Supporting:

X-Ray Crystal Structure, Optical and Electrochemical Properties of $Au_{15}Ag_3(SC_6H_{11})_{14}$ Nanocluster with Core-Shell Structure

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(1) The X-ray structure of $[Au_{15}Ag_3(SC_6H_{11})_{14}]$

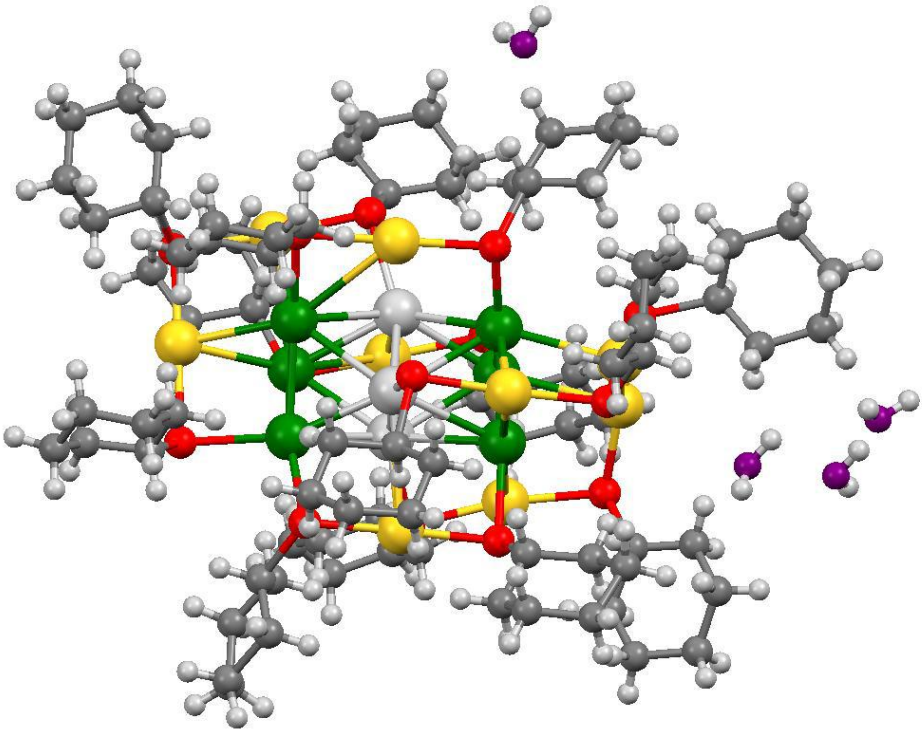

Figure S1. The total number of the $[Au_{15}Ag_3(SC_6H_{11})_{14}]$ (Dark green core Au, dark gray Ag, gold Au in the staple, red S, gray C; white H, pure O)

(2) The purity analysis of the $[Au_{15}Ag_3(SC_6H_{11})_{14}]$ Cluster

The purity analysis was carried out by size exclusion chromatography (SEC) on an Agilent 1200 system using a PL gel column (particle size: 3 μm, pore diameter: 100 Å). A diode array detector (DAD) in situ monitors the optical absorption spectrum (190-950 nm range) of the eluted solution. The purity of the clusters can be verified by comparing the UV-vis spectra at different times of the peak (e.g. peak point, left and right points).

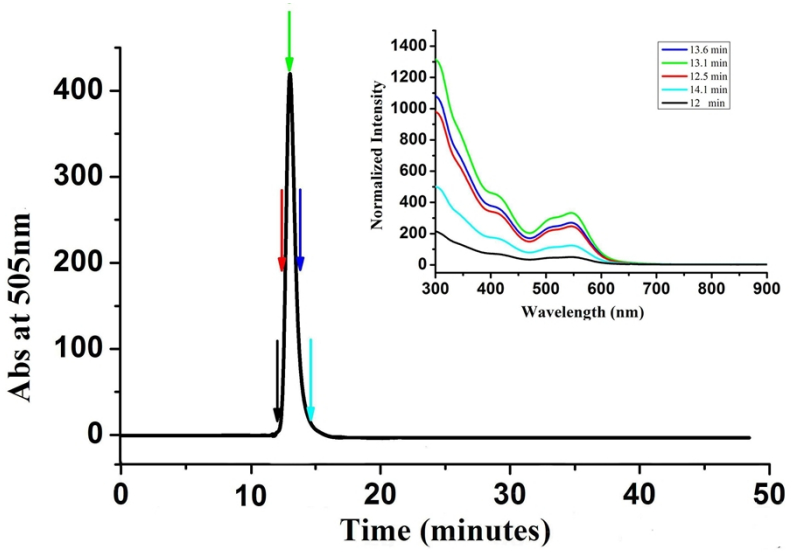

Figure S2. Size exclusion chromatogram of $Au_{15}Ag_3(SC_6H_{11})_{14}$ clusters monitored at 505 nm (eluent, CH_2Cl_2, 0.5 mL/min). (Inset) Online-recorded UV-vis spectra corresponding to the 13.1 min peak and its left/right sides .

(3) The computational details

All the calculations are based on the density functional theory (DFT). First, we optimized the structure of $[Au_{15}Ag_3(SC_6H_{11})_{14}]$（the $-C_6H_{11}$ group in $[Au_{15}Ag_3(SC_6H_{11})_{14}]$ is simplified by methyl ($-CH_3$) group for computing efficiency）using the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional and the double-ζbasis set (DND) with DFT Semi-core Pseudopots (DSPP), as implemented in the $DMol_3$ software package. [An All-Electron Numerical Method for Solving the Local Density Functional for Polyatomic Molecules. J. Chem. Phys. 1990, 92, 508-517. $DMol_3$ is available from Accelrys in version of 6.1.] The we re-optimized the structure of $[Au_{15}Ag_3(SC_6H_{11})_{14}]$ and compute The electronic optical absorption spectra using PBE functional and the triple-ζpolarized TZP basis set with the inclusion of scalar relativity effect via zero-order regular approximation (ZORA) implemented in the ADF package. [ADF 2010.01, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands (http://www.scm.com)].

(4) The stability tests of the $[Au_{15}Ag_3(SC_6H_{11})_{14}]$ Cluster

We We had performed stability tests of $[Au_{15}Ag_3(SC_6H_{11})_{14}]$ in comparison to $Au_{18}(SC_6H_{11})_{14}$ under thermal environments. As shown in the figure S2 below, $Au_{18}(SC_6H_{11})_{14}$ has relative lower stabilities than $Au_{18}(SC_6H_{11})_{14}$. Thermal environment: $Au_{15}Ag_3(SC_6H_{11})_{14}$ (5 mg) and $Au_{18}(SC_6H_{11})_{14}$ (5 mg) was dissolved in toluene at 80 ℃， respectively. In this stability test, the gradual decrease in intensity of the ultraviolet absorption peak of the NC indicates that the NC is gradually destroyed. As shown in the figure S3 below.

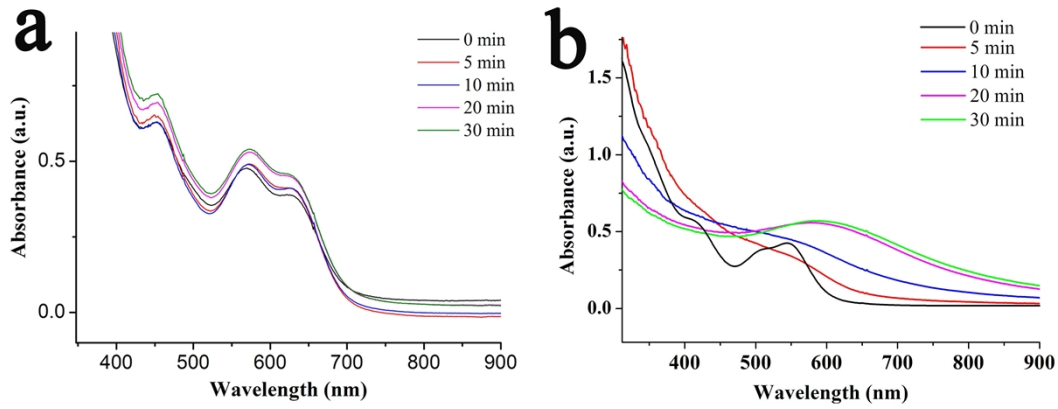

Figure S3: (a) The thermal stability test of the $Au_{15}Ag_3(SC_6H_{11})_{14}$; (b) The thermal stability test of the $Au_{18}(SC_6H_{11})_{14}$.

(5) X-ray Crystallographic Determination

Table S1. Crystal Data and Structure Refinement for the $[Au_{15}Ag_3(SC_6H_{11})_{14}]$ Cluster.

Identification code	$[Au_{15}Ag_3(SC_6H_{11})_{14}]$
Empirical formula	$C_{84}H_{153}Ag_3Au_{15}S_{14}O_2$
Formula weight	4922.00 g/mol
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C 2/c'
Unit cell dimensions	a = 24.9951(16)Å α = 90° b = 18.5586(12) Å β= 90.4780(10)° c = 51.826(5) Å θ= 90°
Volume	24040(3) $Å^3$
Z	8
Calculated density	2.720 mg/m^3
Absorption coefficient	18.980 mm^{-1}
F(000)	17784
Crystal size	0.25x0.23x0.20 mm^3
Theta range for data collection	0.786° to 25.00°
index ranges	−29 ≤ h ≤ 29, −22 ≤ k ≤22, -61≤ l ≤ 61
Reflections collected	168980
Completeness to theta = 25.000	99.8%

Data / parameters / restraints	21138/1057/1281
Goodness-of-fit on F^2	1.071
Final R indices [I>2sigma(I)]	R1 = 0.1342, wR2 = 0.2506
R indices (all data)	R1 = 0.1948, wR2 = 0.2715
Largest diff. peak and hole	7.685 and -5.521e. $Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[Au_{15}Ag_3(SC_6H_{11})_{14}]$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ag(1)	7124(1)	328(2)	8626(1)	27(1)
Ag(2)	7730(1)	1343(2)	8866(1)	26(1)
Ag(3)	6610(1)	1207(2)	9005(1)	41(1)
Au(1)	6398(1)	458(1)	9603(1)	57(1)
Au(2)	7473(1)	-721(1)	9582(1)	66(1)
Au(3)	6881(1)	-275(1)	9112(1)	49(1)
Au(4)	5836(1)	-8(1)	8776(1)	42(1)
Au(5)	7921(1)	-80(1)	8994(1)	50(1)
Au(6)	7441(1)	739(1)	9357(1)	54(1)
Au(7)	7236(1)	2454(1)	9354(1)	44(1)
Au(8)	6954(1)	2445(1)	8720(1)	38(1)
Au(9)	8078(1)	2874(2)	8598(1)	78(1)
Au(10)	6945(1)	3418(1)	8276(1)	61(1)
Au(11)	6186(1)	2315(1)	8017(1)	43(1)
Au(12)	6655(1)	511(1)	8022(1)	36(1)
Au(13)	8309(1)	511(1)	8395(1)	39(1)
Au(14)	6328(1)	1431(1)	8484(1)	35(1)
Au(15)	7333(1)	1660(1)	8333(1)	35(1)
C(1)	5303(8)	1160(30)	9318(9)	92(10)
C(2)	5032(15)	1710(30)	9152(11)	94(10)
C(3)	4444(15)	1570(30)	9119(8)	97(10)
C(4)	4169(12)	1430(30)	9371(9)	101(10)
C(5)	4434(14)	840(30)	9525(9)	97(10)
C(6)	5022(15)	970(30)	9564(8)	94(10)
C(13)	8780(30)	-980(40)	9421(13)	81(9)
C(14)	8900(30)	-250(40)	9509(13)	84(9)
C(15)	9470(30)	-150(40)	9609(13)	86(9)
C(16)	9540(30)	-660(40)	9837(13)	88(9)

C(17)	9400(30)	-1450(40)	9755(13)	87(9)
C(18)	8890(30)	-1510(40)	9635(12)	84(9)
C(19)	5730(20)	-1060(40)	9297(12)	75(8)
C(20)	5180(20)	-1220(30)	9256(12)	74(8)
C(21)	4880(20)	-1260(30)	9497(11)	75(8)
C(22)	5130(20)	-1820(30)	9680(12)	77(9)
C(23)	5730(20)	-1780(40)	9711(12)	77(9)
C(24)	6000(20)	-1670(30)	9462(11)	76(9)
C(25)	5250(20)	490(30)	8235(10)	61(8)
C(26)	4920(20)	1070(30)	8100(10)	64(8)
C(27)	4750(20)	810(30)	7836(11)	67(8)
C(28)	4470(20)	80(30)	7866(11)	67(8)
C(29)	4790(20)	-460(30)	8008(11)	67(8)
C(30)	4960(20)	-180(30)	8269(10)	64(8)
C(31)	6522(10)	-1124(12)	8272(6)	52(7)
C(32)	6241(14)	-1276(15)	8020(6)	56(7)
C(33)	5861(12)	-1901(16)	8039(7)	56(7)
C(34)	6118(15)	-2561(12)	8151(7)	59(7)
C(35)	6409(15)	-2416(14)	8400(6)	57(7)
C(36)	6777(11)	-1781(17)	8387(7)	57(7)
C(37)	6860(20)	1600(30)	7534(9)	51(7)
C(38)	6759(19)	2210(30)	7372(9)	50(7)
C(39)	7240(20)	2400(30)	7196(9)	52(7)
C(40)	7430(20)	1740(30)	7046(9)	53(7)
C(41)	7490(20)	1070(30)	7204(9)	52(7)
C(42)	7040(20)	890(30)	7385(10)	53(7)
C(55)	9045(10)	1940(20)	8811(8)	95(10)
C(56)	9305(16)	1540(30)	9028(8)	94(10)
C(57)	9842(15)	1240(20)	8956(9)	96(10)
C(58)	10204(10)	1790(30)	8841(9)	94(10)
C(59)	9944(13)	2210(30)	8627(8)	96(10)
C(60)	9406(16)	2510(20)	8698(9)	96(10)
C(61)	6430(20)	3770(30)	9124(11)	62(8)
C(62)	6360(20)	4380(30)	8942(11)	62(8)
C(63)	5850(20)	4860(30)	8986(11)	65(8)
C(64)	5380(20)	4300(30)	8978(11)	68(8)
C(65)	5460(20)	3680(30)	9127(11)	67(8)
C(66)	5960(20)	3240(30)	9085(11)	65(8)
C(67)	8172(9)	1800(30)	9761(10)	117(12)
C(68)	8330(17)	2580(20)	9798(11)	118(12)
C(69)	8902(18)	2660(20)	9885(10)	119(13)
C(70)	9033(19)	2200(30)	10115(9)	120(13)
C(71)	8870(19)	1430(20)	10081(10)	120(13)
C(72)	8299(18)	1350(20)	9993(11)	118(12)

C(73)	8774(19)	-1090(30)	8644(9)	46(6)
C(74)	9262(19)	-1120(30)	8482(10)	50(7)
C(75)	9341(19)	-1960(30)	8426(9)	49(7)
C(76)	8862(18)	-2410(30)	8343(9)	48(6)
C(77)	8367(18)	-2180(20)	8505(9)	43(6)
C(78)	8268(18)	-1400(20)	8549(8)	40(6)
C(79)	8520(18)	1820(30)	8001(9)	46(7)
C(80)	9060(18)	1530(30)	7945(10)	50(7)
C(81)	9470(20)	2080(30)	7904(10)	53(7)
C(82)	9320(20)	2590(30)	7681(10)	55(7)
C(83)	8750(20)	2960(30)	7716(10)	56(7)
C(84)	8370(20)	2350(30)	7785(9)	51(7)
S(1)	6012(5)	1392(8)	9378(2)	53(3)
S(2)	6777(7)	-420(10)	9856(3)	79(4)
S(3)	8091(6)	-1161(9)	9283(3)	72(4)
S(4)	6153(5)	-986(7)	8997(2)	47(3)
S(5)	5474(4)	927(6)	8547(2)	38(3)
S(6)	7044(4)	-427(6)	8238(2)	32(2)
S(7)	6300(4)	1361(6)	7746(2)	38(3)
S(8)	6031(7)	3288(8)	8277(3)	65(4)
S(9)	7844(8)	3637(8)	8268(4)	91(6)
S(10)	8415(5)	2283(10)	8951(3)	82(6)
S(11)	7056(5)	3307(6)	9048(2)	46(3)
S(12)	7462(6)	1645(8)	9676(2)	57(4)
S(13)	8707(5)	-93(6)	8729(2)	43(3)
S(14)	7995(4)	1195(6)	8057(2)	37(3)
C(50)	7540(18)	4900(30)	8540(13)	146(16)
C(7)	7067(18)	110(20)	10125(6)	94(7)
C(44)	5690(30)	4680(30)	8265(8)	153(17)
C(49)	7960(30)	4582(14)	8367(11)	147(16)
C(48)	5950(30)	4200(30)	7835(11)	153(17)
C(43)	5720(20)	4030(20)	8094(11)	153(17)
C(45)	5420(30)	5320(30)	8136(11)	153(17)
C(51)	7660(20)	5660(30)	8615(12)	145(16)
C(46)	5660(30)	5480(20)	7877(12)	152(17)
C(52)	8220(30)	5760(30)	8717(10)	147(16)
C(54)	8510(20)	4670(30)	8472(13)	149(16)
C(47)	5680(30)	4830(30)	7705(8)	154(17)
C(53)	8637(18)	5440(30)	8546(13)	149(16)
C(9)	7652(16)	-120(30)	10509(8)	105(9)
C(12)	6650(15)	430(30)	10296(9)	102(8)
C(8)	7419(19)	-420(20)	10264(9)	102(8)
C(11)	6870(20)	720(20)	10545(7)	106(9)
C(10)	7230(20)	190(30)	10682(5)	108(9)

O(4)	7320(20)	4050(30)	7590(9)	112
O(3)	6480(20)	4190(30)	7215(11)	139
O(1)	9640(20)	7930(30)	7701(9)	112
O(2)	2780(20)	1970(30)	9199(9)	112

Table S3. Bond lengths [Å] and angles [deg] for $[Au_{15}Ag_3(SC_6H_{11})_{14}]$.

Ag(1)-S(6)	2.458(11)
Ag(1)-Ag(2)	2.711(4)
Ag(1)-Au(3)	2.826(3)
Ag(1)-Au(5)	2.848(3)
Ag(1)-Ag(3)	2.865(4)
Ag(1)-Au(14)	2.946(3)
Ag(1)-Au(15)	2.951(3)
Ag(1)-Au(13)	3.220(3)
Ag(1)-Au(12)	3.353(3)
Ag(1)-Au(4)	3.376(3)
Ag(2)-S(10)	2.481(14)
Ag(2)-Au(5)	2.764(4)
Ag(2)-Au(6)	2.882(3)
Ag(2)-Ag(3)	2.908(4)
Ag(2)-Au(8)	2.914(3)
Ag(2)-Au(15)	2.982(3)
Ag(2)-Au(13)	3.237(3)
Ag(2)-Au(9)	3.283(4)
Ag(3)-S(1)	2.478(12)
Ag(3)-Au(14)	2.818(4)
Ag(3)-Au(8)	2.868(4)
Ag(3)-Au(3)	2.885(4)
Ag(3)-Au(6)	2.887(4)
Ag(3)-Au(4)	3.195(4)
Ag(3)-Au(7)	3.319(4)
Au(1)-S(1)	2.298(15)
Au(1)-S(2)	2.291(18)
Au(1)-Au(6)	2.959(3)
Au(1)-Au(3)	3.137(3)
Au(2)-S(2)	2.324(18)
Au(2)-S(3)	2.343(17)
Au(2)-Au(6)	2.950(3)
Au(2)-Au(3)	2.957(3)
Au(3)-S(4)	2.321(13)

Au(3)-Au(6)	2.662(3)
Au(3)-Au(5)	2.699(3)
Au(3)-Au(4)	3.169(3)
Au(4)-S(5)	2.284(12)
Au(4)-S(4)	2.287(13)
Au(4)-Au(14)	3.312(3)
Au(5)-S(13)	2.408(12)
Au(5)-S(3)	2.536(15)
Au(5)-Au(6)	2.706(3)
Au(6)-S(12)	2.356(14)
Au(6)-Au(7)	3.224(3)
Au(7)-S(11)	2.283(13)
Au(7)-S(12)	2.311(14)
Au(7)-Au(8)	3.355(2)
Au(8)-S(11)	2.347(12)
Au(8)-Au(15)	2.657(2)
Au(8)-Au(14)	2.729(2)
Au(8)-Au(10)	2.924(3)
Au(8)-Au(9)	2.992(3)
Au(9)-S(10)	2.29(2)
Au(9)-S(9)	2.29(2)
Au(9)-Au(15)	3.221(3)
Au(10)-S(9)	2.28(2)
Au(10)-S(8)	2.297(17)
Au(10)-Au(11)	3.090(3)
Au(11)-S(7)	2.282(12)
Au(11)-S(8)	2.287(14)
Au(11)-Au(14)	2.941(2)
Au(12)-S(6)	2.283(11)
Au(12)-S(7)	2.303(11)
Au(12)-Au(14)	3.058(2)
Au(12)-Au(15)	3.159(2)
Au(13)-S(13)	2.282(12)
Au(13)-S(14)	2.299(12)
Au(13)-Au(15)	3.253(3)
Au(14)-S(5)	2.356(11)
Au(14)-Au(15)	2.671(2)
Au(15)-S(14)	2.361(11)
C(1)-C(6)	1.501(10)
C(1)-C(2)	1.501(10)
C(1)-S(1)	1.849(10)
C(1)-H(1)	0.9800
C(2)-C(3)	1.503(10)
C(2)-H(2A)	0.9700

C(2)-H(2B)	0.9700
C(3)-C(4)	1.501(10)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.501(10)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(6)	1.501(10)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(13)-C(18)	1.51(8)
C(13)-C(14)	1.46(8)
C(13)-S(3)	1.89(7)
C(13)-H(13)	0.9800
C(14)-C(15)	1.52(8)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-C(16)	1.52(8)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-C(17)	1.58(9)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.41(8)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-C(20)	1.41(8)
C(19)-C(24)	1.57(8)
C(19)-S(4)	1.89(6)
C(19)-H(19)	0.9800
C(20)-C(21)	1.47(8)
C(20)-H(20)	0.9300
C(21)-C(22)	1.53(8)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-C(23)	1.50(8)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-C(24)	1.48(8)
C(23)-H(23A)	0.9700

C(23)-H(23B)	0.9700
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(25)-C(30)	1.44(7)
C(25)-C(26)	1.52(7)
C(25)-S(5)	1.90(5)
C(25)-H(25)	0.9800
C(26)-C(27)	1.50(7)
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(27)-C(28)	1.54(7)
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(28)-C(29)	1.48(7)
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(29)-C(30)	1.51(7)
C(29)-H(29A)	0.9700
C(29)-H(29B)	0.9700
C(30)-H(30A)	0.9700
C(30)-H(30B)	0.9700
C(31)-C(36)	1.499(10)
C(31)-C(32)	1.503(10)
C(31)-S(6)	1.847(10)
C(31)-H(31)	0.9800
C(32)-C(33)	1.502(10)
C(32)-H(32A)	0.9700
C(32)-H(32B)	0.9700
C(33)-C(34)	1.499(10)
C(33)-H(33A)	0.9700
C(33)-H(33B)	0.9700
C(34)-C(35)	1.499(10)
C(34)-H(34A)	0.9700
C(34)-H(34B)	0.9700
C(35)-C(36)	1.497(10)
C(35)-H(35A)	0.9700
C(35)-H(35B)	0.9700
C(36)-H(36A)	0.9700
C(36)-H(36B)	0.9700
C(37)-C(38)	1.43(6)
C(37)-C(42)	1.59(7)
C(37)-S(7)	1.85(5)
C(37)-H(37)	0.9800
C(38)-C(39)	1.56(6)

C(38)-H(38A)	0.9700
C(38)-H(38B)	0.9700
C(39)-C(40)	1.51(7)
C(39)-H(39A)	0.9700
C(39)-H(39B)	0.9700
C(40)-C(41)	1.50(7)
C(40)-H(40A)	0.9700
C(40)-H(40B)	0.9700
C(41)-C(42)	1.51(6)
C(41)-H(41A)	0.9700
C(41)-H(41B)	0.9700
C(42)-H(42A)	0.9700
C(42)-H(42B)	0.9700
C(55)-C(60)	1.502(10)
C(55)-C(56)	1.501(10)
C(55)-S(10)	1.850(10)
C(55)-H(55)	0.9800
C(56)-C(57)	1.502(10)
C(56)-H(56A)	0.9700
C(56)-H(56B)	0.9700
C(57)-C(58)	1.499(10)
C(57)-H(57A)	0.9700
C(57)-H(57B)	0.9700
C(58)-C(59)	1.498(10)
C(58)-H(58A)	0.9700
C(58)-H(58B)	0.9700
C(59)-C(60)	1.499(10)
C(59)-H(59A)	0.9700
C(59)-H(59B)	0.9700
C(60)-H(60A)	0.9700
C(60)-H(60B)	0.9700
C(61)-C(62)	1.49(7)
C(61)-C(66)	1.54(7)
C(61)-S(11)	1.83(5)
C(61)-H(61)	0.9800
C(62)-C(63)	1.56(7)
C(62)-H(62A)	0.9700
C(62)-H(62B)	0.9700
C(63)-C(64)	1.57(7)
C(63)-H(63A)	0.9700
C(63)-H(63B)	0.9700
C(64)-C(65)	1.41(7)
C(64)-H(64A)	0.9700
C(64)-H(64B)	0.9700

C(65)-C(66)	1.50(7)
C(65)-H(65A)	0.9700
C(65)-H(65B)	0.9700
C(66)-H(66A)	0.9700
C(66)-H(66B)	0.9700
C(67)-C(68)	1.501(10)
C(67)-C(72)	1.504(10)
C(67)-S(12)	1.848(10)
C(67)-H(67)	0.9800
C(68)-C(69)	1.502(10)
C(68)-H(68A)	0.9700
C(68)-H(68B)	0.9700
C(69)-C(70)	1.501(10)
C(69)-H(69A)	0.9700
C(69)-H(69B)	0.9700
C(70)-C(71)	1.498(10)
C(70)-H(70A)	0.9700
C(70)-H(70B)	0.9700
C(71)-C(72)	1.502(10)
C(71)-H(71A)	0.9700
C(71)-H(71B)	0.9700
C(72)-H(72A)	0.9700
C(72)-H(72B)	0.9700
C(73)-C(78)	1.47(6)
C(73)-C(74)	1.49(6)
C(73)-S(13)	1.90(5)
C(73)-H(73)	0.9800
C(74)-C(75)	1.61(6)
C(74)-H(74A)	0.9700
C(74)-H(74B)	0.9700
C(75)-C(76)	1.51(6)
C(75)-H(75A)	0.9700
C(75)-H(75B)	0.9700
C(76)-C(77)	1.56(6)
C(76)-H(76A)	0.9700
C(76)-H(76B)	0.9700
C(77)-C(78)	1.49(6)
C(77)-H(77A)	0.9700
C(77)-H(77B)	0.9700
C(78)-H(78A)	0.9700
C(78)-H(78B)	0.9700
C(79)-C(80)	1.49(6)
C(79)-C(84)	1.54(6)
C(79)-S(14)	1.77(5)

C(79)-H(79)	0.9800
C(80)-C(81)	1.47(6)
C(80)-H(80A)	0.9700
C(80)-H(80B)	0.9700
C(81)-C(82)	1.55(7)
C(81)-H(81A)	0.9700
C(81)-H(81B)	0.9700
C(82)-C(83)	1.59(7)
C(82)-H(82A)	0.9700
C(82)-H(82B)	0.9700
C(83)-C(84)	1.51(7)
C(83)-H(83A)	0.9700
C(83)-H(83B)	0.9700
C(84)-H(84A)	0.9700
C(84)-H(84B)	0.9700
S(2)-C(7)	1.849(10)
S(8)-C(43)	1.851(10)
S(9)-C(49)	1.849(10)
C(50)-C(49)	1.500(10)
C(50)-C(51)	1.501(10)
C(50)-H(50A)	0.9700
C(50)-H(50B)	0.9700
C(7)-C(12)	1.499(10)
C(7)-C(8)	1.503(10)
C(7)-H(7)	0.9800
C(44)-C(43)	1.499(10)
C(44)-C(45)	1.500(10)
C(44)-H(44A)	0.9700
C(44)-H(44B)	0.9700
C(49)-C(54)	1.501(10)
C(49)-H(49)	0.9800
C(48)-C(43)	1.500(10)
C(48)-C(47)	1.502(10)
C(48)-H(48A)	0.9700
C(48)-H(48B)	0.9700
C(43)-H(43)	0.9800
C(45)-C(46)	1.500(10)
C(45)-H(45A)	0.9700
C(45)-H(45B)	0.9700
C(51)-C(52)	1.498(10)
C(51)-H(51A)	0.9700
C(51)-H(51B)	0.9700
C(46)-C(47)	1.502(10)
C(46)-H(46A)	0.9700

C(46)-H(46B)	0.9700
C(52)-C(53)	1.498(10)
C(52)-H(52A)	0.9700
C(52)-H(52B)	0.9700
C(54)-C(53)	1.502(10)
C(54)-H(54A)	0.9700
C(54)-H(54B)	0.9700
C(47)-H(47A)	0.9700
C(47)-H(47B)	0.9700
C(53)-H(53A)	0.9700
C(53)-H(53B)	0.9700
C(9)-C(10)	1.500(10)
C(9)-C(8)	1.503(10)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(12)-C(11)	1.499(10)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(11)-C(10)	1.499(10)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
O(4)-H(4D)	0.8500
O(4)-H(4E)	0.8499
O(3)-H(3C)	0.8498
O(3)-H(3D)	0.8501
O(1)-H(1A)	0.8497
O(1)-H(1C)	0.8499
O(2)-H(2C)	0.8499
O(2)-H(2D)	0.8500

S(6)-Ag(1)-Ag(2)	144.3(3)
S(6)-Ag(1)-Au(3)	119.1(3)
Ag(2)-Ag(1)-Au(3)	89.48(11)
S(6)-Ag(1)-Au(5)	116.7(3)
Ag(2)-Ag(1)-Au(5)	59.57(10)
Au(3)-Ag(1)-Au(5)	56.80(8)
S(6)-Ag(1)-Ag(3)	148.3(3)
Ag(2)-Ag(1)-Ag(3)	62.80(11)
Au(3)-Ag(1)-Ag(3)	60.91(10)
Au(5)-Ag(1)-Ag(3)	90.42(11)

S(6)-Ag(1)-Au(14)	98.1(3)
Ag(2)-Ag(1)-Au(14)	90.29(11)
Au(3)-Ag(1)-Au(14)	110.41(11)
Au(5)-Ag(1)-Au(14)	145.05(12)
Ag(3)-Ag(1)-Au(14)	57.99(9)
S(6)-Ag(1)-Au(15)	94.0(3)
Ag(2)-Ag(1)-Au(15)	63.41(9)
Au(3)-Ag(1)-Au(15)	146.15(12)
Au(5)-Ag(1)-Au(15)	116.20(11)
Ag(3)-Ag(1)-Au(15)	87.58(11)
Au(14)-Ag(1)-Au(15)	53.86(7)
S(6)-Ag(1)-Au(13)	79.9(2)
Ag(2)-Ag(1)-Au(13)	65.50(9)
Au(3)-Ag(1)-Au(13)	125.33(11)
Au(5)-Ag(1)-Au(13)	68.74(8)
Ag(3)-Ag(1)-Au(13)	127.86(12)
Au(14)-Ag(1)-Au(13)	117.04(10)
Au(15)-Ag(1)-Au(13)	63.46(7)
S(6)-Ag(1)-Au(12)	42.9(3)
Ag(2)-Ag(1)-Au(12)	123.12(12)
Au(3)-Ag(1)-Au(12)	142.80(11)
Au(5)-Ag(1)-Au(12)	152.85(11)
Ag(3)-Ag(1)-Au(12)	115.27(12)
Au(14)-Ag(1)-Au(12)	57.64(7)
Au(15)-Ag(1)-Au(12)	59.74(7)
Au(13)-Ag(1)-Au(12)	87.54(8)
S(6)-Ag(1)-Au(4)	90.6(2)
Ag(2)-Ag(1)-Au(4)	123.62(12)
Au(3)-Ag(1)-Au(4)	60.67(7)
Au(5)-Ag(1)-Au(4)	117.41(10)
Ag(3)-Ag(1)-Au(4)	60.92(9)
Au(14)-Ag(1)-Au(4)	62.74(7)
Au(15)-Ag(1)-Au(4)	116.47(10)
Au(13)-Ag(1)-Au(4)	170.44(11)
Au(12)-Ag(1)-Au(4)	84.61(8)
S(10)-Ag(2)-Ag(1)	162.2(4)
S(10)-Ag(2)-Au(5)	120.7(5)
Ag(1)-Ag(2)-Au(5)	62.69(10)
S(10)-Ag(2)-Au(6)	107.1(5)
Ag(1)-Ag(2)-Au(6)	89.48(11)
Au(5)-Ag(2)-Au(6)	57.23(8)
S(10)-Ag(2)-Ag(3)	132.9(3)
Ag(1)-Ag(2)-Ag(3)	61.20(11)
Au(5)-Ag(2)-Ag(3)	91.23(12)

Au(6)-Ag(2)-Ag(3)	59.83(9)
S(10)-Ag(2)-Au(8)	90.6(4)
Ag(1)-Ag(2)-Au(8)	90.04(11)
Au(5)-Ag(2)-Au(8)	147.79(12)
Au(6)-Ag(2)-Au(8)	109.34(11)
Ag(3)-Ag(2)-Au(8)	59.02(10)
S(10)-Ag(2)-Au(15)	104.5(5)
Ag(1)-Ag(2)-Au(15)	62.21(9)
Au(5)-Ag(2)-Au(15)	117.87(11)
Au(6)-Ag(2)-Au(15)	144.18(11)
Ag(3)-Ag(2)-Au(15)	86.20(10)
Au(8)-Ag(2)-Au(15)	53.55(7)
S(10)-Ag(2)-Au(13)	99.1(3)
Ag(1)-Ag(2)-Au(13)	64.85(9)
Au(5)-Ag(2)-Au(13)	69.44(8)
Au(6)-Ag(2)-Au(13)	126.66(12)
Ag(3)-Ag(2)-Au(13)	125.64(12)
Au(8)-Ag(2)-Au(13)	116.10(10)
Au(15)-Ag(2)-Au(13)	62.92(7)
S(10)-Ag(2)-Au(9)	44.1(5)
Ag(1)-Ag(2)-Au(9)	123.83(12)
Au(5)-Ag(2)-Au(9)	152.05(12)
Au(6)-Ag(2)-Au(9)	141.26(12)
Ag(3)-Ag(2)-Au(9)	116.04(13)
Au(8)-Ag(2)-Au(9)	57.37(8)
Au(15)-Ag(2)-Au(9)	61.64(8)
Au(13)-Ag(2)-Au(9)	88.47(8)
S(1)-Ag(3)-Au(14)	125.4(3)
S(1)-Ag(3)-Ag(1)	153.0(4)
Au(14)-Ag(3)-Ag(1)	62.44(9)
S(1)-Ag(3)-Au(8)	118.4(4)
Au(14)-Ag(3)-Au(8)	57.35(8)
Ag(1)-Ag(3)-Au(8)	87.97(11)
S(1)-Ag(3)-Au(3)	97.2(4)
Au(14)-Ag(3)-Au(3)	112.45(13)
Ag(1)-Ag(3)-Au(3)	58.87(10)
Au(8)-Ag(3)-Au(3)	142.36(13)
S(1)-Ag(3)-Au(6)	89.1(3)
Au(14)-Ag(3)-Au(6)	145.44(14)
Ag(1)-Ag(3)-Au(6)	86.41(12)
Au(8)-Ag(3)-Au(6)	110.48(12)
Au(3)-Ag(3)-Au(6)	54.92(9)
S(1)-Ag(3)-Ag(2)	140.4(3)
Au(14)-Ag(3)-Ag(2)	88.99(11)

Ag(1)-Ag(3)-Ag(2)	56.01(10)
Au(8)-Ag(3)-Ag(2)	60.59(10)
Au(3)-Ag(3)-Ag(2)	84.59(12)
Au(6)-Ag(3)-Ag(2)	59.63(10)
S(1)-Ag(3)-Au(4)	91.2(3)
Au(14)-Ag(3)-Au(4)	66.51(9)
Ag(1)-Ag(3)-Au(4)	67.47(10)
Au(8)-Ag(3)-Au(4)	123.80(12)
Au(3)-Ag(3)-Au(4)	62.58(9)
Au(6)-Ag(3)-Au(4)	116.97(13)
Ag(2)-Ag(3)-Au(4)	123.38(13)
S(1)-Ag(3)-Au(7)	76.3(3)
Au(14)-Ag(3)-Au(7)	122.12(13)
Ag(1)-Ag(3)-Au(7)	123.93(13)
Au(8)-Ag(3)-Au(7)	65.20(9)
Au(3)-Ag(3)-Au(7)	116.82(12)
Au(6)-Ag(3)-Au(7)	62.13(9)
Ag(2)-Ag(3)-Au(7)	67.97(10)
Au(4)-Ag(3)-Au(7)	167.39(12)
S(1)-Au(1)-S(2)	175.5(5)
S(1)-Au(1)-Au(6)	90.9(3)
S(2)-Au(1)-Au(6)	90.6(4)
S(1)-Au(1)-Au(3)	94.5(3)
S(2)-Au(1)-Au(3)	89.7(4)
Au(6)-Au(1)-Au(3)	51.68(6)
S(2)-Au(2)-S(3)	171.5(6)
S(2)-Au(2)-Au(6)	90.2(4)
S(3)-Au(2)-Au(6)	94.3(4)
S(2)-Au(2)-Au(3)	93.7(4)
S(3)-Au(2)-Au(3)	83.2(4)
Au(6)-Au(2)-Au(3)	53.57(7)
S(4)-Au(3)-Au(6)	158.8(3)
S(4)-Au(3)-Au(5)	140.6(3)
Au(6)-Au(3)-Au(5)	60.62(8)
S(4)-Au(3)-Ag(1)	99.8(3)
Au(6)-Au(3)-Ag(1)	91.68(9)
Au(5)-Au(3)-Ag(1)	62.02(8)
S(4)-Au(3)-Ag(3)	108.1(3)
Au(6)-Au(3)-Ag(3)	62.59(9)
Au(5)-Au(3)-Ag(3)	93.07(10)
Ag(1)-Au(3)-Ag(3)	60.22(10)
S(4)-Au(3)-Au(2)	116.0(3)
Au(6)-Au(3)-Au(2)	63.08(8)
Au(5)-Au(3)-Au(2)	75.38(8)

Ag(1)-Au(3)-Au(2)	137.28(10)
Ag(3)-Au(3)-Au(2)	122.69(11)
S(4)-Au(3)-Au(1)	98.5(3)
Au(6)-Au(3)-Au(1)	60.71(7)
Au(5)-Au(3)-Au(1)	120.22(9)
Ag(1)-Au(3)-Au(1)	129.67(11)
Ag(3)-Au(3)-Au(1)	69.58(9)
Au(2)-Au(3)-Au(1)	69.31(8)
S(4)-Au(3)-Au(4)	46.1(3)
Au(6)-Au(3)-Au(4)	125.46(10)
Au(5)-Au(3)-Au(4)	130.22(8)
Ag(1)-Au(3)-Au(4)	68.29(8)
Ag(3)-Au(3)-Au(4)	63.50(9)
Au(2)-Au(3)-Au(4)	154.40(9)
Au(1)-Au(3)-Au(4)	93.29(8)
S(5)-Au(4)-S(4)	176.5(4)
S(5)-Au(4)-Au(3)	136.5(3)
S(4)-Au(4)-Au(3)	47.0(3)
S(5)-Au(4)-Ag(3)	83.9(3)
S(4)-Au(4)-Ag(3)	99.6(3)
Au(3)-Au(4)-Ag(3)	53.92(8)
S(5)-Au(4)-Au(14)	45.3(3)
S(4)-Au(4)-Au(14)	137.8(3)
Au(3)-Au(4)-Au(14)	94.00(6)
Ag(3)-Au(4)-Au(14)	51.29(7)
S(5)-Au(4)-Ag(1)	96.6(3)
S(4)-Au(4)-Ag(1)	86.2(3)
Au(3)-Au(4)-Ag(1)	51.04(6)
Ag(3)-Au(4)-Ag(1)	51.61(8)
Au(14)-Au(4)-Ag(1)	52.25(6)
S(13)-Au(5)-S(3)	101.3(5)
S(13)-Au(5)-Au(3)	156.9(3)
S(3)-Au(5)-Au(3)	85.3(3)
S(13)-Au(5)-Au(6)	140.5(3)
S(3)-Au(5)-Au(6)	96.2(4)
Au(3)-Au(5)-Au(6)	59.01(8)
S(13)-Au(5)-Ag(2)	90.7(3)
S(3)-Au(5)-Ag(2)	157.8(4)
Au(3)-Au(5)-Ag(2)	91.05(9)
Au(6)-Au(5)-Ag(2)	63.57(9)
S(13)-Au(5)-Ag(1)	100.9(3)
S(3)-Au(5)-Ag(1)	135.9(4)
Au(3)-Au(5)-Ag(1)	61.18(8)
Au(6)-Au(5)-Ag(1)	90.29(9)

Ag(2)-Au(5)-Ag(1)	57.74(9)
S(12)-Au(6)-Au(3)	147.9(3)
S(12)-Au(6)-Au(5)	151.7(3)
Au(3)-Au(6)-Au(5)	60.38(8)
S(12)-Au(6)-Ag(2)	109.7(3)
Au(3)-Au(6)-Ag(2)	89.29(9)
Au(5)-Au(6)-Ag(2)	59.20(8)
S(12)-Au(6)-Ag(3)	103.8(4)
Au(3)-Au(6)-Ag(3)	62.50(10)
Au(5)-Au(6)-Ag(3)	92.88(10)
Ag(2)-Au(6)-Ag(3)	60.55(9)
S(12)-Au(6)-Au(2)	112.2(3)
Au(3)-Au(6)-Au(2)	63.35(8)
Au(5)-Au(6)-Au(2)	75.41(9)
Ag(2)-Au(6)-Au(2)	134.46(11)
Ag(3)-Au(6)-Au(2)	122.87(11)
S(12)-Au(6)-Au(1)	80.7(3)
Au(3)-Au(6)-Au(1)	67.61(8)
Au(5)-Au(6)-Au(1)	126.72(10)
Ag(2)-Au(6)-Au(1)	132.68(10)
Ag(3)-Au(6)-Au(1)	72.13(9)
Au(2)-Au(6)-Au(1)	71.89(8)
S(12)-Au(6)-Au(7)	45.7(3)
Au(3)-Au(6)-Au(7)	127.73(9)
Au(5)-Au(6)-Au(7)	128.46(9)
Ag(2)-Au(6)-Au(7)	69.64(8)
Ag(3)-Au(6)-Au(7)	65.52(9)
Au(2)-Au(6)-Au(7)	155.88(9)
Au(1)-Au(6)-Au(7)	92.02(8)
S(11)-Au(7)-S(12)	176.0(5)
S(11)-Au(7)-Au(6)	136.0(3)
S(12)-Au(7)-Au(6)	46.9(3)
S(11)-Au(7)-Ag(3)	90.9(3)
S(12)-Au(7)-Ag(3)	92.9(3)
Au(6)-Au(7)-Ag(3)	52.35(8)
S(11)-Au(7)-Au(8)	44.3(3)
S(12)-Au(7)-Au(8)	138.8(3)
Au(6)-Au(7)-Au(8)	91.87(7)
Ag(3)-Au(7)-Au(8)	50.90(7)
S(11)-Au(8)-Au(15)	151.9(3)
S(11)-Au(8)-Au(14)	148.5(3)
Au(15)-Au(8)-Au(14)	59.44(6)
S(11)-Au(8)-Ag(3)	101.8(3)
Au(15)-Au(8)-Ag(3)	93.44(10)

Au(14)-Au(8)-Ag(3)	60.40(8)
S(11)-Au(8)-Ag(2)	102.9(3)
Au(15)-Au(8)-Ag(2)	64.53(8)
Au(14)-Au(8)-Ag(2)	90.61(8)
Ag(3)-Au(8)-Ag(2)	60.39(9)
S(11)-Au(8)-Au(10)	98.5(3)
Au(15)-Au(8)-Au(10)	75.31(7)
Au(14)-Au(8)-Au(10)	94.18(8)
Ag(3)-Au(8)-Au(10)	154.18(10)
Ag(2)-Au(8)-Au(10)	129.66(9)
S(11)-Au(8)-Au(9)	82.8(3)
Au(15)-Au(8)-Au(9)	69.22(7)
Au(14)-Au(8)-Au(9)	128.64(8)
Ag(3)-Au(8)-Au(9)	127.46(11)
Ag(2)-Au(8)-Au(9)	67.52(9)
Au(10)-Au(8)-Au(9)	70.74(9)
S(11)-Au(8)-Au(7)	42.8(3)
Au(15)-Au(8)-Au(7)	131.88(8)
Au(14)-Au(8)-Au(7)	123.86(8)
Ag(3)-Au(8)-Au(7)	63.91(8)
Ag(2)-Au(8)-Au(7)	67.40(7)
Au(10)-Au(8)-Au(7)	140.10(8)
Au(9)-Au(8)-Au(7)	90.92(8)
S(10)-Au(9)-S(9)	169.3(6)
S(10)-Au(9)-Au(8)	92.5(3)
S(9)-Au(9)-Au(8)	95.1(5)
S(10)-Au(9)-Au(15)	102.3(4)
S(9)-Au(9)-Au(15)	88.4(4)
Au(8)-Au(9)-Au(15)	50.48(5)
S(10)-Au(9)-Ag(2)	49.0(3)
S(9)-Au(9)-Ag(2)	141.6(5)
Au(8)-Au(9)-Ag(2)	55.10(7)
Au(15)-Au(9)-Ag(2)	54.58(7)
S(9)-Au(10)-S(8)	175.7(6)
S(9)-Au(10)-Au(8)	97.1(5)
S(8)-Au(10)-Au(8)	86.2(3)
S(9)-Au(10)-Au(11)	135.3(4)
S(8)-Au(10)-Au(11)	47.5(4)
Au(8)-Au(10)-Au(11)	86.14(7)
S(7)-Au(11)-S(8)	177.0(5)
S(7)-Au(11)-Au(14)	93.4(3)
S(8)-Au(11)-Au(14)	88.6(3)
S(7)-Au(11)-Au(10)	134.6(3)
S(8)-Au(11)-Au(10)	47.7(4)

Au(14)-Au(11)-Au(10)	86.71(7)
S(6)-Au(12)-S(7)	171.0(4)
S(6)-Au(12)-Au(14)	99.0(3)
S(7)-Au(12)-Au(14)	90.0(3)
S(6)-Au(12)-Au(15)	92.3(3)
S(7)-Au(12)-Au(15)	93.3(3)
Au(14)-Au(12)-Au(15)	50.86(5)
S(6)-Au(12)-Ag(1)	47.2(3)
S(7)-Au(12)-Ag(1)	141.3(3)
Au(14)-Au(12)-Ag(1)	54.47(7)
Au(15)-Au(12)-Ag(1)	53.78(6)
S(13)-Au(13)-S(14)	173.4(4)
S(13)-Au(13)-Ag(1)	93.6(3)
S(14)-Au(13)-Ag(1)	91.9(3)
S(13)-Au(13)-Ag(2)	81.9(3)
S(14)-Au(13)-Ag(2)	99.2(3)
Ag(1)-Au(13)-Ag(2)	49.65(7)
S(13)-Au(13)-Au(15)	135.9(3)
S(14)-Au(13)-Au(15)	46.5(3)
Ag(1)-Au(13)-Au(15)	54.23(7)
Ag(2)-Au(13)-Au(15)	54.71(6)
S(5)-Au(14)-Au(15)	163.6(3)
S(5)-Au(14)-Au(8)	136.7(3)
Au(15)-Au(14)-Au(8)	58.95(6)
S(5)-Au(14)-Ag(3)	91.6(3)
Au(15)-Au(14)-Ag(3)	94.31(9)
Au(8)-Au(14)-Ag(3)	62.25(9)
S(5)-Au(14)-Au(11)	103.4(3)
Au(15)-Au(14)-Au(11)	77.25(7)
Au(8)-Au(14)-Au(11)	92.82(7)
Ag(3)-Au(14)-Au(11)	153.97(11)
S(5)-Au(14)-Ag(1)	107.4(3)
Au(15)-Au(14)-Ag(1)	63.16(8)
Au(8)-Au(14)-Ag(1)	89.05(8)
Ag(3)-Au(14)-Ag(1)	59.57(10)
Au(11)-Au(14)-Ag(1)	132.15(9)
S(5)-Au(14)-Au(12)	97.8(3)
Au(15)-Au(14)-Au(12)	66.53(6)
Au(8)-Au(14)-Au(12)	125.43(7)
Ag(3)-Au(14)-Au(12)	127.00(10)
Au(11)-Au(14)-Au(12)	72.49(6)
Ag(1)-Au(14)-Au(12)	67.88(7)
S(5)-Au(14)-Au(4)	43.6(3)
Au(15)-Au(14)-Au(4)	127.99(8)

Au(8)-Au(14)-Au(4)	124.41(7)
Ag(3)-Au(14)-Au(4)	62.21(9)
Au(11)-Au(14)-Au(4)	141.47(8)
Ag(1)-Au(14)-Au(4)	65.00(7)
Au(12)-Au(14)-Au(4)	90.57(6)
S(14)-Au(15)-Au(8)	156.0(3)
S(14)-Au(15)-Au(14)	141.7(3)
Au(8)-Au(15)-Au(14)	61.61(6)
S(14)-Au(15)-Ag(1)	97.7(3)
Au(8)-Au(15)-Ag(1)	90.32(8)
Au(14)-Au(15)-Ag(1)	62.98(8)
S(14)-Au(15)-Ag(2)	105.1(3)
Au(8)-Au(15)-Ag(2)	61.91(8)
Au(14)-Au(15)-Ag(2)	90.29(8)
Ag(1)-Au(15)-Ag(2)	54.38(8)
S(14)-Au(15)-Au(12)	79.6(3)
Au(8)-Au(15)-Au(12)	124.17(7)
Au(14)-Au(15)-Au(12)	62.61(6)
Ag(1)-Au(15)-Au(12)	66.48(7)
Ag(2)-Au(15)-Au(12)	120.83(9)
S(14)-Au(15)-Au(9)	96.2(3)
Au(8)-Au(15)-Au(9)	60.31(6)
Au(14)-Au(15)-Au(9)	121.90(8)
Ag(1)-Au(15)-Au(9)	118.14(10)
Ag(2)-Au(15)-Au(9)	63.78(9)
Au(12)-Au(15)-Au(9)	174.35(8)
S(14)-Au(15)-Au(13)	44.9(3)
Au(8)-Au(15)-Au(13)	123.84(8)
Au(14)-Au(15)-Au(13)	124.95(8)
Ag(1)-Au(15)-Au(13)	62.31(7)
Ag(2)-Au(15)-Au(13)	62.36(7)
Au(12)-Au(15)-Au(13)	90.35(6)
Au(9)-Au(15)-Au(13)	89.27(7)
C(6)-C(1)-C(2)	116(3)
C(6)-C(1)-S(1)	112(3)
C(2)-C(1)-S(1)	111(3)
C(6)-C(1)-H(1)	105.9
C(2)-C(1)-H(1)	105.9
S(1)-C(1)-H(1)	105.9
C(1)-C(2)-C(3)	112.5(11)
C(1)-C(2)-H(2A)	109.1
C(3)-C(2)-H(2A)	109.1
C(1)-C(2)-H(2B)	109.1
C(3)-C(2)-H(2B)	109.1

H(2A)-C(2)-H(2B)	107.8
C(4)-C(3)-C(2)	112.6(11)
C(4)-C(3)-H(3A)	109.1
C(2)-C(3)-H(3A)	109.1
C(4)-C(3)-H(3B)	109.1
C(2)-C(3)-H(3B)	109.1
H(3A)-C(3)-H(3B)	107.8
C(5)-C(4)-C(3)	112.7(11)
C(5)-C(4)-H(4A)	109.1
C(3)-C(4)-H(4A)	109.1
C(5)-C(4)-H(4B)	109.1
C(3)-C(4)-H(4B)	109.1
H(4A)-C(4)-H(4B)	107.8
C(4)-C(5)-C(6)	112.6(11)
C(4)-C(5)-H(5A)	109.1
C(6)-C(5)-H(5A)	109.1
C(4)-C(5)-H(5B)	109.1
C(6)-C(5)-H(5B)	109.1
H(5A)-C(5)-H(5B)	107.8
C(1)-C(6)-C(5)	112.8(10)
C(1)-C(6)-H(6A)	109.0
C(5)-C(6)-H(6A)	109.0
C(1)-C(6)-H(6B)	109.0
C(5)-C(6)-H(6B)	109.0
H(6A)-C(6)-H(6B)	107.8
C(18)-C(13)-C(14)	110(6)
C(18)-C(13)-S(3)	108(5)
C(14)-C(13)-S(3)	118(5)
C(18)-C(13)-H(13)	106.6
C(14)-C(13)-H(13)	106.6
S(3)-C(13)-H(13)	106.6
C(13)-C(14)-C(15)	114(6)
C(13)-C(14)-H(14A)	108.8
C(15)-C(14)-H(14A)	108.8
C(13)-C(14)-H(14B)	108.8
C(15)-C(14)-H(14B)	108.8
H(14A)-C(14)-H(14B)	107.7
C(16)-C(15)-C(14)	107(6)
C(16)-C(15)-H(15A)	110.3
C(14)-C(15)-H(15A)	110.3
C(16)-C(15)-H(15B)	110.3
C(14)-C(15)-H(15B)	110.3
H(15A)-C(15)-H(15B)	108.5
C(15)-C(16)-C(17)	110(6)

C(15)-C(16)-H(16A)	109.6
C(17)-C(16)-H(16A)	109.6
C(15)-C(16)-H(16B)	109.6
C(17)-C(16)-H(16B)	109.6
H(16A)-C(16)-H(16B)	108.1
C(18)-C(17)-C(16)	112(6)
C(18)-C(17)-H(17A)	109.1
C(16)-C(17)-H(17A)	109.1
C(18)-C(17)-H(17B)	109.1
C(16)-C(17)-H(17B)	109.1
H(17A)-C(17)-H(17B)	107.9
C(13)-C(18)-C(17)	116(6)
C(13)-C(18)-H(18A)	108.4
C(17)-C(18)-H(18A)	108.4
C(13)-C(18)-H(18B)	108.4
C(17)-C(18)-H(18B)	108.4
H(18A)-C(18)-H(18B)	107.4
C(20)-C(19)-C(24)	110(5)
C(20)-C(19)-S(4)	116(5)
C(24)-C(19)-S(4)	105(4)
C(20)-C(19)-H(19)	108.7
C(24)-C(19)-H(19)	108.7
S(4)-C(19)-H(19)	108.7
C(19)-C(20)-C(21)	113(6)
C(19)-C(20)-H(20)	123.5
C(21)-C(20)-H(20)	123.5
C(20)-C(21)-C(22)	111(5)
C(20)-C(21)-H(21A)	109.5
C(22)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
C(22)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	108.1
C(21)-C(22)-C(23)	116(5)
C(21)-C(22)-H(22A)	108.4
C(23)-C(22)-H(22A)	108.4
C(21)-C(22)-H(22B)	108.4
C(23)-C(22)-H(22B)	108.4
H(22A)-C(22)-H(22B)	107.4
C(24)-C(23)-C(22)	112(5)
C(24)-C(23)-H(23A)	109.3
C(22)-C(23)-H(23A)	109.3
C(24)-C(23)-H(23B)	109.3
C(22)-C(23)-H(23B)	109.3
H(23A)-C(23)-H(23B)	107.9

C(23)-C(24)-C(19)	113(5)
C(23)-C(24)-H(24A)	109.1
C(19)-C(24)-H(24A)	109.1
C(23)-C(24)-H(24B)	109.1
C(19)-C(24)-H(24B)	109.1
H(24A)-C(24)-H(24B)	107.8
C(30)-C(25)-C(26)	114(5)
C(30)-C(25)-S(5)	114(4)
C(26)-C(25)-S(5)	104(4)
C(30)-C(25)-H(25)	108.3
C(26)-C(25)-H(25)	108.3
S(5)-C(25)-H(25)	108.3
C(27)-C(26)-C(25)	109(5)
C(27)-C(26)-H(26A)	109.8
C(25)-C(26)-H(26A)	109.8
C(27)-C(26)-H(26B)	109.8
C(25)-C(26)-H(26B)	109.8
H(26A)-C(26)-H(26B)	108.3
C(26)-C(27)-C(28)	108(5)
C(26)-C(27)-H(27A)	110.0
C(28)-C(27)-H(27A)	110.0
C(26)-C(27)-H(27B)	110.0
C(28)-C(27)-H(27B)	110.0
H(27A)-C(27)-H(27B)	108.4
C(29)-C(28)-C(27)	113(5)
C(29)-C(28)-H(28A)	108.9
C(27)-C(28)-H(28A)	108.9
C(29)-C(28)-H(28B)	108.9
C(27)-C(28)-H(28B)	108.9
H(28A)-C(28)-H(28B)	107.7
C(30)-C(29)-C(28)	111(5)
C(30)-C(29)-H(29A)	109.4
C(28)-C(29)-H(29A)	109.4
C(30)-C(29)-H(29B)	109.4
C(28)-C(29)-H(29B)	109.4
H(29A)-C(29)-H(29B)	108.0
C(25)-C(30)-C(29)	109(5)
C(25)-C(30)-H(30A)	109.9
C(29)-C(30)-H(30A)	109.9
C(25)-C(30)-H(30B)	109.9
C(29)-C(30)-H(30B)	109.9
H(30A)-C(30)-H(30B)	108.3
C(36)-C(31)-C(32)	112.9(10)
C(36)-C(31)-S(6)	108.0(19)

C(32)-C(31)-S(6)	112.0(19)
C(36)-C(31)-H(31)	107.9
C(32)-C(31)-H(31)	107.9
S(6)-C(31)-H(31)	107.9
C(33)-C(32)-C(31)	112.3(10)
C(33)-C(32)-H(32A)	109.1
C(31)-C(32)-H(32A)	109.1
C(33)-C(32)-H(32B)	109.1
C(31)-C(32)-H(32B)	109.1
H(32A)-C(32)-H(32B)	107.9
C(34)-C(33)-C(32)	112.7(10)
C(34)-C(33)-H(33A)	109.0
C(32)-C(33)-H(33A)	109.0
C(34)-C(33)-H(33B)	109.0
C(32)-C(33)-H(33B)	109.0
H(33A)-C(33)-H(33B)	107.8
C(33)-C(34)-C(35)	113.0(10)
C(33)-C(34)-H(34A)	109.0
C(35)-C(34)-H(34A)	109.0
C(33)-C(34)-H(34B)	109.0
C(35)-C(34)-H(34B)	109.0
H(34A)-C(34)-H(34B)	107.8
C(36)-C(35)-C(34)	113.3(10)
C(36)-C(35)-H(35A)	108.9
C(34)-C(35)-H(35A)	108.9
C(36)-C(35)-H(35B)	108.9
C(34)-C(35)-H(35B)	108.9
H(35A)-C(35)-H(35B)	107.7
C(35)-C(36)-C(31)	113.5(10)
C(35)-C(36)-H(36A)	108.9
C(31)-C(36)-H(36A)	108.9
C(35)-C(36)-H(36B)	108.9
C(31)-C(36)-H(36B)	108.9
H(36A)-C(36)-H(36B)	107.7
C(38)-C(37)-C(42)	115(4)
C(38)-C(37)-S(7)	114(4)
C(42)-C(37)-S(7)	108(3)
C(38)-C(37)-H(37)	106.6
C(42)-C(37)-H(37)	106.6
S(7)-C(37)-H(37)	106.6
C(37)-C(38)-C(39)	113(4)
C(37)-C(38)-H(38A)	109.1
C(39)-C(38)-H(38A)	109.1
C(37)-C(38)-H(38B)	109.1

C(39)-C(38)-H(38B)	109.1
H(38A)-C(38)-H(38B)	107.8
C(40)-C(39)-C(38)	111(4)
C(40)-C(39)-H(39A)	109.5
C(38)-C(39)-H(39A)	109.5
C(40)-C(39)-H(39B)	109.5
C(38)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	108.1
C(39)-C(40)-C(41)	115(4)
C(39)-C(40)-H(40A)	108.5
C(41)-C(40)-H(40A)	108.5
C(39)-C(40)-H(40B)	108.5
C(41)-C(40)-H(40B)	108.5
H(40A)-C(40)-H(40B)	107.5
C(42)-C(41)-C(40)	116(4)
C(42)-C(41)-H(41A)	108.3
C(40)-C(41)-H(41A)	108.3
C(42)-C(41)-H(41B)	108.3
C(40)-C(41)-H(41B)	108.3
H(41A)-C(41)-H(41B)	107.4
C(41)-C(42)-C(37)	110(4)
C(41)-C(42)-H(42A)	109.7
C(37)-C(42)-H(42A)	109.7
C(41)-C(42)-H(42B)	109.7
C(37)-C(42)-H(42B)	109.7
H(42A)-C(42)-H(42B)	108.2
C(60)-C(55)-C(56)	112.6(11)
C(60)-C(55)-S(10)	116(3)
C(56)-C(55)-S(10)	104(3)
C(60)-C(55)-H(55)	108.1
C(56)-C(55)-H(55)	108.1
S(10)-C(55)-H(55)	108.1
C(57)-C(56)-C(55)	112.5(10)
C(57)-C(56)-H(56A)	109.1
C(55)-C(56)-H(56A)	109.1
C(57)-C(56)-H(56B)	109.1
C(55)-C(56)-H(56B)	109.1
H(56A)-C(56)-H(56B)	107.8
C(58)-C(57)-C(56)	112.8(10)
C(58)-C(57)-H(57A)	109.0
C(56)-C(57)-H(57A)	109.0
C(58)-C(57)-H(57B)	109.0
C(56)-C(57)-H(57B)	109.0
H(57A)-C(57)-H(57B)	107.8

C(59)-C(58)-C(57)	113.2(11)
C(59)-C(58)-H(58A)	108.9
C(57)-C(58)-H(58A)	108.9
C(59)-C(58)-H(58B)	108.9
C(57)-C(58)-H(58B)	108.9
H(58A)-C(58)-H(58B)	107.8
C(58)-C(59)-C(60)	113.2(11)
C(58)-C(59)-H(59A)	108.9
C(60)-C(59)-H(59A)	108.9
C(58)-C(59)-H(59B)	108.9
C(60)-C(59)-H(59B)	108.9
H(59A)-C(59)-H(59B)	107.7
C(59)-C(60)-C(55)	112.7(10)
C(59)-C(60)-H(60A)	109.1
C(55)-C(60)-H(60A)	109.1
C(59)-C(60)-H(60B)	109.1
C(55)-C(60)-H(60B)	109.1
H(60A)-C(60)-H(60B)	107.8
C(62)-C(61)-C(66)	108(5)
C(62)-C(61)-S(11)	108(4)
C(66)-C(61)-S(11)	109(4)
C(62)-C(61)-H(61)	110.3
C(66)-C(61)-H(61)	110.3
S(11)-C(61)-H(61)	110.3
C(61)-C(62)-C(63)	116(5)
C(61)-C(62)-H(62A)	108.3
C(63)-C(62)-H(62A)	108.3
C(61)-C(62)-H(62B)	108.3
C(63)-C(62)-H(62B)	108.3
H(62A)-C(62)-H(62B)	107.4
C(62)-C(63)-C(64)	103(4)
C(62)-C(63)-H(63A)	111.2
C(64)-C(63)-H(63A)	111.2
C(62)-C(63)-H(63B)	111.2
C(64)-C(63)-H(63B)	111.2
H(63A)-C(63)-H(63B)	109.1
C(65)-C(64)-C(63)	116(5)
C(65)-C(64)-H(64A)	108.4
C(63)-C(64)-H(64A)	108.4
C(65)-C(64)-H(64B)	108.4
C(63)-C(64)-H(64B)	108.4
H(64A)-C(64)-H(64B)	107.4
C(64)-C(65)-C(66)	118(5)
C(64)-C(65)-H(65A)	107.7

C(66)-C(65)-H(65A)	107.7
C(64)-C(65)-H(65B)	107.7
C(66)-C(65)-H(65B)	107.7
H(65A)-C(65)-H(65B)	107.1
C(65)-C(66)-C(61)	106(5)
C(65)-C(66)-H(66A)	110.6
C(61)-C(66)-H(66A)	110.6
C(65)-C(66)-H(66B)	110.6
C(61)-C(66)-H(66B)	110.6
H(66A)-C(66)-H(66B)	108.7
C(68)-C(67)-C(72)	112.5(11)
C(68)-C(67)-S(12)	116(3)
C(72)-C(67)-S(12)	107(3)
C(68)-C(67)-H(67)	106.9
C(72)-C(67)-H(67)	106.9
S(12)-C(67)-H(67)	106.9
C(67)-C(68)-C(69)	112.5(10)
C(67)-C(68)-H(68A)	109.1
C(69)-C(68)-H(68A)	109.1
C(67)-C(68)-H(68B)	109.1
C(69)-C(68)-H(68B)	109.1
H(68A)-C(68)-H(68B)	107.8
C(68)-C(69)-C(70)	112.6(11)
C(68)-C(69)-H(69A)	109.1
C(70)-C(69)-H(69A)	109.1
C(68)-C(69)-H(69B)	109.1
C(70)-C(69)-H(69B)	109.1
H(69A)-C(69)-H(69B)	107.8
C(71)-C(70)-C(69)	112.9(11)
C(71)-C(70)-H(70A)	109.0
C(69)-C(70)-H(70A)	109.0
C(71)-C(70)-H(70B)	109.0
C(69)-C(70)-H(70B)	109.0
H(70A)-C(70)-H(70B)	107.8
C(70)-C(71)-C(72)	112.9(11)
C(70)-C(71)-H(71A)	109.0
C(72)-C(71)-H(71A)	109.0
C(70)-C(71)-H(71B)	109.0
C(72)-C(71)-H(71B)	109.0
H(71A)-C(71)-H(71B)	107.8
C(71)-C(72)-C(67)	112.5(10)
C(71)-C(72)-H(72A)	109.1
C(67)-C(72)-H(72A)	109.1
C(71)-C(72)-H(72B)	109.1

C(67)-C(72)-H(72B)	109.1
H(72A)-C(72)-H(72B)	107.8
C(78)-C(73)-C(74)	120(4)
C(78)-C(73)-S(13)	112(3)
C(74)-C(73)-S(13)	104(3)
C(78)-C(73)-H(73)	106.5
C(74)-C(73)-H(73)	106.5
S(13)-C(73)-H(73)	106.5
C(73)-C(74)-C(75)	104(4)
C(73)-C(74)-H(74A)	110.9
C(75)-C(74)-H(74A)	110.9
C(73)-C(74)-H(74B)	110.9
C(75)-C(74)-H(74B)	110.9
H(74A)-C(74)-H(74B)	108.9
C(76)-C(75)-C(74)	119(4)
C(76)-C(75)-H(75A)	107.5
C(74)-C(75)-H(75A)	107.5
C(76)-C(75)-H(75B)	107.5
C(74)-C(75)-H(75B)	107.5
H(75A)-C(75)-H(75B)	107.0
C(75)-C(76)-C(77)	109(4)
C(75)-C(76)-H(76A)	109.9
C(77)-C(76)-H(76A)	109.9
C(75)-C(76)-H(76B)	109.9
C(77)-C(76)-H(76B)	109.9
H(76A)-C(76)-H(76B)	108.3
C(78)-C(77)-C(76)	119(4)
C(78)-C(77)-H(77A)	107.6
C(76)-C(77)-H(77A)	107.6
C(78)-C(77)-H(77B)	107.6
C(76)-C(77)-H(77B)	107.6
H(77A)-C(77)-H(77B)	107.0
C(73)-C(78)-C(77)	107(4)
C(73)-C(78)-H(78A)	110.3
C(77)-C(78)-H(78A)	110.3
C(73)-C(78)-H(78B)	110.3
C(77)-C(78)-H(78B)	110.3
H(78A)-C(78)-H(78B)	108.6
C(80)-C(79)-C(84)	108(4)
C(80)-C(79)-S(14)	118(3)
C(84)-C(79)-S(14)	111(3)
C(80)-C(79)-H(79)	106.4
C(84)-C(79)-H(79)	106.4
S(14)-C(79)-H(79)	106.4

C(79)-C(80)-C(81)	114(4)
C(79)-C(80)-H(80A)	108.7
C(81)-C(80)-H(80A)	108.7
C(79)-C(80)-H(80B)	108.7
C(81)-C(80)-H(80B)	108.7
H(80A)-C(80)-H(80B)	107.6
C(80)-C(81)-C(82)	112(4)
C(80)-C(81)-H(81A)	109.3
C(82)-C(81)-H(81A)	109.3
C(80)-C(81)-H(81B)	109.3
C(82)-C(81)-H(81B)	109.3
H(81A)-C(81)-H(81B)	108.0
C(81)-C(82)-C(83)	113(4)
C(81)-C(82)-H(82A)	108.9
C(83)-C(82)-H(82A)	108.9
C(81)-C(82)-H(82B)	108.9
C(83)-C(82)-H(82B)	108.9
H(82A)-C(82)-H(82B)	107.7
C(84)-C(83)-C(82)	106(4)
C(84)-C(83)-H(83A)	110.5
C(82)-C(83)-H(83A)	110.5
C(84)-C(83)-H(83B)	110.5
C(82)-C(83)-H(83B)	110.5
H(83A)-C(83)-H(83B)	108.7
C(83)-C(84)-C(79)	120(4)
C(83)-C(84)-H(84A)	107.3
C(79)-C(84)-H(84A)	107.3
C(83)-C(84)-H(84B)	107.3
C(79)-C(84)-H(84B)	107.3
H(84A)-C(84)-H(84B)	106.9
C(1)-S(1)-Au(1)	107.7(17)
C(1)-S(1)-Ag(3)	114.8(17)
Au(1)-S(1)-Ag(3)	92.2(5)
C(7)-S(2)-Au(1)	102.2(15)
C(7)-S(2)-Au(2)	107.3(16)
Au(1)-S(2)-Au(2)	97.4(6)
C(13)-S(3)-Au(2)	107(2)
C(13)-S(3)-Au(5)	103(2)
Au(2)-S(3)-Au(5)	90.4(6)
C(19)-S(4)-Au(4)	106(2)
C(19)-S(4)-Au(3)	106(2)
Au(4)-S(4)-Au(3)	86.9(4)
C(25)-S(5)-Au(4)	103.3(18)
C(25)-S(5)-Au(14)	108.6(18)

Au(4)-S(5)-Au(14)	91.1(4)
C(31)-S(6)-Au(12)	106.4(11)
C(31)-S(6)-Ag(1)	112.0(11)
Au(12)-S(6)-Ag(1)	89.9(4)
C(37)-S(7)-Au(11)	106.3(16)
C(37)-S(7)-Au(12)	104.0(16)
Au(11)-S(7)-Au(12)	101.4(4)
C(43)-S(8)-Au(11)	111(2)
C(43)-S(8)-Au(10)	110(2)
Au(11)-S(8)-Au(10)	84.8(5)
C(49)-S(9)-Au(10)	108(2)
C(49)-S(9)-Au(9)	110(2)
Au(10)-S(9)-Au(9)	96.9(6)
C(55)-S(10)-Au(9)	99.1(16)
C(55)-S(10)-Ag(2)	106.2(15)
Au(9)-S(10)-Ag(2)	86.9(5)
C(61)-S(11)-Au(7)	109.6(19)
C(61)-S(11)-Au(8)	112.8(19)
Au(7)-S(11)-Au(8)	92.9(4)
C(67)-S(12)-Au(7)	107.3(17)
C(67)-S(12)-Au(6)	107.2(18)
Au(7)-S(12)-Au(6)	87.4(4)
C(73)-S(13)-Au(13)	109.8(16)
C(73)-S(13)-Au(5)	102.5(15)
Au(13)-S(13)-Au(5)	94.3(4)
C(79)-S(14)-Au(13)	103.7(16)
C(79)-S(14)-Au(15)	112.5(16)
Au(13)-S(14)-Au(15)	88.5(4)
C(49)-C(50)-C(51)	112.8(11)
C(49)-C(50)-H(50A)	109.0
C(51)-C(50)-H(50A)	109.0
C(49)-C(50)-H(50B)	109.0
C(51)-C(50)-H(50B)	109.0
H(50A)-C(50)-H(50B)	107.8
C(12)-C(7)-C(8)	112.8(10)
C(12)-C(7)-S(2)	113(3)
C(8)-C(7)-S(2)	104(3)
C(12)-C(7)-H(7)	109.1
C(8)-C(7)-H(7)	109.1
S(2)-C(7)-H(7)	109.1
C(43)-C(44)-C(45)	113.0(11)
C(43)-C(44)-H(44A)	109.0
C(45)-C(44)-H(44A)	109.0
C(43)-C(44)-H(44B)	109.0

C(45)-C(44)-H(44B)	109.0
H(44A)-C(44)-H(44B)	107.8
C(50)-C(49)-C(54)	112.8(11)
C(50)-C(49)-S(9)	116(4)
C(54)-C(49)-S(9)	110(4)
C(50)-C(49)-H(49)	105.8
C(54)-C(49)-H(49)	105.8
S(9)-C(49)-H(49)	105.8
C(43)-C(48)-C(47)	112.7(11)
C(43)-C(48)-H(48A)	109.0
C(47)-C(48)-H(48A)	109.0
C(43)-C(48)-H(48B)	109.0
C(47)-C(48)-H(48B)	109.0
H(48A)-C(48)-H(48B)	107.8
C(48)-C(43)-C(44)	113.0(11)
C(48)-C(43)-S(8)	117(4)
C(44)-C(43)-S(8)	109(4)
C(48)-C(43)-H(43)	105.9
C(44)-C(43)-H(43)	105.9
S(8)-C(43)-H(43)	105.9
C(46)-C(45)-C(44)	112.9(11)
C(46)-C(45)-H(45A)	109.0
C(44)-C(45)-H(45A)	109.0
C(46)-C(45)-H(45B)	109.0
C(44)-C(45)-H(45B)	109.0
H(45A)-C(45)-H(45B)	107.8
C(52)-C(51)-C(50)	113.0(11)
C(52)-C(51)-H(51A)	109.0
C(50)-C(51)-H(51A)	109.0
C(52)-C(51)-H(51B)	109.0
C(50)-C(51)-H(51B)	109.0
H(51A)-C(51)-H(51B)	107.8
C(45)-C(46)-C(47)	112.7(11)
C(45)-C(46)-H(46A)	109.0
C(47)-C(46)-H(46A)	109.0
C(45)-C(46)-H(46B)	109.0
C(47)-C(46)-H(46B)	109.0
H(46A)-C(46)-H(46B)	107.8
C(53)-C(52)-C(51)	113.2(11)
C(53)-C(52)-H(52A)	108.9
C(51)-C(52)-H(52A)	108.9
C(53)-C(52)-H(52B)	108.9
C(51)-C(52)-H(52B)	108.9
H(52A)-C(52)-H(52B)	107.8

C(53)-C(54)-C(49)	112.6(11)
C(53)-C(54)-H(54A)	109.1
C(49)-C(54)-H(54A)	109.1
C(53)-C(54)-H(54B)	109.1
C(49)-C(54)-H(54B)	109.1
H(54A)-C(54)-H(54B)	107.8
C(46)-C(47)-C(48)	112.6(11)
C(46)-C(47)-H(47A)	109.1
C(48)-C(47)-H(47A)	109.1
C(46)-C(47)-H(47B)	109.1
C(48)-C(47)-H(47B)	109.1
H(47A)-C(47)-H(47B)	107.8
C(52)-C(53)-C(54)	112.9(11)
C(52)-C(53)-H(53A)	109.0
C(54)-C(53)-H(53A)	109.0
C(52)-C(53)-H(53B)	109.0
C(54)-C(53)-H(53B)	109.0
H(53A)-C(53)-H(53B)	107.8
C(10)-C(9)-C(8)	112.4(11)
C(10)-C(9)-H(9A)	109.1
C(8)-C(9)-H(9A)	109.1
C(10)-C(9)-H(9B)	109.1
C(8)-C(9)-H(9B)	109.1
H(9A)-C(9)-H(9B)	107.8
C(7)-C(12)-C(11)	113.1(10)
C(7)-C(12)-H(12A)	109.0
C(11)-C(12)-H(12A)	109.0
C(7)-C(12)-H(12B)	109.0
C(11)-C(12)-H(12B)	109.0
H(12A)-C(12)-H(12B)	107.8
C(7)-C(8)-C(9)	112.3(10)
C(7)-C(8)-H(8A)	109.1
C(9)-C(8)-H(8A)	109.1
C(7)-C(8)-H(8B)	109.1
C(9)-C(8)-H(8B)	109.1
H(8A)-C(8)-H(8B)	107.9
C(10)-C(11)-C(12)	113.2(11)
C(10)-C(11)-H(11A)	108.9
C(12)-C(11)-H(11A)	108.9
C(10)-C(11)-H(11B)	108.9
C(12)-C(11)-H(11B)	108.9
H(11A)-C(11)-H(11B)	107.7
C(11)-C(10)-C(9)	112.9(11)
C(11)-C(10)-H(10A)	109.0

C(9)-C(10)-H(10A)	109.0
C(11)-C(10)-H(10B)	109.0
C(9)-C(10)-H(10B)	109.0
H(10A)-C(10)-H(10B)	107.8
H(4D)-O(4)-H(4E)	109.5
H(3C)-O(3)-H(3D)	109.5
H(1A)-O(1)-H(1C)	109.5
H(2C)-O(2)-H(2D)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for $[Au_{15}Ag_3(SC_6H_{11})_{14}]$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ag(1)	34(2)	31(2)	16(1)	3(1)	3(1)	-6(1)
Ag(2)	21(1)	38(2)	20(1)	2(1)	0(1)	-7(1)
Ag(3)	38(2)	59(2)	25(2)	1(2)	5(1)	-2(2)
Au(1)	61(1)	80(2)	31(1)	-8(1)	10(1)	-22(1)
Au(2)	69(2)	83(2)	47(1)	28(1)	-7(1)	-12(1)
Au(3)	48(1)	60(1)	39(1)	10(1)	1(1)	-8(1)
Au(4)	35(1)	55(1)	37(1)	0(1)	6(1)	-4(1)
Au(5)	46(1)	59(1)	44(1)	4(1)	2(1)	3(1)
Au(6)	58(1)	67(1)	36(1)	3(1)	2(1)	-4(1)
Au(7)	42(1)	54(1)	35(1)	-8(1)	0(1)	-3(1)
Au(8)	37(1)	43(1)	32(1)	-5(1)	4(1)	-5(1)
Au(9)	54(1)	97(2)	83(2)	-50(2)	30(1)	-38(1)
Au(10)	87(2)	45(1)	52(1)	-1(1)	12(1)	-14(1)
Au(11)	53(1)	37(1)	38(1)	2(1)	1(1)	-5(1)
Au(12)	36(1)	40(1)	31(1)	0(1)	4(1)	-7(1)
Au(13)	37(1)	42(1)	39(1)	-2(1)	7(1)	-7(1)
Au(14)	32(1)	44(1)	31(1)	-1(1)	3(1)	-4(1)
Au(15)	33(1)	44(1)	29(1)	-1(1)	6(1)	-6(1)
C(1)	91(12)	94(13)	90(13)	-1(10)	1(9)	-3(9)
C(2)	93(13)	95(13)	94(13)	-1(9)	0(9)	-2(10)

C(3)	94(13)	100(13)	98(13)	0(9)	-1(9)	-4(10)
C(4)	97(13)	104(13)	102(13)	-1(10)	2(9)	-4(9)
C(5)	95(13)	98(13)	97(13)	-2(9)	3(9)	-7(10)
C(6)	93(13)	95(13)	95(13)	-1(9)	3(9)	-6(10)
C(13)	81(12)	83(12)	77(12)	-2(9)	2(9)	2(9)
C(14)	85(12)	85(12)	82(12)	-2(9)	1(9)	-1(10)
C(15)	85(12)	87(12)	86(13)	-4(9)	-1(10)	-1(9)
C(16)	86(12)	89(12)	89(12)	0(9)	-1(9)	1(9)
C(17)	85(12)	88(12)	87(12)	1(9)	0(9)	5(10)
C(18)	83(12)	86(12)	82(12)	1(9)	1(9)	3(9)
C(19)	72(11)	80(12)	74(12)	7(9)	5(9)	-6(9)
C(20)	70(11)	80(12)	72(11)	8(9)	8(9)	-3(9)
C(21)	71(11)	82(12)	72(12)	9(9)	7(9)	-4(9)
C(22)	74(11)	82(12)	75(11)	9(9)	6(9)	-3(10)
C(23)	75(11)	80(12)	76(11)	8(9)	6(9)	-2(9)
C(24)	73(11)	79(12)	74(12)	4(9)	5(9)	-4(9)
C(25)	61(11)	62(11)	61(11)	2(9)	1(9)	-1(9)
C(26)	67(11)	63(10)	61(11)	3(9)	-1(9)	-3(9)
C(27)	69(11)	69(11)	65(11)	2(9)	-1(9)	-2(9)
C(28)	69(11)	66(11)	67(11)	1(9)	-6(9)	-1(9)
C(29)	67(11)	67(11)	67(11)	-1(9)	-6(9)	2(9)
C(30)	64(11)	63(11)	64(11)	1(9)	-4(9)	0(9)
C(31)	53(11)	52(10)	51(11)	-4(9)	1(9)	-1(9)
C(32)	57(11)	57(10)	53(10)	-8(9)	0(9)	2(9)
C(33)	56(11)	58(11)	55(11)	-7(9)	-1(9)	2(8)
C(34)	60(11)	56(10)	61(11)	-4(9)	1(9)	-1(9)
C(35)	60(11)	54(10)	59(11)	0(9)	3(9)	3(9)
C(36)	56(11)	55(11)	59(11)	-1(9)	1(9)	1(8)
C(37)	53(11)	51(10)	50(10)	1(8)	3(9)	-2(9)
C(38)	51(10)	50(10)	48(10)	1(9)	5(8)	-3(9)
C(39)	52(11)	54(10)	50(10)	1(8)	7(9)	-3(9)
C(40)	56(11)	52(10)	51(10)	0(8)	7(9)	-3(9)
C(41)	54(11)	52(10)	50(11)	0(9)	5(9)	1(9)
C(42)	53(11)	52(10)	53(11)	1(9)	2(9)	-1(9)
C(55)	93(12)	94(13)	98(13)	-4(9)	1(9)	-3(9)
C(56)	93(13)	92(13)	97(13)	-3(9)	6(9)	-1(9)
C(57)	93(13)	96(13)	99(13)	0(9)	8(9)	-1(9)
C(58)	91(12)	94(13)	97(13)	0(9)	3(9)	-1(9)
C(59)	92(13)	97(13)	99(13)	0(9)	1(9)	0(9)
C(60)	92(13)	98(13)	98(13)	0(9)	-1(10)	-2(9)
C(61)	62(10)	62(11)	63(11)	-3(9)	0(9)	7(9)
C(62)	63(10)	61(11)	64(11)	-2(9)	-1(9)	6(9)
C(63)	64(11)	63(11)	69(12)	0(9)	-1(9)	6(8)
C(64)	65(10)	66(11)	73(12)	-1(9)	-2(10)	4(9)

C(65)	65(10)	63(11)	72(12)	-2(9)	1(10)	4(9)
C(66)	63(11)	64(11)	69(12)	-3(9)	0(9)	3(8)
C(67)	118(15)	117(15)	117(15)	3(10)	-7(9)	-1(9)
C(68)	119(15)	117(15)	118(15)	3(10)	-5(9)	0(10)
C(69)	119(15)	118(15)	119(15)	4(9)	-7(10)	-3(9)
C(70)	120(15)	119(15)	120(15)	3(10)	-7(9)	-1(9)
C(71)	121(15)	119(15)	121(15)	4(10)	-9(9)	-2(10)
C(72)	118(15)	118(15)	119(15)	4(9)	-7(10)	-1(9)
C(73)	50(10)	44(10)	44(10)	-2(9)	2(8)	-1(8)
C(74)	49(10)	49(10)	51(11)	-2(9)	3(9)	-2(9)
C(75)	49(9)	50(10)	48(11)	-3(9)	4(9)	0(8)
C(76)	48(10)	48(10)	47(10)	-1(9)	5(9)	0(8)
C(77)	47(9)	43(10)	40(10)	1(9)	4(9)	0(9)
C(78)	45(9)	41(10)	35(10)	1(9)	7(9)	0(8)
C(79)	46(10)	45(10)	49(10)	-5(8)	1(9)	2(9)
C(80)	45(10)	53(10)	53(11)	0(9)	5(9)	-2(8)
C(81)	52(10)	52(11)	55(11)	5(9)	6(9)	-3(8)
C(82)	56(10)	55(10)	54(11)	3(9)	3(9)	-2(9)
C(83)	57(10)	56(10)	56(11)	3(9)	0(9)	-1(8)
C(84)	52(10)	50(10)	52(11)	-2(9)	-1(9)	1(8)
S(1)	41(7)	74(9)	45(7)	-12(7)	12(6)	-17(6)
S(2)	78(8)	87(8)	70(7)	15(7)	1(6)	-24(7)
S(3)	49(8)	86(11)	80(11)	32(9)	-7(7)	-2(8)
S(4)	42(7)	53(8)	47(7)	5(6)	6(5)	-7(6)
S(5)	37(6)	36(6)	41(6)	-2(5)	8(5)	2(5)
S(6)	23(5)	34(6)	40(6)	-4(5)	4(4)	-5(4)
S(7)	36(6)	39(6)	40(6)	4(5)	2(5)	-8(5)
S(8)	97(12)	54(8)	44(8)	-2(6)	-9(7)	20(8)
S(9)	114(14)	51(9)	109(14)	-31(9)	46(12)	-24(9)
S(10)	37(7)	101(13)	109(13)	-66(11)	18(8)	-29(8)
S(11)	53(7)	39(6)	45(7)	-10(5)	5(6)	-3(6)
S(12)	69(9)	74(9)	30(6)	0(6)	-3(6)	-25(8)
S(13)	38(6)	38(6)	52(7)	-2(5)	5(5)	-7(5)
S(14)	38(6)	45(6)	29(6)	-7(5)	7(5)	-14(5)
C(50)	147(17)	145(18)	147(18)	-3(10)	1(10)	1(9)
C(7)	94(10)	97(10)	92(9)	3(8)	-6(8)	-12(8)
C(44)	154(19)	152(18)	152(18)	1(9)	2(10)	3(10)
C(49)	146(18)	146(18)	148(18)	-4(10)	2(9)	-1(9)
C(48)	155(19)	151(18)	153(18)	0(9)	2(10)	0(10)
C(43)	155(19)	152(18)	151(18)	0(9)	1(10)	1(10)
C(45)	154(19)	152(18)	153(18)	2(9)	3(10)	2(10)
C(51)	146(17)	143(18)	146(18)	-2(10)	2(10)	-1(10)
C(46)	154(19)	151(18)	151(18)	1(9)	2(10)	0(10)
C(52)	148(18)	145(18)	149(18)	-3(10)	0(9)	1(9)

C(54)	147(17)	147(18)	152(18)	-6(10)	3(10)	-2(10)
C(47)	156(19)	153(18)	153(18)	0(9)	1(10)	1(10)
C(53)	147(17)	148(18)	151(18)	-5(10)	2(10)	-2(9)
C(9)	110(12)	105(12)	100(11)	2(10)	-11(9)	-6(9)
C(12)	102(11)	105(12)	99(11)	-4(9)	-1(9)	-12(9)
C(8)	105(11)	104(12)	97(11)	4(9)	-13(9)	-8(9)
C(11)	106(12)	107(12)	104(11)	-5(9)	-4(9)	-11(9)
C(10)	110(12)	108(13)	104(11)	-1(9)	-6(9)	-10(10)
O(4)	126	100	108	23	-4	-5
O(3)	151	119	147	45	-51	-25
O(1)	126	100	108	23	-4	-5
O(2)	126	100	108	23	-4	-5