Supplementary Information:

1. Experimental

Synthesis and crystallization of $Au_{24}(SR)_{20}$ (R = CH_2Ph-^tBu). The $[Au_{23}(S\text{-}c\text{-}C_6H_{11})_{16}]^-$ nanocluster was used as the starting material for obtaining the $[Au_{24}(SCH_2Ph\text{-}^tBu)_{20}]^0$ nanocluster via a ligand exchange reaction with $HSCH_2Ph$-^{t}Bu thiol. In a typical reaction, ~3 mg Au_{23} clusters were dissolved in ~0.5 mL dichloromethane containing 0.5 mL $HSCH_2Ph$-^{t}Bu thiol. The mixture was stirred for 36 h at 40 °C under reflux conditions. The resulting nanocluster product was then washed with methanol several times and finally extracted with dichloromethane. Single crystal growth of the nanoclusters was performed by first dissolving ~2 mg $[Au_{24}(SCH_2Ph\text{-}^tBu)_{20}]^0$ clusters in 0.5 mL dichloromethane, followed by vapour diffusion of pentane into the cluster solution for 1-2 days. ESI mass spectra of Au_{24} clusters were recorded using a Waters Q-TOF mass spectrometer equipped with Z-spray source with source temperature kept at 70 °C. The cluster sample was directly infused into the chamber at 5 μL/min. The spray voltage was kept at 2.20 kV and the cone voltage at 60 V. To prepare the ESI sample, $[Au_{24}(SCH_2Ph\text{-}^tBu)_{20}]^0$ clusters were dissolved in toluene (~1 mg/mL) and diluted (2:1 v) by dry ethanol containing 50 mM CsOAc to ionize the clusters by forming Cs^+-cluster adducts.

X-ray crystallographic determination of $Au_{24}(SR)_{20}$. Single X-ray diffraction data of $Au_{24}(SR)_{20}$ was collected on a Bruker X8 Prospector Ultra equipped with an Apex II CCD detector and an IμS micro-focus CuKα X-ray source (λ = 1.54178 Å). A piece of red rod-shaped crystal with dimensions 0.18 x 0.12 x 0.03 mm was mounted onto a MiTeGen micromount with fluorolube. The data were collected under room temperature (296 K).

A triclinic unit cell with dimensions a = 15.9929(8), b = 21.5942(12), c = 21.8042(11), α = 66.888(3)°, β = 74.051(3)°, and γ = 73.462(3)° was derived from the least-square refinement of 9411 reflections in the range of 2.27 < θ < 53.61. Centrosymmetric space group P-1 was determined based on mean |E*E-1| statistic (1.048).

The data was collected to 0.95 Å. After integration of the data by Bruker program SAINT[1], empirical absorption correction was applied using program SADABS[1]. Maximum and minimum transmittance (T_{max}, T_{min}) values are 0.5043 and 0.0873 respectively.

The structure was successfully solved with direct method using Bruker program SHELXTL.[2] All the Au, S, and some of the C atoms were located easily. Although most of the C atoms were generated via subsequent difference Fourier syntheses, some of the t-Bu carbons could not be found. In that case, three t-Bu benzene fragments were constrained as rigid model adapted from Cambridge database. In terms of other t-Bu benzene fragments, numerous restraints were applied to optimize the bond lengths, bond angles, and atomic displacement parameters. In particular, attempts to refine C119, C120, and C124 were not successful. This is probably due to either severe disorder or high absorption coefficient (Mu=26.44 mm^{-1}). So they were left unrefined. Estimated atomic displacement parameters (0.4 or 0.5) were given. All the non-hydrogen atoms except t-Bu carbons were refined anisotropically. Idealized atom positions were calculated for all hydrogen atoms (with d-(C_{CH3}-H) = 0.96 Å, d-($C_{aromatic}$-H)=0.93 Å, d-(C_{CH2}-H)=0.97 Å). All the refinement parameters are summarized in Table S1.

1. APEX II software suite, Bruker-AXS (2006).
2. SHELXTL, G. M. Sheldrick, *ActaCrystallogr*. A, **64**, 112 (2008).

2. DFT Calculations

Density functional theory (DFT) calculations were performed with $Au_{24}(SCH_3)_{20}$ in which methanethiolate replaces the actual bulky ligand. Starting from the X-ray structures, we first carried out geometry optimization of the model clusters by freezing the $Au_{24}S_{20}$ core structure while relaxing the structures of ligands. We calculated geometry optimization and analyzed electronic properties of the cluster without molecular symmetry. Geometry optimizations based on a quasi-Newton–Raphson method were carried out at the level of Kohn–Sham density functional theory (KS-DFT) employing the hybrid functional B3LYP for $Au_{24}(SCH_3)_{20}$. Of note, we also compared PBE0 and B3LYP functionals for $Au_{24}(SCH_3)_{20}$ and found that the B3LYP functional gave a slightly closer match with the experimental

optical spectrum. The double-ζ valence quality plus polarization basis in the TURBOMOLE basis set library was adopted in the calculations along with a 60-electron relativistic effective core potentials for the gold atom. The absorption spectra were simulated within time-dependent KS linear response theory. All the calculations used the TURBOMOLE Ver. 6.3 package of ab initio quantum chemistry programs.

3. Supplementary Figures

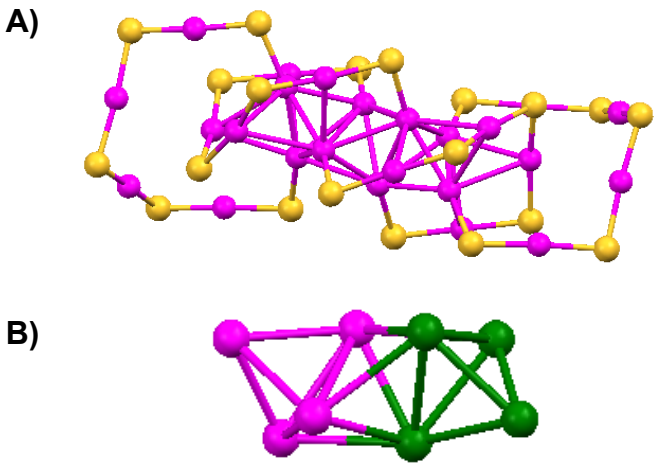

Figure S1. Theoretical structure (Iso 3) of $Au_{24}(SCH_3)_{20}$, (A) the $Au_{24}S_{20}$ framework consisting of four tetrameric Au_4S_5 staples and a Au_8 kernel, (B) configuration of the Au_8 kernel. (Coordinates were provided by Prof. Y. Pei).

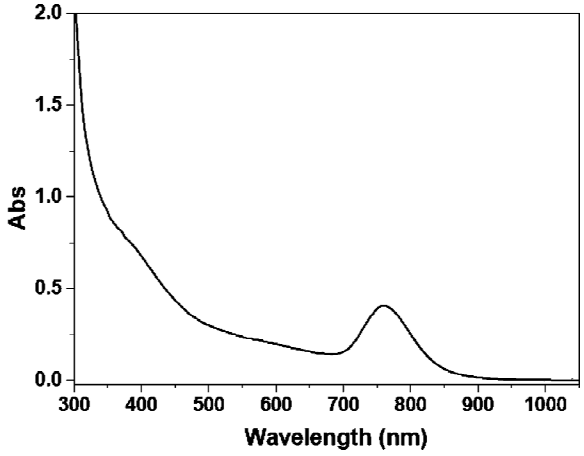

Figure S2. UV-Vis spectrum of $[Au_{24}(SCH_2CH_2Ph)_{20}]^0$ (ref 72, see main text).

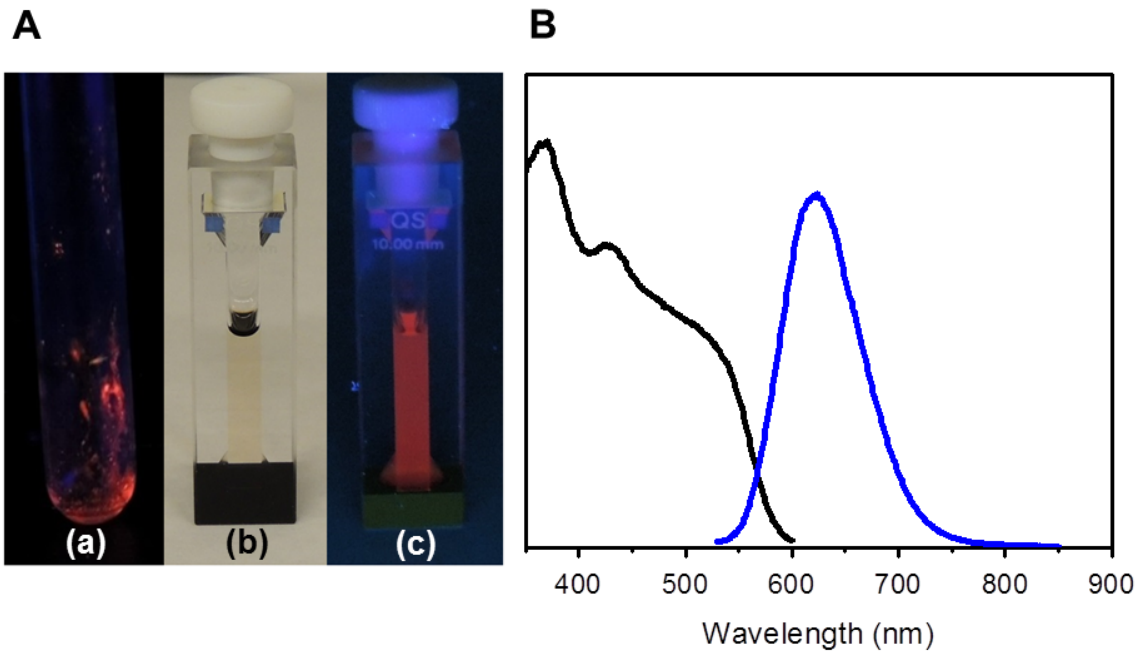

Figure S3. (A) Photoluminescence of $Au_{24}(SCH_2Ph\text{-}t\text{-}Bu)_{20}$ nanoclusters: (a) Solid Au_{24} crystals under UV light (λ = 365 nm) with red emission, (b) Photograph of a ~0.1 OD (at 500 nm) solution of Au_{24} in toluene under visible light, (c) The same solution under under UV (λ = 365 nm). (B) Photoluminescence spectrum (blue curve) of Au_{24} in toluene (blue curve, excit.=514 nm, slit width: 5 nm, concentration: 0.08 OD absorbance at 514 nm measured by UV-vis) and the excitation spectrum (black curve) corresponding to the 618 nm emission band.

4. Supplementary Tables for $Au_{24}(SR)_{20}$ structural parameters

Table S1. Crystal data and structure refinement for $Au_{24}(SR)_{20}$.

Identification code	Au24(SR)20	
Empirical formula	C220 H300 Au24 S20	
Formula weight	8313.00	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 15.9929(8) Å	α= 66.888(3)°.
	b = 21.5942(12) Å	β= 74.051(3)°.
	c = 21.8042(11) Å	γ = 73.462(3)°.
Volume	6524.8(6) $Å^3$	
Z	1	
Density (calculated)	2.116 Mg/m^3	
Absorption coefficient	26.437 mm^{-1}	
F(000)	3836	
Crystal size	0.18 x 0.12 x 0.03 mm^3	
Theta range for data collection	2.24 to 54.53°.	
Index ranges	-16<=h<=16, -22<=k<=22, -22<=l<=23	
Reflections collected	56832	
Independent reflections	15678 [R(int) = 0.0640]	
Completeness to theta = 54.53°	97.4 %	
Absorption correction	Multi scan (SADABS)	
Max. and min. transmission	0.5043 and 0.0873	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15678 / 429 / 914	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0545, wR2 = 0.1578	
R indices (all data)	R1 = 0.0916, wR2 = 0.1944	
Largest diff. peak and hole	2.039 and -0.816 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $Au_{24}(SR)_{20}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(24)	2979(17)	6872(12)	1868(10)	100(9)
C(25)	2211(16)	6749(13)	2348(13)	150(16)
C(26)	2036(14)	6866(13)	2958(12)	200(30)
C(27)	2612(16)	7089(12)	3140(10)	200(30)
C(28)	3383(15)	7198(14)	2671(12)	200(20)
C(29)	3554(15)	7089(14)	2063(11)	136(13)
C(127)	2420(20)	7224(19)	3808(12)	370(50)
C(128)	2400(30)	7960(20)	3670(20)	410(60)
C(129)	2920(30)	6660(20)	4278(12)	490(80)
C(130)	1450(30)	7150(30)	4190(15)	640(120)
C(42)	-390(20)	3569(16)	4140(15)	176(15)
C(43)	180(20)	3347(17)	4602(18)	203(18)
C(44)	570(20)	2662(18)	4875(15)	250(20)
C(45)	417(18)	2155(16)	4726(14)	280(30)
C(46)	-160(20)	2372(18)	4278(16)	240(20)
C(47)	-540(20)	3050(20)	4003(14)	208(19)
C(123)	850(30)	1398(16)	5020(20)	520(90)
C(124)	1410(30)	1140(20)	4460(30)	500
C(125)	220(30)	1042(17)	5560(30)	520(90)
C(126)	1560(30)	1320(20)	5430(30)	540(90)
C(36)	-1098(19)	2954(15)	2207(13)	158(16)
C(37)	-1830(20)	3113(11)	2681(15)	210(20)
C(38)	-2141(18)	2617(13)	3272(14)	250(20)
C(39)	-1778(17)	1937(12)	3420(12)	230(20)
C(40)	-1070(20)	1775(12)	2944(14)	240(20)
C(41)	-748(19)	2266(16)	2362(13)	220(20)
C(119)	-2110(30)	1386(16)	4072(15)	400
C(120)	-1400(30)	1020(20)	4481(16)	400
C(121)	-2650(30)	1040(20)	3910(20)	510(90)
C(122)	-2840(30)	1730(20)	4556(16)	420(60)
Au(1)	3763(1)	5388(1)	597(1)	79(1)

Au(2)	4339(1)	4202(1)	287(1)	78(1)
Au(3)	1868(1)	4754(1)	1596(1)	87(1)
Au(4)	1858(1)	6336(1)	274(1)	86(1)
Au(5)	3766(1)	6844(1)	-526(1)	88(1)
Au(6)	5713(1)	4537(1)	725(1)	80(1)
Au(7)	3911(1)	3905(1)	1791(1)	86(1)
Au(8)	2739(1)	5032(1)	39(1)	83(1)
Au(9)	3127(1)	5128(1)	2328(1)	96(1)
Au(10)	9(1)	4191(1)	2392(1)	104(1)
Au(11)	1114(1)	4638(1)	3192(1)	105(1)
Au(12)	927(1)	4263(1)	696(1)	100(1)
S(1)	-336(6)	4809(5)	3102(5)	118(3)
S(2)	2627(5)	3627(4)	1792(4)	89(2)
S(3)	1655(5)	4836(4)	-345(4)	97(2)
S(4)	3847(5)	5861(4)	1377(3)	88(2)
S(5)	1113(5)	5882(4)	1359(4)	92(2)
S(6)	2521(6)	4444(5)	3371(4)	111(3)
S(7)	285(6)	3559(5)	1707(4)	110(3)
S(8)	2457(6)	6914(4)	-829(4)	100(2)
S(9)	5168(6)	4143(4)	1890(4)	101(2)
S(10)	4966(5)	3081(4)	263(4)	92(2)
C(1)	3050(20)	6703(15)	1224(16)	107(10)
C(2)	1840(20)	7804(16)	-937(18)	120(12)
C(3)	2320(20)	4100(19)	-645(17)	119(11)
C(4)	27(17)	5846(14)	1233(14)	85(8)
C(5)	4440(20)	2468(15)	1045(19)	127(13)
C(6)	2430(30)	4901(19)	3959(15)	128(13)
C(7)	-850(20)	3547(17)	1644(16)	117(11)
C(8)	-880(30)	4270(20)	3924(18)	142(14)
C(9)	2230(20)	3111(18)	2689(14)	111(11)
C(10)	5890(30)	3330(20)	2282(17)	134(13)
C(12)	2500(20)	2364(13)	2790(15)	122(12)
C(13)	1940(20)	2061(17)	2681(16)	157(17)
C(14)	2170(30)	1367(19)	2750(20)	210(30)
C(15)	2990(30)	992(13)	2913(19)	190(30)
C(16)	3540(20)	1287(19)	3050(20)	200(30)

C(17)	3320(20)	1980(20)	2980(20)	180(20)
C(18)	5420(20)	2902(18)	2963(14)	138(15)
C(19)	5730(30)	2200(20)	3169(18)	210(30)
C(20)	5380(30)	1788(17)	3800(20)	260(40)
C(21)	4720(40)	2070(20)	4220(20)	290(50)
C(22)	4420(40)	2770(20)	4024(19)	270(40)
C(23)	4730(30)	3182(16)	3383(18)	170(20)
C(30)	1675(19)	8078(15)	-411(14)	120(9)
C(31)	846(16)	8097(13)	1(16)	138(10)
C(32)	664(17)	8353(17)	519(17)	156(12)
C(33)	1290(20)	8613(18)	617(17)	148(11)
C(34)	2131(19)	8566(18)	230(18)	139(10)
C(35)	2315(16)	8307(16)	-293(16)	130(10)
C(48)	5083(17)	1815(13)	1259(16)	107(10)
C(49)	5480(20)	1693(16)	1795(16)	137(15)
C(50)	6080(20)	1090(20)	2016(16)	171(19)
C(51)	6290(30)	596(16)	1710(20)	160(20)
C(52)	5900(30)	726(18)	1170(20)	180(20)
C(53)	5310(20)	1332(19)	940(17)	142(15)
C(54)	2769(18)	4359(14)	-1375(12)	97(9)
C(55)	2309(16)	4589(16)	-1897(15)	141(14)
C(56)	2740(20)	4780(18)	-2565(14)	139(14)
C(57)	3640(20)	4760(20)	-2716(13)	128(13)
C(58)	4105(15)	4500(20)	-2192(17)	144(16)
C(59)	3671(19)	4318(18)	-1526(15)	127(13)
C(60)	-417(16)	6545(12)	783(12)	88(8)
C(61)	-948(17)	7046(15)	1023(12)	117(11)
C(62)	-1391(18)	7640(14)	604(17)	124(12)
C(63)	-1300(20)	7723(15)	-73(16)	124(12)
C(64)	-750(20)	7224(16)	-314(11)	116(11)
C(65)	-323(17)	6631(13)	106(13)	98(9)
C(66)	2080(20)	4494(17)	4673(13)	139(12)
C(67)	2700(20)	4000(20)	5027(17)	204(19)
C(68)	2440(20)	3580(20)	5690(17)	199(19)
C(69)	1550(30)	3656(18)	5979(13)	150(14)
C(70)	930(20)	4160(20)	5633(18)	170(16)

C(71)	1190(20)	4566(19)	4969(18)	161(15)
C(72)	-1820(30)	8410(30)	-560(20)	158(15)
C(73)	-2350(40)	8140(30)	-830(30)	240(30)
C(74)	-1210(40)	8710(30)	-1210(30)	230(30)
C(75)	-2200(30)	8940(30)	-170(30)	190(20)
C(76)	1030(30)	8920(30)	1200(30)	165(17)
C(77)	390(50)	8650(40)	1850(40)	280(30)
C(78)	410(40)	9650(40)	960(30)	260(30)
C(79)	1760(40)	9010(30)	1370(30)	240(30)
C(83)	7900(40)	110(40)	2000(30)	270(30)
C(84)	7560(50)	-440(40)	1380(40)	320(40)
C(85)	6730(50)	-490(40)	2590(40)	280(40)
C(86)	1250(50)	2460(40)	6710(50)	420(60)
C(87)	460(30)	3360(30)	7010(30)	220(20)
C(88)	1300(30)	3100(30)	6700(30)	200(20)
C(91)	3910(60)	4790(50)	-3900(40)	360(50)
C(102)	5070(50)	4870(40)	-3590(30)	270(30)
C(104)	1880(40)	2970(40)	7120(40)	360(50)
C(101)	4100(40)	5030(30)	-3450(30)	172(18)
C(103)	3810(50)	5770(40)	-3830(40)	300(40)
C(107)	7050(40)	-160(30)	1930(40)	210(20)
C(115)	4390(40)	1540(30)	4990(30)	380(60)
C(116)	4560(70)	1920(50)	5330(60)	500(80)
C(117)	3510(70)	1660(70)	4910(80)	630(120)
C(118)	4870(60)	860(50)	5130(50)	440(70)
C(131)	3290(30)	160(20)	3030(30)	270(30)
C(132)	2600(50)	-40(50)	3500(40)	380(50)
C(133)	4050(50)	-40(60)	3250(40)	460(70)
C(134)	3330(50)	130(40)	2440(30)	320(40)

Table S3. Bond lengths [Å] and angles [°] for $Au_{24}(SR)_{20}$.

C(24)-C(29)	1.3663	C(46)-H(46A)	0.9300
C(24)-C(25)	1.3912	C(47)-H(47A)	0.9300
C(24)-C(1)	1.55(4)	C(123)-C(125)	1.4466
C(25)-C(26)	1.3876	C(123)-C(124)	1.4935
C(25)-H(25A)	0.9300	C(123)-C(126)	1.5736
C(26)-C(27)	1.3574	C(124)-H(12G)	0.9600
C(26)-H(26A)	0.9300	C(124)-H(12H)	0.9600
C(27)-C(28)	1.3799	C(124)-H(12I)	0.9600
C(27)-C(127)	1.5302	C(125)-H(12J)	0.9600
C(28)-C(29)	1.3754	C(125)-H(12K)	0.9600
C(28)-H(28A)	0.9300	C(125)-H(12L)	0.9600
C(29)-H(29A)	0.9300	C(126)-H(12M)	0.9600
C(127)-C(129)	1.4466	C(126)-H(12N)	0.9600
C(127)-C(128)	1.4935	C(126)-H(12O)	0.9600
C(127)-C(130)	1.5736	C(36)-C(41)	1.3663
C(128)-H(12A)	0.9600	C(36)-C(37)	1.3912
C(128)-H(12B)	0.9600	C(36)-C(7)	1.45(4)
C(128)-H(12C)	0.9600	C(37)-C(38)	1.3877
C(129)-H(12D)	0.9600	C(37)-H(37A)	0.9300
C(129)-H(12E)	0.9600	C(38)-C(39)	1.3573
C(129)-H(12F)	0.9600	C(38)-H(38A)	0.9300
C(130)-H(13A)	0.9600	C(39)-C(40)	1.3800
C(130)-H(13B)	0.9600	C(39)-C(119)	1.5301
C(130)-H(13C)	0.9600	C(40)-C(41)	1.3753
C(42)-C(47)	1.3663	C(40)-H(40A)	0.9300
C(42)-C(43)	1.3912	C(41)-H(41A)	0.9300
C(42)-C(8)	1.45(5)	C(119)-C(121)	1.4466
C(43)-C(44)	1.3877	C(119)-C(120)	1.4936
C(43)-H(43A)	0.9300	C(119)-C(122)	1.5737
C(44)-C(45)	1.3574	C(120)-H(12P)	0.9600
C(44)-H(44A)	0.9300	C(120)-H(12Q)	0.9600
C(45)-C(46)	1.3800	C(120)-H(12R)	0.9600
C(45)-C(123)	1.5301	C(121)-H(12S)	0.9600
C(46)-C(47)	1.3753	C(121)-H(12T)	0.9600

C(121)-H(12U)	0.9600	Au(6)-S(9)	2.335(7)
C(122)-H(12V)	0.9600	Au(6)-Au(1)#1	2.7231(16)
C(122)-H(12W)	0.9600	Au(6)-Au(2)#1	2.7477(15)
C(122)-H(12X)	0.9600	Au(6)-Au(8)#1	2.7554(17)
Au(1)-S(4)	2.351(7)	Au(6)-Au(5)#1	3.0289(17)
Au(1)-Au(8)	2.7000(16)	Au(7)-S(9)	2.294(8)
Au(1)-Au(6)#1	2.7231(16)	Au(7)-S(2)	2.297(8)
Au(1)-Au(2)	2.7458(16)	Au(7)-Au(9)	3.1075(19)
Au(1)-Au(5)	3.1370(15)	Au(8)-S(3)	2.321(7)
Au(1)-Au(6)	3.1626(17)	Au(8)-Au(6)#1	2.7554(17)
Au(1)-Au(7)	3.2330(15)	Au(9)-S(6)	2.294(8)
Au(1)-Au(4)	3.2348(17)	Au(9)-S(4)	2.298(7)
Au(1)-Au(2)#1	3.2700(16)	Au(10)-S(7)	2.278(9)
Au(2)-S(10)	2.357(7)	Au(10)-S(1)	2.282(10)
Au(2)-Au(8)	2.7281(17)	Au(10)-Au(11)	3.327(2)
Au(2)-Au(6)#1	2.7477(15)	Au(11)-S(6)	2.283(10)
Au(2)-Au(6)	2.9762(17)	Au(11)-S(1)	2.292(10)
Au(2)-Au(7)	2.9993(16)	Au(12)-S(3)	2.281(8)
Au(2)-Au(5)#1	3.2561(17)	Au(12)-S(7)	2.290(9)
Au(2)-Au(1)#1	3.2700(16)	S(1)-C(8)	1.84(4)
Au(3)-S(5)	2.311(8)	S(2)-C(9)	1.87(3)
Au(3)-S(2)	2.316(7)	S(3)-C(3)	1.88(3)
Au(3)-Au(8)	3.1787(17)	S(4)-C(1)	1.87(3)
Au(3)-Au(11)	3.2864(18)	S(5)-C(4)	1.86(3)
Au(3)-Au(10)	3.3002(18)	S(6)-C(6)	1.86(3)
Au(3)-Au(7)	3.3109(18)	S(7)-C(7)	1.86(4)
Au(3)-Au(9)	3.3114(19)	S(8)-C(2)	1.85(3)
Au(3)-Au(12)	3.3776(19)	S(9)-C(10)	1.83(4)
Au(4)-S(5)	2.296(7)	S(10)-C(5)	1.86(3)
Au(4)-S(8)	2.306(8)	S(10)-Au(5)#1	2.316(8)
Au(4)-Au(8)	2.9413(17)	C(1)-H(1A)	0.9700
Au(4)-Au(5)	3.3223(17)	C(1)-H(1B)	0.9700
Au(5)-S(8)	2.311(8)	C(2)-C(30)	1.42(4)
Au(5)-S(10)#1	2.316(8)	C(2)-H(2A)	0.9700
Au(5)-Au(6)#1	3.0289(17)	C(2)-H(2B)	0.9700
Au(5)-Au(2)#1	3.2561(17)	C(3)-C(54)	1.51(4)

C(3)-H(3A)	0.9700	C(20)-C(21)	1.37(2)
C(3)-H(3B)	0.9700	C(20)-H(20A)	0.9300
C(4)-C(60)	1.53(3)	C(21)-C(22)	1.38(2)
C(4)-H(4A)	0.9700	C(21)-C(115)	1.66(3)
C(4)-H(4B)	0.9700	C(22)-C(23)	1.37(2)
C(5)-C(48)	1.48(4)	C(22)-H(22A)	0.9300
C(5)-H(5A)	0.9700	C(23)-H(23A)	0.9300
C(5)-H(5B)	0.9700	C(30)-C(35)	1.37(2)
C(6)-C(66)	1.50(4)	C(30)-C(31)	1.38(2)
C(6)-H(6A)	0.9700	C(31)-C(32)	1.37(2)
C(6)-H(6B)	0.9700	C(31)-H(31A)	0.9300
C(7)-H(7A)	0.9700	C(32)-C(33)	1.37(2)
C(7)-H(7B)	0.9700	C(32)-H(32A)	0.9300
C(8)-H(8A)	0.9700	C(33)-C(34)	1.38(2)
C(8)-H(8B)	0.9700	C(33)-C(76)	1.56(5)
C(9)-C(12)	1.49(4)	C(34)-C(35)	1.38(2)
C(9)-H(9A)	0.9700	C(34)-H(34A)	0.9300
C(9)-H(9B)	0.9700	C(35)-H(35A)	0.9300
C(10)-C(18)	1.53(4)	C(48)-C(49)	1.38(2)
C(10)-H(10A)	0.9700	C(48)-C(53)	1.38(2)
C(10)-H(10B)	0.9700	C(49)-C(50)	1.38(2)
C(12)-C(13)	1.37(2)	C(49)-H(49A)	0.9300
C(12)-C(17)	1.40(2)	C(50)-C(51)	1.38(2)
C(13)-C(14)	1.40(2)	C(50)-H(50A)	0.9300
C(13)-H(13D)	0.9300	C(51)-C(52)	1.39(2)
C(14)-C(15)	1.39(2)	C(51)-C(107)	1.71(7)
C(14)-H(14A)	0.9300	C(52)-C(53)	1.37(2)
C(15)-C(16)	1.37(2)	C(52)-H(52A)	0.9300
C(15)-C(131)	1.64(3)	C(53)-H(53A)	0.9300
C(16)-C(17)	1.38(2)	C(54)-C(59)	1.37(2)
C(16)-H(16A)	0.9300	C(54)-C(55)	1.38(2)
C(17)-H(17A)	0.9300	C(55)-C(56)	1.38(2)
C(18)-C(19)	1.38(2)	C(55)-H(55A)	0.9300
C(18)-C(23)	1.38(2)	C(56)-C(57)	1.38(2)
C(19)-C(20)	1.37(2)	C(56)-H(56A)	0.9300
C(19)-H(19A)	0.9300	C(57)-C(58)	1.37(2)

C(57)-C(101)	1.52(6)	C(75)-H(75B)	0.9600
C(58)-C(59)	1.38(2)	C(75)-H(75C)	0.9600
C(58)-H(58A)	0.9300	C(76)-C(79)	1.41(7)
C(59)-H(59A)	0.9300	C(76)-C(77)	1.51(7)
C(60)-C(61)	1.36(2)	C(76)-C(78)	1.59(7)
C(60)-C(65)	1.38(2)	C(77)-H(77A)	0.9600
C(61)-C(62)	1.38(2)	C(77)-H(77B)	0.9600
C(61)-H(61A)	0.9300	C(77)-H(77C)	0.9600
C(62)-C(63)	1.38(2)	C(78)-H(78A)	0.9600
C(62)-H(62A)	0.9300	C(78)-H(78B)	0.9600
C(63)-C(64)	1.37(2)	C(78)-H(78C)	0.9600
C(63)-C(72)	1.60(5)	C(79)-H(79A)	0.9600
C(64)-C(65)	1.37(2)	C(79)-H(79B)	0.9600
C(64)-H(64A)	0.9300	C(79)-H(79C)	0.9600
C(65)-H(65A)	0.9300	C(83)-C(107)	1.67(8)
C(66)-C(67)	1.38(2)	C(83)-H(83A)	0.9600
C(66)-C(71)	1.38(2)	C(83)-H(83B)	0.9600
C(67)-C(68)	1.40(2)	C(83)-H(83C)	0.9600
C(67)-H(67A)	0.9300	C(84)-C(107)	1.48(8)
C(68)-C(69)	1.38(2)	C(84)-H(84A)	0.9600
C(68)-H(68A)	0.9300	C(84)-H(84B)	0.9600
C(69)-C(70)	1.37(2)	C(84)-H(84C)	0.9600
C(69)-C(88)	1.58(7)	C(85)-C(107)	1.35(8)
C(70)-C(71)	1.38(2)	C(85)-H(85A)	0.9600
C(70)-H(70A)	0.9300	C(85)-H(85B)	0.9600
C(71)-H(71A)	0.9300	C(85)-H(85C)	0.9600
C(72)-C(73)	1.51(7)	C(86)-C(88)	1.40(4)
C(72)-C(74)	1.51(6)	C(86)-H(86A)	0.9600
C(72)-C(75)	1.57(6)	C(86)-H(86B)	0.9600
C(73)-H(73A)	0.9600	C(86)-H(86C)	0.9600
C(73)-H(73B)	0.9600	C(87)-C(88)	1.39(4)
C(73)-H(73C)	0.9600	C(87)-H(87A)	0.9600
C(74)-H(74A)	0.9600	C(87)-H(87B)	0.9600
C(74)-H(74B)	0.9600	C(87)-H(87C)	0.9600
C(74)-H(74C)	0.9600	C(88)-C(104)	1.40(4)
C(75)-H(75A)	0.9600	C(91)-C(101)	1.41(9)

C(91)-H(91A)	0.9600	C(116)-H(11C)	0.9600
C(91)-H(91B)	0.9600	C(117)-H(11D)	0.9600
C(91)-H(91C)	0.9600	C(117)-H(11E)	0.9600
C(102)-C(101)	1.47(7)	C(117)-H(11F)	0.9600
C(102)-H(10C)	0.9600	C(118)-H(11G)	0.9600
C(102)-H(10D)	0.9600	C(118)-H(11H)	0.9600
C(102)-H(10E)	0.9600	C(118)-H(11I)	0.9600
C(104)-H(10F)	0.9600	C(131)-C(134)	1.32(5)
C(104)-H(10G)	0.9600	C(131)-C(132)	1.32(5)
C(104)-H(10H)	0.9600	C(131)-C(133)	1.32(5)
C(101)-C(103)	1.49(8)	C(132)-H(13E)	0.9600
C(103)-H(10I)	0.9600	C(132)-H(13F)	0.9600
C(103)-H(10J)	0.9600	C(132)-H(13G)	0.9600
C(103)-H(10K)	0.9600	C(133)-H(13H)	0.9600
C(115)-C(118)	1.40(7)	C(133)-H(13I)	0.9600
C(115)-C(117)	1.41(7)	C(133)-H(13J)	0.9600
C(115)-C(116)	1.41(7)	C(134)-H(13K)	0.9600
C(116)-H(11A)	0.9600	C(134)-H(13L)	0.9600
C(116)-H(11B)	0.9600	C(134)-H(13M)	0.9600

-----Bond angles----

C(29)-C(24)-C(25)	114.0	C(24)-C(29)-H(29A)	118.3
C(29)-C(24)-C(1)	131(2)	C(28)-C(29)-H(29A)	118.3
C(25)-C(24)-C(1)	115(2)	C(129)-C(127)-C(128)	124.1
C(26)-C(25)-C(24)	122.6	C(129)-C(127)-C(27)	108.9
C(26)-C(25)-H(25A)	118.7	C(128)-C(127)-C(27)	110.0
C(24)-C(25)-H(25A)	118.7	C(129)-C(127)-C(130)	100.1
C(27)-C(26)-C(25)	122.5	C(128)-C(127)-C(130)	102.3
C(27)-C(26)-H(26A)	118.7	C(27)-C(127)-C(130)	110.2
C(25)-C(26)-H(26A)	118.7	C(127)-C(128)-H(12A)	109.5
C(26)-C(27)-C(28)	115.1	C(127)-C(128)-H(12B)	109.5
C(26)-C(27)-C(127)	123.0	H(12A)-C(128)-H(12B)	109.5
C(28)-C(27)-C(127)	121.9	C(127)-C(128)-H(12C)	109.5
C(29)-C(28)-C(27)	122.5	H(12A)-C(128)-H(12C)	109.5
C(29)-C(28)-H(28A)	118.7	H(12B)-C(128)-H(12C)	109.5
C(27)-C(28)-H(28A)	118.7	C(127)-C(129)-H(12D)	109.5
C(24)-C(29)-C(28)	123.3	C(127)-C(129)-H(12E)	109.5

H(12D)-C(129)-H(12E)	109.5	H(12G)-C(124)-H(12H)	109.5
C(127)-C(129)-H(12F)	109.5	C(123)-C(124)-H(12I)	109.5
H(12D)-C(129)-H(12F)	109.5	H(12G)-C(124)-H(12I)	109.5
H(12E)-C(129)-H(12F)	109.5	H(12H)-C(124)-H(12I)	109.5
C(127)-C(130)-H(13A)	109.5	C(123)-C(125)-H(12J)	109.5
C(127)-C(130)-H(13B)	109.5	C(123)-C(125)-H(12K)	109.5
H(13A)-C(130)-H(13B)	109.5	H(12J)-C(125)-H(12K)	109.5
C(127)-C(130)-H(13C)	109.5	C(123)-C(125)-H(12L)	109.5
H(13A)-C(130)-H(13C)	109.5	H(12J)-C(125)-H(12L)	109.5
H(13B)-C(130)-H(13C)	109.5	H(12K)-C(125)-H(12L)	109.5
C(47)-C(42)-C(43)	114.0	C(123)-C(126)-H(12M)	109.5
C(47)-C(42)-C(8)	124(3)	C(123)-C(126)-H(12N)	109.5
C(43)-C(42)-C(8)	122(3)	H(12M)-C(126)-H(12N)	109.5
C(44)-C(43)-C(42)	122.6	C(123)-C(126)-H(12O)	109.5
C(44)-C(43)-H(43A)	118.7	H(12M)-C(126)-H(12O)	109.5
C(42)-C(43)-H(43A)	118.7	H(12N)-C(126)-H(12O)	109.5
C(45)-C(44)-C(43)	122.5	C(41)-C(36)-C(37)	114.0
C(45)-C(44)-H(44A)	118.7	C(41)-C(36)-C(7)	132(3)
C(43)-C(44)-H(44A)	118.7	C(37)-C(36)-C(7)	114(3)
C(44)-C(45)-C(46)	115.1	C(38)-C(37)-C(36)	122.6
C(44)-C(45)-C(123)	123.1	C(38)-C(37)-H(37A)	118.7
C(46)-C(45)-C(123)	121.9	C(36)-C(37)-H(37A)	118.7
C(47)-C(46)-C(45)	122.5	C(39)-C(38)-C(37)	122.5
C(47)-C(46)-H(46A)	118.7	C(39)-C(38)-H(38A)	118.7
C(45)-C(46)-H(46A)	118.7	C(37)-C(38)-H(38A)	118.7
C(42)-C(47)-C(46)	123.3	C(38)-C(39)-C(40)	115.1
C(42)-C(47)-H(47A)	118.4	C(38)-C(39)-C(119)	123.0
C(46)-C(47)-H(47A)	118.4	C(40)-C(39)-C(119)	121.9
C(125)-C(123)-C(124)	124.1	C(41)-C(40)-C(39)	122.5
C(125)-C(123)-C(45)	108.9	C(41)-C(40)-H(40A)	118.7
C(124)-C(123)-C(45)	110.0	C(39)-C(40)-H(40A)	118.7
C(125)-C(123)-C(126)	100.1	C(36)-C(41)-C(40)	123.3
C(124)-C(123)-C(126)	102.3	C(36)-C(41)-H(41A)	118.3
C(45)-C(123)-C(126)	110.2	C(40)-C(41)-H(41A)	118.3
C(123)-C(124)-H(12G)	109.5	C(121)-C(119)-C(120)	124.1
C(123)-C(124)-H(12H)	109.5	C(121)-C(119)-C(39)	108.9

C(120)-C(119)-C(39)	110.0	Au(5)-Au(1)-Au(6)	111.54(5)
C(121)-C(119)-C(122)	100.1	S(4)-Au(1)-Au(7)	88.11(18)
C(120)-C(119)-C(122)	102.3	Au(8)-Au(1)-Au(7)	91.07(4)
C(39)-C(119)-C(122)	110.2	Au(6)#1-Au(1)-Au(7)	119.81(5)
C(119)-C(120)-H(12P)	109.5	Au(2)-Au(1)-Au(7)	59.56(4)
C(119)-C(120)-H(12Q)	109.5	Au(5)-Au(1)-Au(7)	174.81(5)
H(12P)-C(120)-H(12Q)	109.5	Au(6)-Au(1)-Au(7)	64.47(4)
C(119)-C(120)-H(12R)	109.5	S(4)-Au(1)-Au(4)	95.25(19)
H(12P)-C(120)-H(12R)	109.5	Au(8)-Au(1)-Au(4)	58.59(4)
H(12Q)-C(120)-H(12R)	109.5	Au(6)#1-Au(1)-Au(4)	89.69(5)
C(119)-C(121)-H(12S)	109.5	Au(2)-Au(1)-Au(4)	118.71(5)
C(119)-C(121)-H(12T)	109.5	Au(5)-Au(1)-Au(4)	62.83(4)
H(12S)-C(121)-H(12T)	109.5	Au(6)-Au(1)-Au(4)	173.11(5)
C(119)-C(121)-H(12U)	109.5	Au(7)-Au(1)-Au(4)	121.39(5)
H(12S)-C(121)-H(12U)	109.5	S(4)-Au(1)-Au(2)#1	89.12(19)
H(12T)-C(121)-H(12U)	109.5	Au(8)-Au(1)-Au(2)#1	119.64(5)
C(119)-C(122)-H(12V)	109.5	Au(6)#1-Au(1)-Au(2)#1	58.71(4)
C(119)-C(122)-H(12W)	109.5	Au(2)-Au(1)-Au(2)#1	86.78(5)
H(12V)-C(122)-H(12W)	109.5	Au(5)-Au(1)-Au(2)#1	61.05(4)
C(119)-C(122)-H(12X)	109.5	Au(6)-Au(1)-Au(2)#1	50.54(3)
H(12V)-C(122)-H(12X)	109.5	Au(7)-Au(1)-Au(2)#1	115.00(5)
H(12W)-C(122)-H(12X)	109.5	Au(4)-Au(1)-Au(2)#1	123.53(4)
S(4)-Au(1)-Au(8)	148.2(2)	S(10)-Au(2)-Au(8)	131.2(2)
S(4)-Au(1)-Au(6)#1	143.34(19)	S(10)-Au(2)-Au(1)	166.4(2)
Au(8)-Au(1)-Au(6)#1	61.07(4)	Au(8)-Au(2)-Au(1)	59.11(4)
S(4)-Au(1)-Au(2)	141.41(19)	S(10)-Au(2)-Au(6)#1	131.51(19)
Au(8)-Au(1)-Au(2)	60.12(4)	Au(8)-Au(2)-Au(6)#1	60.42(4)
Au(6)#1-Au(1)-Au(2)	60.32(4)	Au(1)-Au(2)-Au(6)#1	59.43(4)
S(4)-Au(1)-Au(5)	88.46(18)	S(10)-Au(2)-Au(6)	103.1(2)
Au(8)-Au(1)-Au(5)	93.90(5)	Au(8)-Au(2)-Au(6)	125.60(5)
Au(6)#1-Au(1)-Au(5)	61.77(4)	Au(1)-Au(2)-Au(6)	66.97(4)
Au(2)-Au(1)-Au(5)	122.03(5)	Au(6)#1-Au(2)-Au(6)	87.14(4)
S(4)-Au(1)-Au(6)	88.40(19)	S(10)-Au(2)-Au(7)	99.85(19)
Au(8)-Au(1)-Au(6)	119.70(5)	Au(8)-Au(2)-Au(7)	95.72(5)
Au(6)#1-Au(1)-Au(6)	83.92(5)	Au(1)-Au(2)-Au(7)	68.33(4)
Au(2)-Au(1)-Au(6)	60.00(4)	Au(6)#1-Au(2)-Au(7)	127.68(5)

Au(6)-Au(2)-Au(7)	69.63(4)	S(2)-Au(3)-Au(12)	79.29(19)
S(10)-Au(2)-Au(5)#1	45.32(19)	Au(8)-Au(3)-Au(12)	63.12(4)
Au(8)-Au(2)-Au(5)#1	176.25(6)	Au(11)-Au(3)-Au(12)	124.71(5)
Au(1)-Au(2)-Au(5)#1	124.57(5)	Au(10)-Au(3)-Au(12)	64.11(4)
Au(6)#1-Au(2)-Au(5)#1	120.11(5)	Au(7)-Au(3)-Au(12)	114.92(5)
Au(6)-Au(2)-Au(5)#1	57.95(4)	Au(9)-Au(3)-Au(12)	169.84(6)
Au(7)-Au(2)-Au(5)#1	86.71(4)	S(5)-Au(4)-S(8)	172.6(3)
S(10)-Au(2)-Au(1)#1	87.01(19)	S(5)-Au(4)-Au(8)	97.7(2)
Au(8)-Au(2)-Au(1)#1	123.10(4)	S(8)-Au(4)-Au(8)	88.8(2)
Au(1)-Au(2)-Au(1)#1	93.22(5)	S(5)-Au(4)-Au(1)	94.11(19)
Au(6)#1-Au(2)-Au(1)#1	62.70(4)	S(8)-Au(4)-Au(1)	92.7(2)
Au(6)-Au(2)-Au(1)#1	51.43(4)	Au(8)-Au(4)-Au(1)	51.58(4)
Au(7)-Au(2)-Au(1)#1	120.46(5)	S(5)-Au(4)-Au(5)	139.7(2)
Au(5)#1-Au(2)-Au(1)#1	57.46(3)	S(8)-Au(4)-Au(5)	44.0(2)
S(5)-Au(3)-S(2)	177.9(3)	Au(8)-Au(4)-Au(5)	85.87(4)
S(5)-Au(3)-Au(8)	91.11(19)	Au(1)-Au(4)-Au(5)	57.14(3)
S(2)-Au(3)-Au(8)	86.94(18)	S(8)-Au(5)-S(10)#1	173.0(3)
S(5)-Au(3)-Au(11)	84.78(19)	S(8)-Au(5)-Au(6)#1	83.9(2)
S(2)-Au(3)-Au(11)	97.27(18)	S(10)#1-Au(5)-Au(6)#1	102.61(19)
Au(8)-Au(3)-Au(11)	171.62(6)	S(8)-Au(5)-Au(1)	95.18(19)
S(5)-Au(3)-Au(10)	91.20(19)	S(10)#1-Au(5)-Au(1)	90.94(17)
S(2)-Au(3)-Au(10)	89.30(19)	Au(6)#1-Au(5)-Au(1)	52.38(4)
Au(8)-Au(3)-Au(10)	126.86(5)	S(8)-Au(5)-Au(2)#1	140.2(2)
Au(11)-Au(3)-Au(10)	60.67(4)	S(10)#1-Au(5)-Au(2)#1	46.34(19)
S(5)-Au(3)-Au(7)	136.6(2)	Au(6)#1-Au(5)-Au(2)#1	56.39(4)
S(2)-Au(3)-Au(7)	43.90(19)	Au(1)-Au(5)-Au(2)#1	61.49(4)
Au(8)-Au(3)-Au(7)	81.81(4)	S(8)-Au(5)-Au(4)	43.91(19)
Au(11)-Au(3)-Au(7)	96.17(4)	S(10)#1-Au(5)-Au(4)	138.75(19)
Au(10)-Au(3)-Au(7)	126.98(5)	Au(6)#1-Au(5)-Au(4)	83.08(4)
S(5)-Au(3)-Au(9)	87.1(2)	Au(1)-Au(5)-Au(4)	60.03(4)
S(2)-Au(3)-Au(9)	94.28(19)	Au(2)#1-Au(5)-Au(4)	121.19(4)
Au(8)-Au(3)-Au(9)	109.00(5)	S(9)-Au(6)-Au(1)#1	161.7(2)
Au(11)-Au(3)-Au(9)	63.57(4)	S(9)-Au(6)-Au(2)#1	135.6(2)
Au(10)-Au(3)-Au(9)	124.13(5)	Au(1)#1-Au(6)-Au(2)#1	60.25(4)
Au(7)-Au(3)-Au(9)	55.97(4)	S(9)-Au(6)-Au(8)#1	133.2(2)
S(5)-Au(3)-Au(12)	99.1(2)	Au(1)#1-Au(6)-Au(8)#1	59.05(4)

Au(2)#1-Au(6)-Au(8)#1	59.44(4)	Au(2)-Au(8)-Au(6)#1	60.14(4)
S(9)-Au(6)-Au(2)	97.4(2)	S(3)-Au(8)-Au(4)	101.2(2)
Au(1)#1-Au(6)-Au(2)	69.86(4)	Au(1)-Au(8)-Au(4)	69.83(4)
Au(2)#1-Au(6)-Au(2)	92.86(4)	Au(2)-Au(8)-Au(4)	130.60(5)
Au(8)#1-Au(6)-Au(2)	128.76(5)	Au(6)#1-Au(8)-Au(4)	95.46(5)
S(9)-Au(6)-Au(5)#1	97.3(2)	S(3)-Au(8)-Au(3)	100.7(2)
Au(1)#1-Au(6)-Au(5)#1	65.85(4)	Au(1)-Au(8)-Au(3)	72.38(4)
Au(2)#1-Au(6)-Au(5)#1	126.04(5)	Au(2)-Au(8)-Au(3)	94.73(4)
Au(8)#1-Au(6)-Au(5)#1	95.21(5)	Au(6)#1-Au(8)-Au(3)	132.13(5)
Au(2)-Au(6)-Au(5)#1	65.66(4)	Au(4)-Au(8)-Au(3)	69.64(4)
S(9)-Au(6)-Au(1)	85.6(2)	S(6)-Au(9)-S(4)	170.9(3)
Au(1)#1-Au(6)-Au(1)	96.08(5)	S(6)-Au(9)-Au(7)	92.9(2)
Au(2)#1-Au(6)-Au(1)	66.76(4)	S(4)-Au(9)-Au(7)	92.16(19)
Au(8)#1-Au(6)-Au(1)	126.17(5)	S(6)-Au(9)-Au(3)	90.3(2)
Au(2)-Au(6)-Au(1)	53.03(4)	S(4)-Au(9)-Au(3)	98.72(18)
Au(5)#1-Au(6)-Au(1)	118.40(5)	Au(7)-Au(9)-Au(3)	62.01(4)
S(9)-Au(7)-S(2)	175.0(3)	S(7)-Au(10)-S(1)	177.1(3)
S(9)-Au(7)-Au(2)	97.63(19)	S(7)-Au(10)-Au(3)	89.8(2)
S(2)-Au(7)-Au(2)	87.23(18)	S(1)-Au(10)-Au(3)	93.1(2)
S(9)-Au(7)-Au(9)	78.2(2)	S(7)-Au(10)-Au(11)	139.0(2)
S(2)-Au(7)-Au(9)	100.3(2)	S(1)-Au(10)-Au(11)	43.4(2)
Au(2)-Au(7)-Au(9)	118.69(5)	Au(3)-Au(10)-Au(11)	59.46(4)
S(9)-Au(7)-Au(1)	84.59(19)	S(6)-Au(11)-S(1)	175.5(3)
S(2)-Au(7)-Au(1)	99.20(17)	S(6)-Au(11)-Au(3)	91.1(2)
Au(2)-Au(7)-Au(1)	52.12(3)	S(1)-Au(11)-Au(3)	93.3(2)
Au(9)-Au(7)-Au(1)	66.67(4)	S(6)-Au(11)-Au(10)	139.7(2)
S(9)-Au(7)-Au(3)	136.4(2)	S(1)-Au(11)-Au(10)	43.2(2)
S(2)-Au(7)-Au(3)	44.37(18)	Au(3)-Au(11)-Au(10)	59.87(4)
Au(2)-Au(7)-Au(3)	87.16(4)	S(3)-Au(12)-S(7)	172.5(3)
Au(9)-Au(7)-Au(3)	62.02(4)	S(3)-Au(12)-Au(3)	96.1(2)
Au(1)-Au(7)-Au(3)	64.50(4)	S(7)-Au(12)-Au(3)	87.6(2)
S(3)-Au(8)-Au(1)	170.0(2)	C(8)-S(1)-Au(10)	106.0(14)
S(3)-Au(8)-Au(2)	128.0(2)	C(8)-S(1)-Au(11)	105.9(14)
Au(1)-Au(8)-Au(2)	60.77(4)	Au(10)-S(1)-Au(11)	93.3(4)
S(3)-Au(8)-Au(6)#1	127.1(2)	C(9)-S(2)-Au(7)	106.0(11)
Au(1)-Au(8)-Au(6)#1	59.88(4)	C(9)-S(2)-Au(3)	108.2(12)

Au(7)-S(2)-Au(3)	91.7(3)	H(2A)-C(2)-H(2B)	106.8
C(3)-S(3)-Au(12)	101.0(11)	C(54)-C(3)-S(3)	111(2)
C(3)-S(3)-Au(8)	99.8(11)	C(54)-C(3)-H(3A)	109.5
Au(12)-S(3)-Au(8)	96.6(3)	S(3)-C(3)-H(3A)	109.5
C(1)-S(4)-Au(9)	104.3(10)	C(54)-C(3)-H(3B)	109.5
C(1)-S(4)-Au(1)	107.1(11)	S(3)-C(3)-H(3B)	109.5
Au(9)-S(4)-Au(1)	97.2(3)	H(3A)-C(3)-H(3B)	108.0
C(4)-S(5)-Au(4)	103.5(9)	C(60)-C(4)-S(5)	111.5(19)
C(4)-S(5)-Au(3)	102.9(9)	C(60)-C(4)-H(4A)	109.3
Au(4)-S(5)-Au(3)	98.9(3)	S(5)-C(4)-H(4A)	109.3
C(6)-S(6)-Au(11)	105.6(13)	C(60)-C(4)-H(4B)	109.3
C(6)-S(6)-Au(9)	104.7(12)	S(5)-C(4)-H(4B)	109.3
Au(11)-S(6)-Au(9)	98.8(3)	H(4A)-C(4)-H(4B)	108.0
C(7)-S(7)-Au(10)	103.1(12)	C(48)-C(5)-S(10)	110(2)
C(7)-S(7)-Au(12)	109.0(10)	C(48)-C(5)-H(5A)	109.8
Au(10)-S(7)-Au(12)	101.8(4)	S(10)-C(5)-H(5A)	109.8
C(2)-S(8)-Au(4)	101.6(11)	C(48)-C(5)-H(5B)	109.8
C(2)-S(8)-Au(5)	105.3(13)	S(10)-C(5)-H(5B)	109.8
Au(4)-S(8)-Au(5)	92.1(3)	H(5A)-C(5)-H(5B)	108.2
C(10)-S(9)-Au(7)	108.3(14)	C(66)-C(6)-S(6)	111(3)
C(10)-S(9)-Au(6)	108.8(12)	C(66)-C(6)-H(6A)	109.5
Au(7)-S(9)-Au(6)	95.0(3)	S(6)-C(6)-H(6A)	109.5
C(5)-S(10)-Au(5)#1	105.3(13)	C(66)-C(6)-H(6B)	109.5
C(5)-S(10)-Au(2)	108.1(12)	S(6)-C(6)-H(6B)	109.5
Au(5)#1-S(10)-Au(2)	88.3(3)	H(6A)-C(6)-H(6B)	108.1
C(24)-C(1)-S(4)	102.5(19)	C(36)-C(7)-S(7)	105(2)
C(24)-C(1)-H(1A)	111.3	C(36)-C(7)-H(7A)	110.7
S(4)-C(1)-H(1A)	111.3	S(7)-C(7)-H(7A)	110.7
C(24)-C(1)-H(1B)	111.3	C(36)-C(7)-H(7B)	110.7
S(4)-C(1)-H(1B)	111.3	S(7)-C(7)-H(7B)	110.7
H(1A)-C(1)-H(1B)	109.2	H(7A)-C(7)-H(7B)	108.8
C(30)-C(2)-S(8)	121(2)	C(42)-C(8)-S(1)	113(3)
C(30)-C(2)-H(2A)	107.2	C(42)-C(8)-H(8A)	109.1
S(8)-C(2)-H(2A)	107.2	S(1)-C(8)-H(8A)	109.1
C(30)-C(2)-H(2B)	107.2	C(42)-C(8)-H(8B)	109.1
S(8)-C(2)-H(2B)	107.2	S(1)-C(8)-H(8B)	109.1

H(8A)-C(8)-H(8B)	107.8	C(18)-C(19)-H(19A)	119.9
C(12)-C(9)-S(2)	110(2)	C(21)-C(20)-C(19)	120.1(16)
C(12)-C(9)-H(9A)	109.6	C(21)-C(20)-H(20A)	119.9
S(2)-C(9)-H(9A)	109.6	C(19)-C(20)-H(20A)	119.9
C(12)-C(9)-H(9B)	109.6	C(20)-C(21)-C(22)	119.9(16)
S(2)-C(9)-H(9B)	109.6	C(20)-C(21)-C(115)	117(4)
H(9A)-C(9)-H(9B)	108.1	C(22)-C(21)-C(115)	123(4)
C(18)-C(10)-S(9)	112(3)	C(23)-C(22)-C(21)	119.9(17)
C(18)-C(10)-H(10A)	109.2	C(23)-C(22)-H(22A)	120.0
S(9)-C(10)-H(10A)	109.2	C(21)-C(22)-H(22A)	120.0
C(18)-C(10)-H(10B)	109.2	C(22)-C(23)-C(18)	120.0(16)
S(9)-C(10)-H(10B)	109.2	C(22)-C(23)-H(23A)	120.0
H(10A)-C(10)-H(10B)	107.9	C(18)-C(23)-H(23A)	120.0
C(13)-C(12)-C(17)	120.2(16)	C(35)-C(30)-C(31)	119.8(16)
C(13)-C(12)-C(9)	118(3)	C(35)-C(30)-C(2)	122(3)
C(17)-C(12)-C(9)	122(3)	C(31)-C(30)-C(2)	118(3)
C(12)-C(13)-C(14)	120.3(16)	C(32)-C(31)-C(30)	119.7(16)
C(12)-C(13)-H(13D)	119.9	C(32)-C(31)-H(31A)	120.1
C(14)-C(13)-H(13D)	119.9	C(30)-C(31)-H(31A)	120.1
C(15)-C(14)-C(13)	119.2(16)	C(31)-C(32)-C(33)	120.5(16)
C(15)-C(14)-H(14A)	120.4	C(31)-C(32)-H(32A)	119.7
C(13)-C(14)-H(14A)	120.4	C(33)-C(32)-H(32A)	119.7
C(16)-C(15)-C(14)	120.6(16)	C(32)-C(33)-C(34)	120.0(16)
C(16)-C(15)-C(131)	118(4)	C(32)-C(33)-C(76)	118(3)
C(14)-C(15)-C(131)	121(4)	C(34)-C(33)-C(76)	122(3)
C(15)-C(16)-C(17)	120.2(16)	C(33)-C(34)-C(35)	119.3(16)
C(15)-C(16)-H(16A)	119.9	C(33)-C(34)-H(34A)	120.4
C(17)-C(16)-H(16A)	119.9	C(35)-C(34)-H(34A)	120.4
C(16)-C(17)-C(12)	119.3(16)	C(30)-C(35)-C(34)	120.5(15)
C(16)-C(17)-H(17A)	120.3	C(30)-C(35)-H(35A)	119.8
C(12)-C(17)-H(17A)	120.3	C(34)-C(35)-H(35A)	119.8
C(19)-C(18)-C(23)	119.5(16)	C(49)-C(48)-C(53)	119.1(15)
C(19)-C(18)-C(10)	117(3)	C(49)-C(48)-C(5)	118(3)
C(23)-C(18)-C(10)	124(3)	C(53)-C(48)-C(5)	123(3)
C(20)-C(19)-C(18)	120.2(16)	C(48)-C(49)-C(50)	120.1(16)
C(20)-C(19)-H(19A)	119.9	C(48)-C(49)-H(49A)	120.0

C(50)-C(49)-H(49A)	120.0	C(62)-C(61)-H(61A)	119.4
C(51)-C(50)-C(49)	120.8(16)	C(61)-C(62)-C(63)	119.5(15)
C(51)-C(50)-H(50A)	119.6	C(61)-C(62)-H(62A)	120.3
C(49)-C(50)-H(50A)	119.6	C(63)-C(62)-H(62A)	120.3
C(50)-C(51)-C(52)	118.8(16)	C(64)-C(63)-C(62)	119.0(15)
C(50)-C(51)-C(107)	125(4)	C(64)-C(63)-C(72)	122(3)
C(52)-C(51)-C(107)	116(4)	C(62)-C(63)-C(72)	119(3)
C(53)-C(52)-C(51)	120.1(16)	C(65)-C(64)-C(63)	121.2(15)
C(53)-C(52)-H(52A)	120.0	C(65)-C(64)-H(64A)	119.4
C(51)-C(52)-H(52A)	120.0	C(63)-C(64)-H(64A)	119.4
C(52)-C(53)-C(48)	121.0(16)	C(64)-C(65)-C(60)	119.8(15)
C(52)-C(53)-H(53A)	119.5	C(64)-C(65)-H(65A)	120.1
C(48)-C(53)-H(53A)	119.5	C(60)-C(65)-H(65A)	120.1
C(59)-C(54)-C(55)	119.0(15)	C(67)-C(66)-C(71)	120.3(16)
C(59)-C(54)-C(3)	119(3)	C(67)-C(66)-C(6)	115(3)
C(55)-C(54)-C(3)	121(3)	C(71)-C(66)-C(6)	124(3)
C(54)-C(55)-C(56)	121.0(15)	C(66)-C(67)-C(68)	119.7(16)
C(54)-C(55)-H(55A)	119.5	C(66)-C(67)-H(67A)	120.1
C(56)-C(55)-H(55A)	119.5	C(68)-C(67)-H(67A)	120.1
C(55)-C(56)-C(57)	119.8(15)	C(69)-C(68)-C(67)	119.5(16)
C(55)-C(56)-H(56A)	120.1	C(69)-C(68)-H(68A)	120.2
C(57)-C(56)-H(56A)	120.1	C(67)-C(68)-H(68A)	120.2
C(58)-C(57)-C(56)	118.7(15)	C(70)-C(69)-C(68)	120.4(16)
C(58)-C(57)-C(101)	122(3)	C(70)-C(69)-C(88)	124(3)
C(56)-C(57)-C(101)	120(3)	C(68)-C(69)-C(88)	116(3)
C(57)-C(58)-C(59)	121.1(15)	C(69)-C(70)-C(71)	120.1(16)
C(57)-C(58)-H(58A)	119.4	C(69)-C(70)-H(70A)	120.0
C(59)-C(58)-H(58A)	119.4	C(71)-C(70)-H(70A)	120.0
C(54)-C(59)-C(58)	120.1(15)	C(66)-C(71)-C(70)	119.8(16)
C(54)-C(59)-H(59A)	120.0	C(66)-C(71)-H(71A)	120.1
C(58)-C(59)-H(59A)	120.0	C(70)-C(71)-H(71A)	120.1
C(61)-C(60)-C(65)	119.3(14)	C(73)-C(72)-C(74)	98(4)
C(61)-C(60)-C(4)	124(2)	C(73)-C(72)-C(75)	127(5)
C(65)-C(60)-C(4)	117(2)	C(74)-C(72)-C(75)	110(4)
C(60)-C(61)-C(62)	121.2(15)	C(73)-C(72)-C(63)	103(4)
C(60)-C(61)-H(61A)	119.4	C(74)-C(72)-C(63)	111(4)

C(75)-C(72)-C(63)	108(4)	H(78B)-C(78)-H(78C)	109.5
C(72)-C(73)-H(73A)	109.5	C(76)-C(79)-H(79A)	109.5
C(72)-C(73)-H(73B)	109.5	C(76)-C(79)-H(79B)	109.5
H(73A)-C(73)-H(73B)	109.5	H(79A)-C(79)-H(79B)	109.5
C(72)-C(73)-H(73C)	109.5	C(76)-C(79)-H(79C)	109.5
H(73A)-C(73)-H(73C)	109.5	H(79A)-C(79)-H(79C)	109.5
H(73B)-C(73)-H(73C)	109.5	H(79B)-C(79)-H(79C)	109.5
C(72)-C(74)-H(74A)	109.5	C(107)-C(83)-H(83A)	109.5
C(72)-C(74)-H(74B)	109.5	C(107)-C(83)-H(83B)	109.5
H(74A)-C(74)-H(74B)	109.5	H(83A)-C(83)-H(83B)	109.5
C(72)-C(74)-H(74C)	109.5	C(107)-C(83)-H(83C)	109.5
H(74A)-C(74)-H(74C)	109.5	H(83A)-C(83)-H(83C)	109.5
H(74B)-C(74)-H(74C)	109.5	H(83B)-C(83)-H(83C)	109.5
C(72)-C(75)-H(75A)	109.5	C(107)-C(84)-H(84A)	109.5
C(72)-C(75)-H(75B)	109.5	C(107)-C(84)-H(84B)	109.5
H(75A)-C(75)-H(75B)	109.5	H(84A)-C(84)-H(84B)	109.5
C(72)-C(75)-H(75C)	109.5	C(107)-C(84)-H(84C)	109.5
H(75A)-C(75)-H(75C)	109.5	H(84A)-C(84)-H(84C)	109.5
H(75B)-C(75)-H(75C)	109.5	H(84B)-C(84)-H(84C)	109.5
C(79)-C(76)-C(77)	108(5)	C(107)-C(85)-H(85A)	109.5
C(79)-C(76)-C(33)	113(5)	C(107)-C(85)-H(85B)	109.5
C(77)-C(76)-C(33)	124(5)	H(85A)-C(85)-H(85B)	109.5
C(79)-C(76)-C(78)	106(5)	C(107)-C(85)-H(85C)	109.5
C(77)-C(76)-C(78)	94(5)	H(85A)-C(85)-H(85C)	109.5
C(33)-C(76)-C(78)	108(4)	H(85B)-C(85)-H(85C)	109.5
C(76)-C(77)-H(77A)	109.5	C(88)-C(86)-H(86A)	109.5
C(76)-C(77)-H(77B)	109.5	C(88)-C(86)-H(86B)	109.5
H(77A)-C(77)-H(77B)	109.5	H(86A)-C(86)-H(86B)	109.5
C(76)-C(77)-H(77C)	109.5	C(88)-C(86)-H(86C)	109.5
H(77A)-C(77)-H(77C)	109.5	H(86A)-C(86)-H(86C)	109.5
H(77B)-C(77)-H(77C)	109.5	H(86B)-C(86)-H(86C)	109.5
C(76)-C(78)-H(78A)	109.5	C(88)-C(87)-H(87A)	109.5
C(76)-C(78)-H(78B)	109.5	C(88)-C(87)-H(87B)	109.5
H(78A)-C(78)-H(78B)	109.5	H(87A)-C(87)-H(87B)	109.5
C(76)-C(78)-H(78C)	109.5	C(88)-C(87)-H(87C)	109.5
H(78A)-C(78)-H(78C)	109.5	H(87A)-C(87)-H(87C)	109.5

H(87B)-C(87)-H(87C)	109.5	H(10J)-C(103)-H(10K)	109.5
C(87)-C(88)-C(104)	107(4)	C(85)-C(107)-C(84)	130(7)
C(87)-C(88)-C(86)	106(4)	C(85)-C(107)-C(83)	102(6)
C(104)-C(88)-C(86)	105(4)	C(84)-C(107)-C(83)	96(6)
C(87)-C(88)-C(69)	109(5)	C(85)-C(107)-C(51)	105(6)
C(104)-C(88)-C(69)	112(6)	C(84)-C(107)-C(51)	117(6)
C(86)-C(88)-C(69)	118(7)	C(83)-C(107)-C(51)	102(5)
C(101)-C(91)-H(91A)	109.5	C(118)-C(115)-C(117)	116(3)
C(101)-C(91)-H(91B)	109.5	C(118)-C(115)-C(116)	116(3)
H(91A)-C(91)-H(91B)	109.5	C(117)-C(115)-C(116)	117(3)
C(101)-C(91)-H(91C)	109.5	C(118)-C(115)-C(21)	114(7)
H(91A)-C(91)-H(91C)	109.5	C(117)-C(115)-C(21)	94(7)
H(91B)-C(91)-H(91C)	109.5	C(116)-C(115)-C(21)	94(7)
C(101)-C(102)-H(10C)	109.5	C(115)-C(116)-H(11A)	109.5
C(101)-C(102)-H(10D)	109.5	C(115)-C(116)-H(11B)	109.5
H(10C)-C(102)-H(10D)	109.5	H(11A)-C(116)-H(11B)	109.5
C(101)-C(102)-H(10E)	109.5	C(115)-C(116)-H(11C)	109.4
H(10C)-C(102)-H(10E)	109.5	H(11A)-C(116)-H(11C)	109.5
H(10D)-C(102)-H(10E)	109.5	H(11B)-C(116)-H(11C)	109.5
C(88)-C(104)-H(10F)	109.5	C(115)-C(117)-H(11D)	109.5
C(88)-C(104)-H(10G)	109.5	C(115)-C(117)-H(11E)	109.5
H(10F)-C(104)-H(10G)	109.5	H(11D)-C(117)-H(11E)	109.5
C(88)-C(104)-H(10H)	109.5	C(115)-C(117)-H(11F)	109.4
H(10F)-C(104)-H(10H)	109.5	H(11D)-C(117)-H(11F)	109.5
H(10G)-C(104)-H(10H)	109.5	H(11E)-C(117)-H(11F)	109.5
C(91)-C(101)-C(102)	102(6)	C(115)-C(118)-H(11G)	109.5
C(91)-C(101)-C(103)	96(6)	C(115)-C(118)-H(11H)	109.5
C(102)-C(101)-C(103)	107(6)	H(11G)-C(118)-H(11H)	109.5
C(91)-C(101)-C(57)	116(6)	C(115)-C(118)-H(11I)	109.4
C(102)-C(101)-C(57)	117(5)	H(11G)-C(118)-H(11I)	109.5
C(103)-C(101)-C(57)	117(5)	H(11H)-C(118)-H(11I)	109.5
C(101)-C(103)-H(10I)	109.5	C(134)-C(131)-C(132)	115(3)
C(101)-C(103)-H(10J)	109.5	C(134)-C(131)-C(133)	115(3)
H(10I)-C(103)-H(10J)	109.5	C(132)-C(131)-C(133)	115(3)
C(101)-C(103)-H(10K)	109.5	C(134)-C(131)-C(15)	104(5)
H(10I)-C(103)-H(10K)	109.5	C(132)-C(131)-C(15)	99(5)

C(133)-C(131)-C(15)	105(7)	C(131)-C(133)-H(13J)	109.5
C(131)-C(132)-H(13E)	109.5	H(13H)-C(133)-H(13J)	109.5
C(131)-C(132)-H(13F)	109.4	H(13I)-C(133)-H(13J)	109.5
H(13E)-C(132)-H(13F)	109.5	C(131)-C(134)-H(13K)	109.5
C(131)-C(132)-H(13G)	109.5	C(131)-C(134)-H(13L)	109.4
H(13E)-C(132)-H(13G)	109.5	H(13K)-C(134)-H(13L)	109.5
H(13F)-C(132)-H(13G)	109.5	C(131)-C(134)-H(13M)	109.5
C(131)-C(133)-H(13H)	109.5	H(13K)-C(134)-H(13M)	109.5
C(131)-C(133)-H(13I)	109.4	H(13L)-C(134)-H(13M)	109.5
H(13H)-C(133)-H(13I)	109.5		

Symmetry transformations used to generate equivalent atoms:

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

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Au_{24}(SR)_{20}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(24)	80(20)	100(20)	100(20)	-29(18)	6(18)	-16(18)
C(25)	160(40)	170(40)	170(40)	-130(30)	20(30)	-40(30)
C(26)	250(60)	120(40)	220(60)	-90(40)	50(50)	-40(40)
C(27)	380(90)	110(30)	80(30)	-50(20)	30(40)	-40(40)
C(28)	200(50)	300(70)	140(40)	-140(50)	10(30)	-60(50)
C(29)	140(30)	170(40)	120(30)	-80(30)	0(20)	-50(30)
C(42)	230(40)	190(40)	130(30)	-40(30)	-40(30)	-90(30)
C(43)	240(40)	180(40)	160(30)	0(30)	-50(30)	-70(30)
C(44)	280(40)	230(40)	180(30)	0(30)	-60(30)	-50(40)
C(45)	300(40)	260(40)	190(40)	0(40)	-50(30)	-10(40)
C(46)	300(40)	220(40)	130(30)	-20(30)	-40(30)	-30(40)
C(47)	270(40)	180(40)	120(30)	0(30)	-30(30)	-60(40)
C(36)	140(30)	140(30)	140(30)	50(20)	-40(20)	-70(20)
C(37)	200(40)	190(30)	150(30)	50(30)	-10(30)	-70(30)
C(38)	250(40)	220(40)	160(30)	40(30)	0(30)	-80(40)
C(39)	250(40)	170(30)	180(40)	70(30)	-10(30)	-90(30)
C(40)	210(40)	160(30)	230(40)	50(30)	-20(30)	-40(30)
C(41)	180(30)	130(30)	230(40)	30(30)	-10(30)	-40(30)
Au(1)	95(1)	67(1)	73(1)	-15(1)	-19(1)	-22(1)
Au(2)	86(1)	62(1)	76(1)	-8(1)	-21(1)	-19(1)
Au(3)	89(1)	79(1)	79(1)	-11(1)	-16(1)	-18(1)
Au(4)	81(1)	74(1)	93(1)	-17(1)	-15(1)	-17(1)
Au(5)	91(1)	72(1)	83(1)	-7(1)	-9(1)	-23(1)
Au(6)	90(1)	70(1)	70(1)	-7(1)	-17(1)	-25(1)
Au(7)	96(1)	75(1)	71(1)	-7(1)	-14(1)	-22(1)
Au(8)	84(1)	74(1)	83(1)	-11(1)	-20(1)	-23(1)
Au(9)	106(1)	90(1)	80(1)	-19(1)	-15(1)	-21(1)
Au(10)	107(1)	109(1)	86(1)	-19(1)	-13(1)	-32(1)
Au(11)	124(1)	97(1)	85(1)	-25(1)	-8(1)	-30(1)
Au(12)	96(1)	114(1)	97(1)	-37(1)	-12(1)	-34(1)
S(1)	120(7)	129(7)	104(6)	-37(5)	-8(5)	-37(6)

S(2)	92(5)	80(4)	80(4)	-13(3)	-12(4)	-22(4)
S(3)	84(5)	114(6)	97(5)	-28(4)	-26(4)	-29(4)
S(4)	99(5)	91(5)	75(4)	-27(4)	-17(4)	-22(4)
S(5)	91(5)	87(5)	86(5)	-15(4)	-17(4)	-20(4)
S(6)	127(7)	106(6)	83(5)	-16(4)	-10(5)	-30(5)
S(7)	113(6)	125(7)	94(6)	-32(5)	-15(5)	-37(5)
S(8)	103(6)	86(5)	95(5)	-11(4)	-16(4)	-23(4)
S(9)	107(6)	108(6)	74(5)	-9(4)	-18(4)	-33(5)
S(10)	97(5)	73(4)	95(5)	-15(4)	-14(4)	-23(4)
C(1)	130(30)	78(19)	100(20)	-17(16)	-2(19)	-25(18)
C(2)	110(30)	90(20)	120(30)	0(20)	-20(20)	-8(19)
C(3)	120(30)	150(30)	100(20)	-60(20)	10(20)	-50(20)
C(4)	71(17)	82(18)	100(20)	-39(16)	-1(15)	-7(15)
C(5)	110(30)	63(19)	160(30)	9(19)	-10(20)	-27(19)
C(6)	170(30)	140(30)	80(20)	-30(20)	-40(20)	-60(30)
C(7)	140(30)	110(30)	90(20)	-26(19)	-10(20)	-40(20)
C(8)	170(40)	150(40)	100(30)	-40(30)	0(30)	-60(30)
C(9)	110(20)	140(30)	80(20)	-9(18)	0(17)	-70(20)
C(10)	140(30)	150(30)	90(30)	-30(20)	-30(20)	-10(30)
C(12)	120(30)	110(30)	100(20)	-10(20)	20(20)	-50(30)
C(13)	170(40)	90(30)	190(40)	20(30)	-80(30)	-40(30)
C(14)	340(90)	110(40)	190(50)	0(30)	-80(50)	-90(50)
C(15)	280(70)	60(20)	110(30)	30(20)	10(40)	10(30)
C(16)	200(50)	70(30)	240(60)	30(30)	0(40)	-30(30)
C(17)	120(40)	150(40)	180(40)	50(30)	-30(30)	-40(30)
C(18)	140(30)	140(40)	90(30)	0(20)	-50(30)	10(30)
C(19)	310(70)	160(50)	100(30)	10(30)	-50(40)	0(50)
C(20)	290(80)	270(80)	120(50)	30(50)	-20(50)	-80(60)
C(21)	330(90)	300(100)	80(40)	30(50)	40(50)	-30(70)
C(22)	410(100)	150(50)	110(40)	30(30)	-20(50)	20(60)
C(23)	190(40)	160(40)	80(30)	-10(30)	0(30)	20(30)
C(30)	89(18)	90(20)	160(30)	-29(18)	-18(16)	-7(16)
C(31)	93(16)	100(20)	210(30)	-70(20)	-1(19)	-8(17)
C(32)	110(20)	140(30)	220(30)	-90(20)	10(20)	-20(20)
C(33)	130(20)	110(20)	200(30)	-60(20)	0(20)	-30(20)
C(34)	120(19)	100(20)	190(30)	-43(19)	-20(20)	-30(20)

C(35)	93(18)	90(20)	180(30)	-36(18)	-17(19)	-8(16)
C(48)	100(20)	100(30)	110(30)	-20(20)	10(20)	-50(20)
C(49)	100(30)	110(30)	150(40)	10(20)	-20(30)	-10(20)
C(50)	170(50)	170(50)	130(40)	-30(40)	-20(30)	0(40)
C(51)	180(40)	110(30)	120(30)	10(30)	-20(30)	20(30)
C(52)	240(60)	120(40)	160(50)	-40(30)	30(40)	-70(40)
C(53)	160(40)	70(20)	170(40)	-30(30)	-30(30)	-20(20)
C(54)	100(20)	100(20)	110(30)	-55(19)	-30(20)	-16(19)
C(55)	100(30)	200(40)	120(30)	-50(30)	0(30)	-50(30)
C(56)	110(30)	190(40)	120(30)	-50(30)	-30(20)	-40(30)
C(57)	110(30)	180(40)	100(30)	-70(30)	20(20)	-60(30)
C(58)	60(20)	270(50)	130(30)	-90(30)	0(20)	-70(30)
C(59)	110(30)	160(30)	130(30)	-50(30)	-30(20)	-60(30)
C(60)	77(19)	90(20)	80(20)	-7(16)	-13(15)	-22(17)
C(61)	100(20)	140(30)	110(30)	-70(30)	-10(20)	10(20)
C(62)	90(20)	100(30)	170(40)	-60(30)	-30(30)	20(20)
C(63)	120(30)	130(30)	110(30)	-10(20)	-40(20)	-30(30)
C(64)	150(30)	120(30)	80(20)	-30(20)	-10(20)	-50(30)
C(65)	110(20)	80(20)	110(20)	-12(17)	-30(20)	-39(18)
C(66)	180(30)	140(30)	90(20)	-20(20)	-30(20)	-60(30)
C(67)	210(40)	220(40)	120(30)	10(30)	-20(30)	-50(30)
C(68)	220(40)	210(40)	110(30)	0(30)	-30(30)	-30(30)
C(69)	200(40)	150(30)	80(20)	-50(20)	20(20)	-40(30)
C(70)	170(30)	180(30)	110(30)	-20(20)	-10(20)	-20(30)
C(71)	170(30)	160(30)	130(30)	-30(20)	-20(30)	-30(30)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for $Au_{24}(SR)_{20}$.

	x	y	z	U(eq)
H(25A)	1799	6583	2258	180
H(26A)	1502	6788	3253	242
H(28A)	3802	7351	2769	237
H(29A)	4090	7167	1771	164
H(12A)	2972	8068	3432	622
H(12B)	2251	8049	4089	622
H(12C)	1962	8247	3394	622
H(12D)	3544	6638	4106	738
H(12E)	2775	6234	4330	738
H(12F)	2770	6719	4710	738
H(13A)	1337	7234	4608	963
H(13B)	1378	6691	4285	963
H(13C)	1036	7473	3911	963
H(43A)	294	3670	4734	244
H(44A)	959	2545	5171	296
H(46A)	-287	2046	4158	286
H(47A)	-930	3163	3708	249
H(12G)	1037	1168	4169	750
H(12H)	1705	676	4649	750
H(12I)	1843	1424	4200	750
H(12J)	-267	1047	5377	786
H(12K)	-2	1268	5891	786
H(12L)	500	576	5770	786
H(12M)	1835	847	5614	815
H(12N)	1281	1497	5799	815
H(12O)	2012	1578	5140	815
H(37A)	-2113	3570	2600	258
H(38A)	-2620	2756	3577	295
H(40A)	-792	1317	3020	291
H(41A)	-270	2124	2058	260

H(12P)	-909	786	4230	600
H(12Q)	-1623	691	4899	600
H(12R)	-1199	1346	4577	600
H(12S)	-2277	805	3615	771
H(12T)	-3113	1380	3699	771
H(12U)	-2897	723	4326	771
H(12V)	-3050	1382	4962	636
H(12W)	-3332	2006	4330	636
H(12X)	-2594	2019	4670	636
H(1A)	3281	7051	817	129
H(1B)	2481	6663	1185	129
H(2A)	2159	8104	-1338	144
H(2B)	1271	7841	-1037	144
H(3A)	2759	3827	-364	143
H(3B)	1926	3808	-598	143
H(4A)	116	5505	1023	103
H(4B)	-361	5706	1670	103
H(5A)	4235	2665	1404	152
H(5B)	3923	2381	959	152
H(6A)	3013	4976	3934	153
H(6B)	2040	5347	3822	153
H(7A)	-1258	3965	1678	141
H(7B)	-840	3505	1215	141
H(8A)	-937	4475	4265	170
H(8B)	-1470	4274	3889	170
H(9A)	2471	3212	2992	134
H(9B)	1585	3234	2797	134
H(10A)	6086	3066	1978	161
H(10B)	6409	3424	2348	161
H(13D)	1396	2319	2561	188
H(14A)	1785	1158	2684	253
H(16A)	4073	1023	3189	246
H(17A)	3698	2182	3055	213
H(19A)	6173	2009	2882	257
H(20A)	5587	1316	3933	307
H(22A)	4002	2968	4324	328

H(23A)	4478	3648	3230	205
H(31A)	413	7938	-73	166
H(32A)	113	8351	806	188
H(34A)	2570	8705	319	167
H(35A)	2875	8289	-566	156
H(49A)	5336	2017	2008	164
H(50A)	6352	1014	2373	206
H(52A)	6044	403	952	220
H(53A)	5066	1418	569	171
H(55A)	1699	4614	-1799	169
H(56A)	2421	4926	-2912	166
H(58A)	4719	4446	-2289	172
H(59A)	3989	4167	-1178	153
H(61A)	-1014	6988	1479	141
H(62A)	-1748	7981	774	149
H(64A)	-657	7289	-774	139
H(65A)	29	6287	-62	118
H(67A)	3301	3950	4825	245
H(68A)	2856	3255	5936	239
H(70A)	341	4237	5845	204
H(71A)	769	4885	4722	193
H(73A)	-2708	8514	-1128	356
H(73B)	-2736	7866	-466	356
H(73C)	-1958	7855	-1086	356
H(74A)	-1535	9125	-1489	341
H(74B)	-990	8385	-1447	341
H(74C)	-726	8807	-1111	341
H(75A)	-2515	9354	-446	286
H(75B)	-1713	9033	-61	286
H(75C)	-2589	8743	246	286
H(77A)	311	8920	2135	419
H(77B)	620	8180	2089	419
H(77C)	-176	8691	1751	419
H(78A)	241	9851	1309	387
H(78B)	-117	9610	857	387
H(78C)	722	9946	557	387

H(79A)	1554	9207	1727	365
H(79B)	2063	9322	978	365
H(79C)	2154	8581	1519	365
H(83A)	8373	-277	2121	411
H(83B)	7702	317	2345	411
H(83C)	8100	439	1574	411
H(84A)	7979	-844	1564	484
H(84B)	7866	-99	1028	484
H(84C)	7155	-544	1202	484
H(85A)	7139	-915	2751	424
H(85B)	6166	-582	2625	424
H(85C)	6672	-209	2853	424
H(86A)	1087	2172	7175	632
H(86B)	1821	2245	6519	632
H(86C)	817	2511	6459	632
H(87A)	297	3025	7447	324
H(87B)	32	3459	6735	324
H(87C)	475	3773	7074	324
H(91A)	4256	4963	-4345	533
H(91B)	3288	4945	-3927	533
H(91C)	4047	4295	-3743	533
H(10C)	5286	5044	-4066	403
H(10D)	5283	4387	-3413	403
H(10E)	5286	5092	-3366	403
H(10F)	1711	2632	7553	545
H(10G)	1873	3386	7189	545
H(10H)	2474	2799	6920	545
H(10I)	4136	5890	-4282	454
H(10J)	3913	6043	-3603	454
H(10K)	3185	5871	-3833	454
H(11A)	4404	1695	5813	750
H(11B)	4213	2373	5200	750
H(11C)	5179	1933	5213	750
H(11D)	3172	1398	5321	946
H(11E)	3502	1524	4543	946
H(11F)	3254	2140	4813	946

H(11G)	4655	587	5586	661
H(11H)	5485	848	5069	661
H(11I)	4779	671	4821	661
H(13E)	2661	-529	3613	565
H(13F)	2063	193	3321	565
H(13G)	2573	56	3896	565
H(13H)	4269	-515	3313	684
H(13I)	3955	35	3674	684
H(13J)	4467	226	2921	684
H(13K)	3508	-344	2462	481
H(13L)	3755	384	2106	481
H(13M)	2757	316	2308	481