118.67(3)
Au(4)-Au(6)-Ag(4)	62.62(3)
Au(1)-Au(6)-Ag(4)	174.70(3)
Au(2)-Au(6)-Ag(4)	116.96(3)
Au(7)-Au(6)-Ag(4)	62.06(3)
Ag(2)-Au(6)-Ag(4)	114.79(4)
Ag(3)-Au(6)-Ag(4)	62.49(3)
Au(5)-Au(6)-Ag(5)	61.89(3)
Au(3)-Au(6)-Ag(5)	115.79(3)
Ag(1)-Au(6)-Ag(5)	119.76(4)
Au(4)-Au(6)-Ag(5)	63.22(3)
Au(1)-Au(6)-Ag(5)	116.18(3)
Au(2)-Au(6)-Ag(5)	174.46(3)
Au(7)-Au(6)-Ag(5)	60.61(3)
Ag(2)-Au(6)-Ag(5)	113.77(3)
Ag(3)-Au(6)-Ag(5)	112.39(3)
Ag(4)-Au(6)-Ag(5)	60.75(3)
Au(5)-Au(6)-Ag(6)	60.62(3)
Au(3)-Au(6)-Ag(6)	175.14(3)
Ag(1)-Au(6)-Ag(6)	118.15(3)
Au(4)-Au(6)-Ag(6)	115.27(3)
Au(1)-Au(6)-Ag(6)	62.15(3)
Au(2)-Au(6)-Ag(6)	116.71(3)
Au(7)-Au(6)-Ag(6)	61.35(3)
Ag(2)-Au(6)-Ag(6)	63.22(3)
Ag(3)-Au(6)-Ag(6)	114.79(3)
Ag(4)-Au(6)-Ag(6)	112.92(4)
Ag(5)-Au(6)-Ag(6)	61.88(4)
Au(6)#1-Au(7)-Au(6)	174.09(5)
Au(6)#1-Au(7)-Ag(5)#1	62.12(2)
Au(6)-Au(7)-Ag(5)#1	121.04(3)
Au(6)#1-Au(7)-Ag(5)	121.04(3)
Au(6)-Au(7)-Ag(5)	62.12(2)

Ag(5)#1-Au(7)-Ag(5)	124.53(6)
Au(6)#1-Au(7)-Ag(2)	114.65(4)
Au(6)-Au(7)-Ag(2)	59.83(2)
Ag(5)#1-Au(7)-Ag(2)	112.43(3)
Ag(5)-Au(7)-Ag(2)	113.01(3)
Au(6)#1-Au(7)-Ag(2)#1	59.82(2)
Au(6)-Au(7)-Ag(2)#1	114.65(4)
Ag(5)#1-Au(7)-Ag(2)#1	113.01(3)
Ag(5)-Au(7)-Ag(2)#1	112.44(3)
Ag(2)-Au(7)-Ag(2)#1	67.78(5)
Au(6)#1-Au(7)-Ag(3)	120.20(2)
Au(6)-Au(7)-Ag(3)	60.05(2)
Ag(5)#1-Au(7)-Ag(3)	66.06(3)
Ag(5)-Au(7)-Ag(3)	111.81(3)
Ag(2)-Au(7)-Ag(3)	61.82(3)
Ag(2)#1-Au(7)-Ag(3)	122.24(4)
Au(6)#1-Au(7)-Ag(3)#1	60.05(2)
Au(6)-Au(7)-Ag(3)#1	120.20(2)
Ag(5)#1-Au(7)-Ag(3)#1	111.81(3)
Ag(5)-Au(7)-Ag(3)#1	66.06(3)
Ag(2)-Au(7)-Ag(3)#1	122.24(4)
Ag(2)#1-Au(7)-Ag(3)#1	61.81(3)
Ag(3)-Au(7)-Ag(3)#1	175.78(6)
Au(6)#1-Au(7)-Ag(6)#1	61.84(2)
Au(6)-Au(7)-Ag(6)#1	114.40(3)
Ag(5)#1-Au(7)-Ag(6)#1	62.54(3)
Ag(5)-Au(7)-Ag(6)#1	172.87(5)
Ag(2)-Au(7)-Ag(6)#1	60.85(3)
Ag(2)#1-Au(7)-Ag(6)#1	62.60(3)
Ag(3)-Au(7)-Ag(6)#1	69.25(3)
Ag(3)#1-Au(7)-Ag(6)#1	113.34(3)
Au(6)#1-Au(7)-Ag(6)	114.40(3)
Au(6)-Au(7)-Ag(6)	61.84(2)
Ag(5)#1-Au(7)-Ag(6)	172.88(5)
Ag(5)-Au(7)-Ag(6)	62.53(3)
Ag(2)-Au(7)-Ag(6)	62.60(3)
Ag(2)#1-Au(7)-Ag(6)	60.85(3)
Ag(3)-Au(7)-Ag(6)	113.34(3)
Ag(3)#1-Au(7)-Ag(6)	69.26(3)
Ag(6)#1-Au(7)-Ag(6)	110.42(6)
Au(6)#1-Au(7)-Ag(4)	124.70(4)
Au(6)-Au(7)-Ag(4)	61.02(2)
Ag(5)#1-Au(7)-Ag(4)	73.79(4)
Ag(5)-Au(7)-Ag(4)	60.89(3)

Ag(2)-Au(7)-Ag(4)	111.91(3)
Ag(2)#1-Au(7)-Ag(4)	172.97(3)
Ag(3)-Au(7)-Ag(4)	61.43(3)
Ag(3)#1-Au(7)-Ag(4)	114.70(4)
Ag(6)#1-Au(7)-Ag(4)	123.81(3)
Ag(6)-Au(7)-Ag(4)	112.48(3)
Au(6)#1-Au(7)-Ag(4)#1	61.02(2)
Au(6)-Au(7)-Ag(4)#1	124.70(4)
Ag(5)#1-Au(7)-Ag(4)#1	60.89(3)
Ag(5)-Au(7)-Ag(4)#1	73.79(4)
Ag(2)-Au(7)-Ag(4)#1	172.97(3)
Ag(2)#1-Au(7)-Ag(4)#1	111.91(3)
Ag(3)-Au(7)-Ag(4)#1	114.70(4)
Ag(3)#1-Au(7)-Ag(4)#1	61.42(3)
Ag(6)#1-Au(7)-Ag(4)#1	112.48(3)
Ag(6)-Au(7)-Ag(4)#1	123.81(3)
Ag(4)-Au(7)-Ag(4)#1	69.31(5)
C(2)-C(1)-C(6)	120.0
C(2)-C(1)-P(1)	117.0(2)
C(6)-C(1)-P(1)	123.0(2)
C(1)-C(2)-C(3)	120.0
C(2)-C(3)-C(4)	120.0
C(5)-C(4)-C(3)	120.0
C(6)-C(5)-C(4)	120.0
C(5)-C(6)-C(1)	120.0
C(12)-C(7)-C(8)	120.0
C(12)-C(7)-P(1)	118.0(2)
C(8)-C(7)-P(1)	122.0(2)
C(9)-C(8)-C(7)	120.0
C(10)-C(9)-C(8)	120.0
C(9)-C(10)-C(11)	120.0
C(10)-C(11)-C(12)	120.0
C(11)-C(12)-C(7)	120.0
C(14)-C(13)-C(18)	120.0
C(14)-C(13)-P(1)	117.2(3)
C(18)-C(13)-P(1)	122.6(3)
C(13)-C(14)-C(15)	120.0
C(16)-C(15)-C(14)	120.0
C(15)-C(16)-C(17)	120.0
C(18)-C(17)-C(16)	120.0
C(17)-C(18)-C(13)	120.0
C(20)-C(19)-C(24)	120.0
C(20)-C(19)-P(2)	123.0(7)
C(24)-C(19)-P(2)	116.7(7)

C(21)-C(20)-C(19)	120.0
C(20)-C(21)-C(22)	120.0
C(23)-C(22)-C(21)	120.0
C(24)-C(23)-C(22)	120.0
C(23)-C(24)-C(19)	120.0
C(26)-C(25)-C(30)	120.0
C(26)-C(25)-P(2)	120.9(7)
C(30)-C(25)-P(2)	119.1(7)
C(27)-C(26)-C(25)	120.0
C(26)-C(27)-C(28)	120.0
C(29)-C(28)-C(27)	120.0
C(28)-C(29)-C(30)	120.0
C(29)-C(30)-C(25)	120.0
C(32)-C(31)-C(36)	120.0
C(32)-C(31)-P(2)	124.2(8)
C(36)-C(31)-P(2)	115.7(8)
C(31)-C(32)-C(33)	120.0
C(34)-C(33)-C(32)	120.0
C(33)-C(34)-C(35)	120.0
C(36)-C(35)-C(34)	120.0
C(35)-C(36)-C(31)	120.0
C(38)-C(37)-C(42)	120.0
C(38)-C(37)-P(3)	121.9(8)
C(42)-C(37)-P(3)	118.0(8)
C(37)-C(38)-C(39)	120.0
C(38)-C(39)-C(40)	120.0
C(41)-C(40)-C(39)	120.0
C(42)-C(41)-C(40)	120.0
C(41)-C(42)-C(37)	120.0
C(44)-C(43)-C(48)	120.0
C(44)-C(43)-P(3)	126.5(4)
C(48)-C(43)-P(3)	113.5(4)
C(45)-C(44)-C(43)	120.0
C(44)-C(45)-C(46)	120.0
C(47)-C(46)-C(45)	120.0
C(48)-C(47)-C(46)	120.0
C(47)-C(48)-C(43)	120.0
C(50)-C(49)-C(54)	120.0
C(50)-C(49)-P(3)	119.1(3)
C(54)-C(49)-P(3)	120.9(3)
C(49)-C(50)-C(51)	120.0
C(52)-C(51)-C(50)	120.0
C(53)-C(52)-C(51)	120.0
C(54)-C(53)-C(52)	120.0

C(53)-C(54)-C(49)	120.0
C(56)-C(55)-C(60)	120.0
C(56)-C(55)-P(4)	122.0(14)
C(60)-C(55)-P(4)	118.0(14)
C(57)-C(56)-C(55)	120.0
C(56)-C(57)-C(58)	120.0
C(59)-C(58)-C(57)	120.0
C(58)-C(59)-C(60)	120.0
C(59)-C(60)-C(55)	120.0
C(62)-C(61)-C(66)	120.0
C(62)-C(61)-P(4)	124.1(2)
C(66)-C(61)-P(4)	115.2(2)
C(63)-C(62)-C(61)	120.0
C(62)-C(63)-C(64)	120.0
C(63)-C(64)-C(65)	120.0
C(66)-C(65)-C(64)	120.0
C(65)-C(66)-C(61)	120.0
C(68)-C(67)-C(72)	120.0
C(68)-C(67)-P(4)	115.6(2)
C(72)-C(67)-P(4)	124.4(2)
C(67)-C(68)-C(69)	120.0
C(70)-C(69)-C(68)	120.0
C(69)-C(70)-C(71)	120.0
C(70)-C(71)-C(72)	120.0
C(71)-C(72)-C(67)	120.0
C(75)-C(74)-C(79)	120.0
C(75)-C(74)-P(5)	121.54(19)
C(79)-C(74)-P(5)	118.05(19)
C(74)-C(75)-C(76)	120.0
C(75)-C(76)-C(77)	120.0
C(76)-C(77)-C(78)	120.0
C(79)-C(78)-C(77)	120.0
C(78)-C(79)-C(74)	120.0
C(81)-C(80)-C(85)	120.0
C(81)-C(80)-P(5)	122.98(19)
C(85)-C(80)-P(5)	117.01(19)
C(82)-C(81)-C(80)	120.0
C(81)-C(82)-C(83)	120.0
C(82)-C(83)-C(84)	120.0
C(83)-C(84)-C(85)	120.0
C(84)-C(85)-C(80)	120.0
C(87)-C(86)-C(91)	120.0
C(87)-C(86)-P(5)	121.33(19)
C(91)-C(86)-P(5)	118.64(19)

C(86)-C(87)-C(88)	120.0
C(89)-C(88)-C(87)	120.0
C(88)-C(89)-C(90)	120.0
C(91)-C(90)-C(89)	120.0
C(90)-C(91)-C(86)	120.0
Ag(2)-Cl(2)-Ag(6)#1	71.42(11)
Ag(3)-Cl(3)-Ag(5)#1	72.47(13)
Ag(3)-Cl(3)-Ag(6)#1	74.63(13)
Ag(5)#1-Cl(3)-Ag(6)#1	61.72(10)
Ag(5)-Cl(4)-Ag(4)#1	83.76(18)
C(1)-P(1)-C(7)	105.6(4)
C(1)-P(1)-C(13)	103.2(4)
C(7)-P(1)-C(13)	106.1(4)
C(1)-P(1)-Au(1)	116.4(3)
C(7)-P(1)-Au(1)	112.0(3)
C(13)-P(1)-Au(1)	112.5(3)
C(31)-P(2)-C(25)	106.0(6)
C(31)-P(2)-C(19)	104.5(5)
C(25)-P(2)-C(19)	100.6(5)
C(31)-P(2)-Au(2)	111.8(4)
C(25)-P(2)-Au(2)	116.1(4)
C(19)-P(2)-Au(2)	116.4(4)
C(37)-P(3)-C(43)	103.3(5)
C(37)-P(3)-C(49)	108.4(5)
C(43)-P(3)-C(49)	104.4(4)
C(37)-P(3)-Au(3)	114.1(5)
C(43)-P(3)-Au(3)	111.8(3)
C(49)-P(3)-Au(3)	114.0(3)
C(61)-P(4)-C(55)	106.4(5)
C(61)-P(4)-C(67)	106.1(4)
C(55)-P(4)-C(67)	102.7(6)
C(61)-P(4)-Au(4)	111.2(2)
C(55)-P(4)-Au(4)	116.8(7)
C(67)-P(4)-Au(4)	112.8(3)
C(86)-P(5)-C(74)	108.5(3)
C(86)-P(5)-C(80)	104.1(3)
C(74)-P(5)-C(80)	104.7(3)
C(86)-P(5)-Au(5)	111.6(3)
C(74)-P(5)-Au(5)	111.5(2)
C(80)-P(5)-Au(5)	115.9(3)

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Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

**Table S5.** Anisotropic displacement parameters ( $\text{A}^2 \times 10^3$ ) for  $[\text{Au}_{13}\text{Ag}_{12}(\text{PPh}_3)_{10}\text{Cl}_8]^+$ . The anisotropic displacement factor exponent takes the form:  $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	<b>U11</b>	<b>U22</b>	<b>U33</b>	<b>U23</b>	<b>U13</b>	<b>U12</b>
Ag(1)	46(1)	62(1)	50(1)	-6(1)	32(1)	-6(1)
Ag(2)	51(1)	50(1)	54(1)	0(1)	35(1)	1(1)
Ag(3)	42(1)	63(1)	34(1)	-3(1)	21(1)	-5(1)
Ag(4)	56(1)	55(1)	60(1)	1(1)	37(1)	-8(1)
Ag(5)	48(1)	73(1)	44(1)	11(1)	28(1)	6(1)
Ag(6)	49(1)	72(1)	47(1)	-19(1)	30(1)	-5(1)
Au(1)	53(1)	47(1)	52(1)	-12(1)	31(1)	-13(1)
Au(2)	52(1)	47(1)	39(1)	0(1)	30(1)	-5(1)
Au(3)	52(1)	49(1)	36(1)	-9(1)	27(1)	-5(1)
Au(4)	49(1)	52(1)	47(1)	-1(1)	27(1)	2(1)
Au(5)	37(1)	65(1)	35(1)	-7(1)	16(1)	-3(1)
Au(6)	36(1)	43(1)	28(1)	-5(1)	19(1)	-4(1)
Au(7)	63(1)	93(1)	57(1)	0	38(1)	0
C(1)	85(13)	74(11)	83(12)	-5(9)	55(11)	-10(9)
C(2)	85(13)	80(12)	97(14)	-1(10)	51(12)	-4(10)
C(3)	90(14)	79(12)	93(14)	5(10)	55(12)	2(11)
C(4)	93(15)	82(13)	97(14)	-3(11)	56(13)	7(11)
C(5)	95(15)	79(13)	101(15)	-3(10)	56(13)	0(11)
C(6)	90(14)	74(12)	95(14)	-4(10)	52(12)	-7(10)
C(7)	124(19)	123(19)	140(20)	6(17)	87(17)	-12(16)
C(8)	140(20)	130(20)	150(20)	13(17)	90(19)	-9(17)
C(9)	150(20)	140(20)	150(20)	13(18)	100(20)	-12(18)
C(10)	140(20)	150(20)	150(20)	12(19)	96(19)	-14(19)
C(11)	140(20)	140(20)	150(20)	7(18)	95(19)	-7(17)
C(12)	130(20)	130(20)	140(20)	5(16)	90(18)	-9(16)
C(13)	103(17)	90(15)	105(17)	-8(12)	43(14)	-19(13)
C(14)	150(20)	130(20)	120(20)	-3(16)	75(19)	-13(17)
C(15)	150(20)	140(20)	130(20)	-3(18)	70(20)	-10(20)
C(16)	150(20)	140(20)	130(20)	-3(17)	80(20)	-1(19)
C(17)	150(20)	140(20)	140(20)	-9(19)	70(20)	2(18)
C(18)	140(20)	130(20)	140(20)	-12(18)	80(20)	-3(19)
C(19)	82(12)	68(10)	70(11)	2(8)	50(10)	-4(9)
C(20)	86(13)	76(12)	80(12)	2(9)	52(11)	-9(10)
C(21)	97(14)	80(13)	87(13)	7(10)	54(12)	-8(11)
C(22)	102(15)	77(13)	93(14)	5(10)	55(13)	-3(11)
C(23)	101(15)	73(12)	93(14)	2(10)	57(12)	3(10)
C(24)	94(13)	75(12)	86(13)	-1(10)	57(11)	-1(10)

C(25)	74(11)	84(12)	70(11)	2(9)	50(10)	-3(9)
C(26)	82(13)	85(12)	70(11)	11(9)	49(11)	-4(10)
C(27)	87(14)	93(13)	83(13)	9(10)	48(12)	0(11)
C(28)	85(14)	103(15)	90(14)	6(11)	53(12)	-2(11)
C(29)	81(14)	103(14)	92(14)	5(11)	55(12)	-6(11)
C(30)	80(13)	89(12)	76(12)	9(10)	53(11)	-4(10)
C(31)	78(12)	77(11)	70(11)	4(9)	55(10)	-10(9)
C(32)	86(13)	78(11)	70(12)	-3(9)	54(11)	-8(9)
C(33)	95(14)	88(13)	79(13)	-3(10)	59(12)	1(11)
C(34)	98(15)	98(14)	87(14)	-4(11)	62(13)	5(12)
C(35)	92(14)	106(15)	87(15)	5(12)	57(13)	11(12)
C(36)	86(14)	96(13)	83(13)	7(10)	56(12)	4(11)
C(37)	82(13)	93(13)	83(13)	-17(10)	60(11)	2(10)
C(38)	90(14)	102(14)	92(14)	-24(11)	59(12)	0(11)
C(39)	97(15)	111(15)	99(15)	-30(12)	67(13)	9(12)
C(40)	94(15)	114(16)	105(16)	-26(12)	66(13)	4(12)
C(41)	89(14)	109(15)	109(16)	-30(12)	62(13)	-2(12)
C(42)	85(14)	102(14)	99(14)	-28(11)	59(13)	3(11)
C(43)	82(12)	73(11)	67(11)	-14(8)	47(10)	6(9)
C(44)	87(13)	73(11)	74(12)	-1(9)	45(11)	-4(9)
C(45)	97(15)	84(13)	79(13)	6(10)	45(12)	-6(11)
C(46)	99(16)	91(14)	86(14)	-1(11)	46(13)	8(12)
C(47)	93(15)	103(15)	89(15)	3(12)	47(13)	11(12)
C(48)	89(14)	95(13)	79(13)	-4(10)	50(12)	11(11)
C(49)	91(13)	85(12)	92(14)	-13(10)	68(12)	-5(10)
C(50)	104(16)	95(14)	99(15)	-13(12)	62(13)	-8(12)
C(51)	113(17)	93(15)	110(17)	-20(13)	63(15)	-11(13)
C(52)	122(19)	96(16)	116(18)	-5(14)	63(16)	-12(13)
C(53)	130(20)	100(17)	112(18)	10(14)	61(16)	-19(14)
C(54)	118(17)	93(15)	103(16)	4(12)	60(14)	-14(13)
C(55)	115(18)	104(18)	112(18)	4(14)	63(15)	-6(14)
C(56)	120(20)	106(18)	120(19)	8(15)	63(16)	-1(15)
C(57)	130(20)	110(20)	130(20)	11(17)	67(18)	-2(16)
C(58)	140(20)	120(20)	130(20)	17(17)	75(19)	-2(18)
C(59)	140(20)	130(20)	130(20)	19(16)	79(18)	-4(18)
C(60)	130(20)	116(18)	116(19)	13(15)	73(17)	-9(15)
C(61)	89(14)	96(14)	105(15)	-2(12)	59(13)	2(12)
C(62)	96(16)	107(16)	116(17)	1(13)	56(14)	0(13)
C(63)	95(16)	119(18)	118(17)	0(14)	60(15)	1(14)
C(64)	99(16)	116(18)	118(18)	0(14)	61(15)	-2(14)
C(65)	96(16)	114(17)	123(18)	6(14)	64(15)	-4(13)
C(66)	91(15)	106(16)	118(17)	4(13)	60(14)	1(12)
C(67)	140(20)	130(20)	130(20)	-20(16)	86(19)	2(17)
C(68)	150(20)	150(20)	140(20)	-25(18)	90(20)	-6(18)

C(69)	150(20)	150(20)	140(20)	-28(18)	90(20)	-7(19)
C(70)	150(30)	150(20)	140(20)	-23(18)	90(20)	-3(19)
C(71)	150(20)	160(30)	140(20)	-27(18)	90(20)	-1(19)
C(72)	150(20)	150(20)	140(20)	-25(18)	90(20)	0(18)
C(74)	81(13)	86(13)	71(12)	1(9)	44(11)	7(10)
C(75)	85(13)	87(12)	81(13)	-5(10)	48(11)	11(10)
C(76)	98(15)	93(14)	89(14)	1(11)	49(12)	10(12)
C(77)	101(16)	97(15)	95(15)	6(12)	53(13)	13(12)
C(78)	100(15)	96(14)	98(15)	13(12)	54(13)	2(12)
C(79)	89(14)	91(14)	89(14)	13(11)	48(12)	3(11)
C(80)	69(11)	88(12)	70(11)	-7(9)	49(10)	-6(9)
C(81)	85(14)	104(14)	79(13)	-9(11)	48(11)	5(11)
C(82)	96(15)	110(16)	78(13)	-16(11)	50(12)	1(12)
C(83)	100(15)	102(15)	86(14)	-18(11)	55(13)	2(12)
C(84)	97(15)	94(14)	87(14)	-20(11)	51(12)	5(11)
C(85)	83(13)	87(13)	78(12)	-15(10)	47(11)	-1(10)
C(86)	75(12)	85(12)	74(12)	-4(10)	46(10)	-3(10)
C(87)	78(13)	94(13)	82(13)	0(10)	45(11)	-13(10)
C(88)	83(13)	107(15)	90(14)	-2(11)	53(12)	-12(11)
C(89)	89(14)	110(15)	94(15)	1(12)	52(13)	-16(12)
C(90)	89(14)	112(16)	91(14)	-4(12)	56(13)	-13(12)
C(91)	81(13)	100(14)	82(13)	-10(11)	52(11)	-5(10)
Cl(1)	61(3)	109(3)	75(3)	-8(2)	47(2)	-15(2)
Cl(2)	66(3)	69(3)	120(4)	43(3)	50(3)	14(2)
Cl(3)	54(3)	256(7)	47(3)	-4(3)	26(2)	-27(3)
Cl(4)	141(6)	188(7)	330(11)	170(7)	166(7)	71(5)
P(1)	73(3)	50(2)	75(3)	-13(2)	43(3)	-19(2)
P(2)	60(2)	54(2)	39(2)	-2(2)	32(2)	-10(2)
P(3)	67(3)	56(2)	40(2)	-12(2)	32(2)	0(2)
P(4)	54(2)	63(2)	56(2)	-1(2)	26(2)	4(2)
P(5)	38(2)	74(3)	42(2)	-8(2)	13(2)	-5(2)

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