Supporting Information

Novel Double-helical-kernel Evolution Pattern of Gold Nanoclusters: Alternate Single-standed Growth at Both Ends

Hongwei Dong,‡[a,b] Lingwen Liao,‡ [a] Shengli Zhuang,‡[a,b] Chuanhao Yao,[a] Jishi Chen,[a] Shubo Tian,[a] Min Zhu,[a b] Xu Liu,[a b] Lingling Li,[c] and Zhikun Wu*[a]

[a] Key Laboratory of Materials Physics, Anhui Key Laboratory of Nanomaterials and Nanotechnology, CAS Center for Excellence in Nanoscience, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei, Anhui 230031, China

[b] University of Science and Technology of China, Hefei, Anhui 230026, China

[c] Instrumental Analysis Center, Shanghai Jiaotong University, Shanghai 200240, China

Experimental

Chemicals

All chemicals and reagents are commercially available and used as received. The water used in all experiments was ultrapure (resistivity 18.2 MΩ cm), produced with a Milli-Q NANO pure water system. cyclohexanethiol (HS-c-C_6H_{11}, 97%, Aldrich), Sodiumborohydride ($NaBH_4$, 99.0%) were purchased from Sigma-Aldrich. Tetrachloroauric(III) acid ($HAuCl_4 \cdot 4H_2O$, 99.7%), tetrahydrofuran (THF, 99.0%), acetonitrile (CH_3CN, 99.0%), methanol (CH_3OH，99.5%), dichloromethane (AR), petroleum ether (AR) and toluene (99.5%) were purchased from Sinopharm chemical reagent co., ltd.

Synthesis of $Au_{34}(S\text{-}c\text{-}C_6H_{11})_{22}$ and $Au_{42}(S\text{-}c\text{-}C_6H_{11})_{26}$ nanoclusters.

The $Au_{34}(S\text{-}c\text{-}C_6H_{11})_{22}$ and $Au_{42}(S\text{-}c\text{-}C_6H_{11})_{26}$ clusters were synthesized by a two-step size focusing method with some modifications.[1]

Step 1: Synthesis of Aux(S-c-C_6H_{11})y. First, 0.125 mmol of $HAuCl_4$ was dissolved in 5 mL of THF, and the solution was cooled down to 0℃. Then, 0.625 mmol of cyclohexanethiol (5 equivalents per mole of Au) was added to the resulting solution. Approximately half an hour later, the color of the tetrahydrofuran phase changed from orange to light yellow, indicating that the Au(III) was reduced to Au(I). To ensure complete complex formation, the reaction was allowed to proceed for another half hour. Then, 1.25 mmol of $NaBH_4$ dissolved in 5 mL of cold nanopure H_2O was quickly poured into the Au-S-c-C_6H_{11} mixture under vigorous stirring. Approximately three hours later, the crude $Au_x(S\text{-}c\text{-}C_6H_{11})_y$ nanoclusters were precipitated out by the addition of excess methanol.

Step 2: The crude Aux(S-c-C_6H_{11})y nanoclusters obtained from step 1 and 310 μL of cyclohexanethiol were dissolved in 1.5 mL of dichloromethane. The solution was heated to 40℃ under gentle stirring. After 41 hours, the reaction was stopped by

adding excess methanol. This mixture was washed with methanol (4-10 times); during this procedure, the redundant cyclohexanethiol, inorganic salt traces and other byproducts were thoroughly removed through centrifugation at 8000 rpm for 2 min. Next, the crude products were separated by preparative thin layer chromatography (developing solvent: dichloromethane:petroleum ether = 1:3, V/V), and $Au_{34}(S\text{-}c\text{-}C_6H_{11})_{22}$ and $Au_{42}(S\text{-}c\text{-}C_6H_{11})_{26}$ nanoclusters were extracted with CH_2Cl_2 from the cut silica gel. Several days later, $Au_{34}(S\text{-}c\text{-}C_6H_{11})_{22}$ nanoclusters were recrystallized from a solution of toluene/acetonitrile, while $Au_{42}(S\text{-}c\text{-}C_6H_{11})_{26}$ nanoclusters were recrystallized from a solution of toluene/methanol at room temperature.

1 (a) Zeng, C.; Chen, Y.; Liu, C.; Nobusada, K.; Rosi, N. L.; Jin, R. *Sci. Adv.* **2015**, *1*, e1500425. (b) Zeng, C. J.; Liu, C.; Chen, Y. X.; Rosi, N. L.; Jin, R. C. *J. Am. Chem. Soc.* **2016**, *138*, 8710; (c) Zeng, C. J.; Chen, Y. X.; Iida, K.; Nobusada, K.; Kirschbaum, K.; Lambright, K. J.; Jin, R. C. *J. Am. Chem. Soc.* **2016**, *138*, 3950 (d) Liao, L.; Chen, J.; Wang, C.; Zhuang, S.; Yan, N.; Yao, C.; Xia, N.; Li, L.; Bao, X.; Wu, Z. *Chem. Commun.* **2016**, *52*, 12036; (e) Liao, L.; Yao, C.; Wang, C.; Tian, S.; Chen, J.; Li, M.-B.; Xia, N.; Yan, N.; Wu, Z. *Anal. Chem.* **2016**, *88*, 11297.

Figures

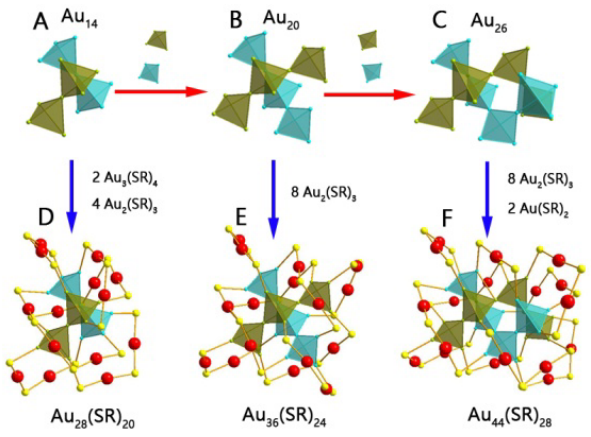

Figure S1. The kernel and total structures of $Au_{28}(TBBT)_{20}$, $Au_{36}(TBBT)_{24}$ and $Au_{44}(TBBT)_{28}$: Au_{14} kernel of $Au_{28}(TBBT)_{20}$ (A); Au_{20} kernel of $Au_{36}(TBBT)_{24}$ (B); Au_{26} kernel of $Au_{44}(TBBT)_{28}$ (C); $Au_{28}(TBBT)_{20}$ framework (D); $Au_{36}(TBBT)_{24}$ framework (E); and $Au_{44}(TBBT)_{28}$ framework (F). For clarity, C and H atoms are omitted. Color labels: yellow = S; others = Au.

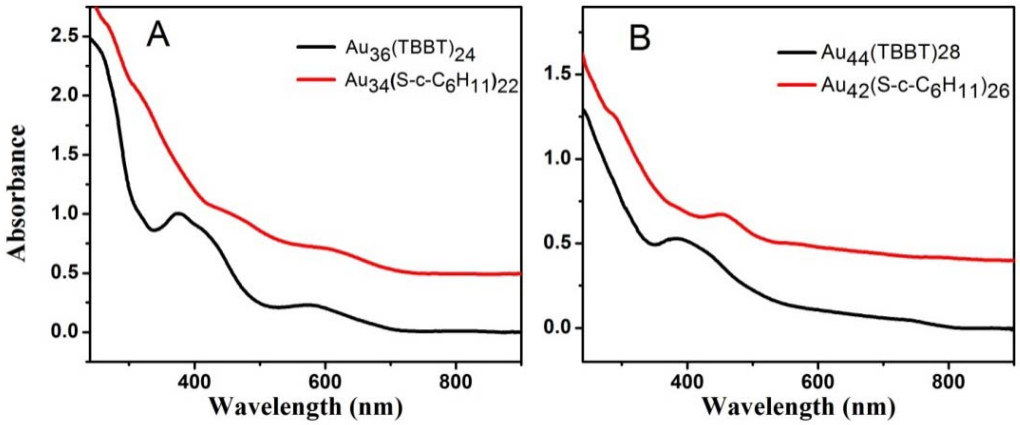

Figure S2. (A) Optical spectra of $Au_{36}(TBBT)_{24}$ (black profile) and $Au_{34}(S\text{-}c\text{-}C_6H_{11})_{22}$ (red); (B) Optical spectra of $Au_{44}(TBBT)_{28}$ (black profile) and $Au_{42}(S\text{-}c\text{-}C_6H_{11})_{26}$.

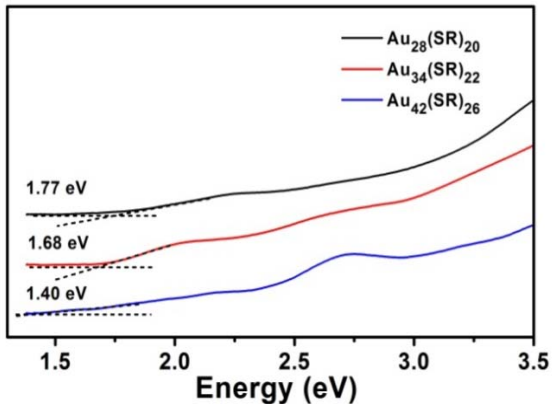

Figure S3. Photon-energy plot of $Au_{28}(S\text{-}c\text{-}C_6H_{11})_{20}$, $Au_{34}(S\text{-}c\text{-}C_6H_{11})_{22}$ and $Au_{42}(S\text{-}c\text{-}C_6H_{11})_{26}$.

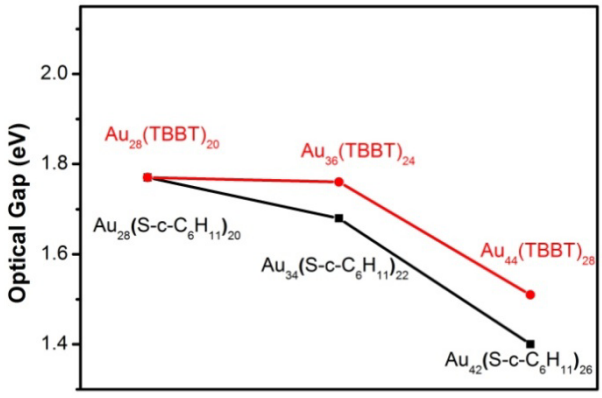

Figure S4. Optical gap comparison of the two series gold nanoclusters.

Instrumentation

UV-visible absorption spectroscopy

The UV/vis/NIR absorption spectra of the Au nanoclusters were acquired on a UV-2600 spectrophotometer (Shimadzu, Japan) in dichloromethane at room

temperature.

X-ray crystallography

The single crystal X-ray diffraction data of both $Au_{34}(S\text{-}c\text{-}C_6H_{11})_{22}$ and $Au_{42}(S\text{-}c\text{-}C_6H_{11})_{26}$ were collected on a Bruker D8 Venture Prospector Ultra equipped with an Apex II charge-coupled device detector and an ImSmicrofocus CuK_α x-ray source (λ= 1.54178 Å) under cold N_2 flow at 173 K.

Electrospray ionization mass spectrometry (ESI MS)

Electrospray ionization (ESI) mass spectra were recorded on a Waters Q-TOF mass spectrometer using a Z-spray source. The sample was first dissolved in toluene (~0.5 g/L), and then diluted (2/1 v/v) with an ethanol solution containing 50 mmol of CsOAc. The sample was directly infused into the chamber at 5 μL/min. The source temperature was maintained at 70 °C, the spray voltage was 2.20 kV and the cone voltage was adjusted to 60 V.

Table S1. Crystal data and structure refinement for $Au_{34}(S\text{-}c\text{-}C_6H_{11})_{22}$

Identification code	160512_zsl6_0ma	
Empirical formula	C138 H254 Au34 Cl12 S22	
Formula weight	9740.98	
Temperature	172.99 K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pbcn	
Unit cell dimensions	a = 26.0266(7) Å	α = 90°.
	b = 27.9405(8) Å	β = 90°.
	c = 28.5247(8) Å	γ = 90°.
Volume	20743.1(10) $Å^3$	
Z	4	
Density (calculated)	3.119 Mg/m^3	
Absorption coefficient	47.657 mm^{-1}	
F(000)	17296	
Theta range for data collection	2.320 to 68.384°.	
Index ranges	-30<=h<=31, -31<=k<=33, -34<=l<=34	
Reflections collected	188505	
Independent reflections	19001 [R(int) = 0.0870]	
Completeness to theta = 67.679°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.1665 and 0.0382	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	19001 / 414 / 930	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0514, wR2 = 0.1336	
R indices (all data)	R1 = 0.0566, wR2 = 0.1379	
Extinction coefficient	n/a	
Largest diff. peak and hole	4.384 and -4.347 e.$Å^{-3}$	

Table S2. Crystal data and structure refinement for $Au_{42}(S\text{-}c\text{-}C_6H_{11})_{26}$.

Identification code	160520	
Empirical formula	C156 H286 Au42 S26	
Formula weight	11267.98	
Temperature	172.99 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 20.6257(11) Å	α = 78.427(3)°.
	b = 20.7452(11) Å	β = 80.789(3)°.
	c = 30.3877(16) Å	γ = 62.667(2)°.
Volume	11281.4(11) $Å^3$	
Z	2	
Density (calculated)	3.317 Mg/m^3	
Absorption coefficient	52.356 mm^{-1}	
F(000)	9912	
Theta range for data collection	2.423 to 66.500°.	
Index ranges	-24<=h<=24, -24<=k<=24, -36<=l<=36	
Reflections collected	151316	
Independent reflections	38006 [R(int) = 0.0913]	
Completeness to theta = 67.679°	93.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.0211 and 0.0001	
Refinement method	Full-matrix-block least-squares on F^2	
Data / restraints / parameters	38006 / 1244 / 2017	
Goodness-of-fit on F^{-2}	1.514	
Final R indices [I>2sigma(I)]	R1 = 0.1663, wR2 = 0.3875	
R indices (all data)	R1 = 0.1989, wR2 = 0.4088	
Extinction coefficient	n/a	
Largest diff. peak and hole	10.495 and -6.544 $e.Å^{-3}$	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for $Au_{34}(SC_6H_{11})_{22}$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Au(1)	5796(1)	7520(1)	2949(1)	19(1)
Au(2)	5000	8049(1)	2500	18(1)
Au(3)	5000	6976(1)	2500	16(1)
Au(4)	5954(1)	6509(1)	3044(1)	21(1)
Au(5)	5955(1)	6941(1)	2098(1)	21(1)
Au(6)	6009(1)	8113(1)	2232(1)	22(1)
Au(7)	5643(1)	8494(1)	3075(1)	24(1)
Au(8)	5000	9266(1)	2500	31(1)
Au(9)	4553(1)	8690(1)	3427(1)	26(1)
Au(10)	4768(1)	7490(1)	3339(1)	20(1)
Au(11)	4876(1)	6513(1)	3342(1)	20(1)
Au(12)	5000	5874(1)	2500	21(1)
Au(13)	5788(1)	6082(1)	4035(1)	27(1)
Au(14)	5802(1)	7087(1)	3797(1)	23(1)
Au(15)	6695(1)	7134(1)	3263(1)	25(1)
Au(16)	7187(1)	6503(1)	2496(1)	34(1)
Au(17)	7144(1)	7874(1)	2572(1)	27(1)
Au(18)	7074(1)	6201(1)	3617(1)	35(1)
Au(19)	5943(1)	8123(1)	4096(1)	27(1)
S(1)	4302(1)	9337(1)	2980(1)	32(1)
S(2)	4663(1)	8065(1)	3941(1)	25(1)
S(3)	5639(1)	7478(1)	4523(1)	28(1)
S(4)	6201(1)	8772(1)	3656(1)	29(1)
S(5)	4966(1)	5849(1)	3851(1)	31(1)
S(6)	6601(1)	6276(1)	4290(1)	31(1)
S(7)	5876(1)	5791(1)	2602(1)	23(1)

S(8)	7645(2)	6056(2)	3022(1)	46(1)
S(9)	6821(1)	6919(1)	1887(1)	30(1)
S(10)	6830(1)	8178(1)	1875(1)	26(1)
S(11)	7485(1)	7543(1)	3244(1)	27(1)
C(1)	4408(6)	9875(5)	3350(5)	37(3)
C(2)	4370(7)	10328(6)	3017(6)	49(4)
C(3)	4415(8)	10768(7)	3318(7)	62(5)
C(4)	4006(8)	10787(7)	3696(7)	63(5)
C(5)	4026(9)	10359(8)	4008(8)	70(5)
C(6)	3996(7)	9899(6)	3717(6)	49(4)
C(7)	4003(6)	7998(5)	4170(5)	38(3)
C(8)	3902(9)	8375(8)	4543(8)	75(6)
C(9)	3384(10)	8337(10)	4743(10)	88(7)
C(10)	3223(9)	7882(8)	4903(8)	71(5)
C(11)	3340(10)	7510(9)	4558(9)	86(7)
C(12)	3889(11)	7541(9)	4361(10)	89(7)
C(13)	6147(5)	7302(5)	4942(5)	33(3)
C(14)	6275(6)	7713(5)	5270(5)	41(3)
C(15)	6702(9)	7546(8)	5606(8)	75(6)
C(16)	6537(8)	7113(7)	5882(7)	62(5)
C(17)	6400(8)	6707(7)	5562(7)	60(4)
C(18)	5975(6)	6859(5)	5207(5)	40(3)
C(19)	5939(6)	9303(5)	3940(5)	39(3)
C(20)	5969(7)	9734(6)	3591(6)	54(4)
C(21)	5800(8)	10180(8)	3840(8)	68(5)
C(22)	6156(8)	10292(7)	4265(7)	61(4)
C(23)	6119(7)	9880(6)	4608(6)	54(4)
C(24)	6277(6)	9409(5)	4374(5)	38(3)
C(25)	4600(6)	5938(6)	4399(5)	45(3)
C(26)	4600(9)	6431(8)	4568(7)	69(5)

C(27)	4266(12)	6456(11)	5011(11)	105(9)
C(28)	4460(9)	6114(8)	5391(8)	74(6)
C(29)	4485(10)	5649(9)	5215(8)	81(6)
C(30)	4806(8)	5604(7)	4785(7)	63(5)
C(31)	6810(5)	5768(5)	4660(5)	35(3)
C(32)	6701(6)	5283(5)	4447(5)	39(3)
C(33)	6921(7)	4886(6)	4746(6)	52(4)
C(34)	7491(7)	4959(6)	4839(7)	54(4)
C(35)	7580(7)	5429(6)	5083(6)	52(4)
C(36)	7385(6)	5838(5)	4770(6)	44(3)
C(37)	5957(5)	5278(5)	3009(5)	33(3)
C(38)	5574(8)	4903(7)	2943(7)	61(5)
C(39)	5673(9)	4467(8)	3244(8)	70(5)
C(40)	6189(7)	4258(6)	3154(6)	52(4)
C(41)	6592(7)	4634(7)	3213(7)	55(4)
C(42)	6502(6)	5079(6)	2923(6)	50(4)
C(43)	8216(6)	6436(6)	3140(5)	45(3)
C(44)	8674(8)	6241(8)	2849(7)	68(5)
C(45)	9137(11)	6512(10)	2951(9)	89(7)
C(46)	9275(10)	6577(10)	3443(9)	84(7)
C(47)	8838(9)	6786(9)	3742(8)	76(6)
C(48)	8371(9)	6462(8)	3650(8)	69(5)
C(49)	6899(6)	6491(5)	1397(5)	36(3)
C(50)	6710(6)	5988(6)	1494(6)	47(4)
C(51)	6849(8)	5656(7)	1102(7)	63(5)
C(52)	7418(8)	5666(7)	1015(7)	64(5)
C(53)	7595(8)	6139(7)	872(7)	65(5)
C(54)	7480(6)	6500(6)	1278(6)	47(4)
C(55)	7002(5)	8818(5)	1864(4)	30(3)
C(56)	7484(6)	8880(5)	1569(5)	41(3)

C(57)	7610(7)	9410(7)	1521(7)	56(4)
C(58)	7674(7)	9637(6)	2012(6)	53(4)
C(59)	7177(7)	9590(6)	2308(7)	55(4)
C(60)	7048(6)	9049(5)	2344(5)	41(3)
C(61)	7416(5)	8022(4)	3688(4)	26(2)
C(62)	7858(6)	8365(6)	3636(6)	47(4)
C(63)	7810(8)	8756(7)	4016(6)	57(4)
C(64)	7843(7)	8516(7)	4510(6)	56(4)
C(65)	7417(6)	8177(6)	4559(5)	44(3)
C(66)	7423(6)	7781(5)	4177(5)	38(3)

Table S4. Bond lengths [Å] and angles [°] for $Au_{34}(SC_6H_{11})_{22}$.

Atom1-Atom2	Length/ Å
Au(1)-Au(2)	2.8492(5)
Au(1)-Au(3)	2.8698(5)
Au(1)-Au(4)	2.8675(6)
Au(1)-Au(5)	2.9468(6)
Au(1)-Au(6)	2.6921(6)
Au(1)-Au(7)	2.7729(6)
Au(1)-Au(10)	2.8961(6)
Au(1)-Au(14)	2.7036(6)
Au(1)-Au(15)	2.7270(6)
Au(2)-Au(1)#1	2.8492(5)
Au(2)-Au(3)	2.9986(9)
Au(2)-Au(6)	2.7416(5)
Au(2)-Au(6)#1	2.7416(5)
Au(2)-Au(7)	2.6519(5)
Au(2)-Au(7)#1	2.6519(5)
Au(2)-Au(10)	2.9214(6)
Au(2)-Au(10)#1	2.9213(6)
Au(3)-Au(1)#1	2.8699(5)
Au(3)-Au(4)#1	3.2044(5)
Au(3)-Au(4)	3.2043(5)
Au(3)-Au(5)	2.7398(4)
Au(3)-Au(5)#1	2.7398(4)
Au(3)-Au(10)	2.8544(5)
Au(3)-Au(10)#1	2.8543(5)
Au(3)-Au(11)#1	2.7489(5)
Au(3)-Au(11)	2.7489(5)
Au(3)-Au(12)	3.0792(8)

Au(4)-Au(5)	2.9565(7)
Au(4)-Au(11)	2.9319(7)
Au(4)-Au(13)	3.1005(7)
Au(4)-Au(14)	2.7169(6)
Au(4)-Au(15)	2.6769(6)
Au(4)-S(7)	2.377(3)
Au(5)-Au(6)	3.2989(7)
Au(5)-Au(10)#1	2.7282(6)
Au(5)-Au(11)#1	2.7727(6)
Au(5)-S(9)	2.334(3)
Au(6)-Au(7)	2.7964(7)
Au(6)-Au(9)#1	2.8758(7)
Au(6)-Au(10)#1	3.1273(7)
Au(6)-Au(17)	3.1811(7)
Au(6)-S(10)	2.372(3)
Au(7)-Au(8)	3.1856(7)
Au(7)-Au(9)	3.0607(7)
Au(7)-Au(19)	3.1893(7)
Au(7)-S(4)	2.336(3)
Au(8)-Au(7)#1	3.1856(7)
Au(8)-Au(9)	3.3070(6)
Au(8)-Au(9)#1	3.3071(6)
Au(8)-S(1)#1	2.283(3)
Au(8)-S(1)	2.283(3)
Au(9)-Au(6)#1	2.8759(7)
Au(9)-S(1)	2.307(3)
Au(9)-S(2)	2.299(3)
Au(10)-Au(5)#1	2.7282(6)
Au(10)-Au(6)#1	3.1273(7)
Au(10)-Au(11)	2.7437(6)

Au(10)-Au(14)	3.1947(7)
Au(10)-S(2)	2.367(3)
Au(11)-Au(5)#1	2.7728(6)
Au(11)-Au(12)	3.0109(6)
Au(11)-Au(13)	3.3151(7)
Au(11)-Au(14)	3.1715(7)
Au(11)-S(5)	2.367(3)
Au(12)-Au(11)#1	3.0109(6)
Au(12)-S(7)#1	2.310(3)
Au(12)-S(7)	2.310(3)
Au(13)-Au(14)	2.8898(7)
Au(13)-S(5)	2.296(3)
Au(13)-S(6)	2.302(3)
Au(14)-Au(15)	2.7822(7)
Au(14)-Au(19)	3.0413(7)
Au(14)-S(3)	2.381(3)
Au(15)-Au(16)	3.0892(7)
Au(15)-Au(17)	3.0859(7)
Au(15)-Au(18)	2.9654(7)
Au(15)-S(11)	2.353(3)
Au(16)-Au(18)	3.3207(8)
Au(16)-S(8)	2.288(4)
Au(16)-S(9)	2.296(3)
Au(17)-S(10)	2.312(3)
Au(17)-S(11)	2.305(3)
Au(18)-S(6)	2.292(3)
Au(18)-S(8)	2.292(4)
Au(19)-S(3)	2.315(3)
Au(19)-S(4)	2.307(3)
S(1)-C(1)	1.857(14)

S(2)-C(7)	1.848(15)
S(3)-C(13)	1.848(14)
S(4)-C(19)	1.823(15)
S(5)-C(25)	1.847(16)
S(6)-C(31)	1.849(14)
S(7)-C(37)	1.856(14)
S(8)-C(43)	1.859(17)
S(9)-C(49)	1.851(14)
S(10)-C(55)	1.846(13)
S(11)-C(61)	1.850(13)
C(1)-H(1)	1.0000
C(1)-C(2)	1.59(2)
C(1)-C(6)	1.50(2)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(2)-C(3)	1.50(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(3)-C(4)	1.52(3)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(4)-C(5)	1.49(3)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(5)-C(6)	1.53(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-H(7)	1.0000
C(7)-C(8)	1.52(3)
C(7)-C(12)	1.42(3)

C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(8)-C(9)	1.47(3)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(9)-C(10)	1.41(3)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(10)-C(11)	1.47(3)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(11)-C(12)	1.54(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-H(13)	1.0000
C(13)-C(14)	1.517(19)
C(13)-C(18)	1.52(2)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(14)-C(15)	1.54(3)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(15)-C(16)	1.50(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(16)-C(17)	1.50(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(17)-C(18)	1.56(2)
C(18)-H(18A)	0.9900

C(18)-H(18B)	0.9900
C(19)-H(19)	1.0000
C(19)-C(20)	1.56(2)
C(19)-C(24)	1.55(2)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(20)-C(21)	1.50(3)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(21)-C(22)	1.56(3)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(22)-C(23)	1.51(3)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(23)-C(24)	1.53(2)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-H(25)	1.0000
C(25)-C(26)	1.46(3)
C(25)-C(30)	1.54(2)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(26)-C(27)	1.53(3)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(27)-C(28)	1.53(4)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(28)-C(29)	1.40(3)

C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(29)-C(30)	1.49(3)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-H(31)	1.0000
C(31)-C(32)	1.513(19)
C(31)-C(36)	1.54(2)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(32)-C(33)	1.51(2)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(33)-C(34)	1.52(2)
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(34)-C(35)	1.50(2)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(35)-C(36)	1.54(2)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-H(37)	1.0000
C(37)-C(38)	1.46(2)
C(37)-C(42)	1.54(2)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(38)-C(39)	1.51(3)
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900

C(39)-C(40)	1.49(3)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(40)-C(41)	1.49(2)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(41)-C(42)	1.51(2)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-H(43)	1.0000
C(43)-C(44)	1.55(3)
C(43)-C(48)	1.51(3)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(44)-C(45)	1.45(3)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(45)-C(46)	1.46(3)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(46)-C(47)	1.54(3)
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(47)-C(48)	1.54(3)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-H(49)	1.0000
C(49)-C(50)	1.51(2)
C(49)-C(54)	1.55(2)
C(50)-H(50A)	0.9900

C(50)-H(50B)	0.9900
C(50)-C(51)	1.50(2)
C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900
C(51)-C(52)	1.50(3)
C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900
C(52)-C(53)	1.46(3)
C(53)-H(53A)	0.9900
C(53)-H(53B)	0.9900
C(53)-C(54)	1.57(3)
C(54)-H(54A)	0.9900
C(54)-H(54B)	0.9900
C(55)-H(55)	1.0000
C(55)-C(56)	1.518(19)
C(55)-C(60)	1.519(19)
C(56)-H(56A)	0.9900
C(56)-H(56B)	0.9900
C(56)-C(57)	1.52(2)
C(57)-H(57A)	0.9900
C(57)-H(57B)	0.9900
C(57)-C(58)	1.55(2)
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
C(58)-C(59)	1.55(3)
C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(59)-C(60)	1.55(2)
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900

C(61)-H(61)	1.0000
C(61)-C(62)	1.505(19)
C(61)-C(66)	1.550(18)
C(62)-H(62A)	0.9900
C(62)-H(62B)	0.9900
C(62)-C(63)	1.54(2)
C(63)-H(63A)	0.9900
C(63)-H(63B)	0.9900
C(63)-C(64)	1.56(3)
C(64)-H(64A)	0.9900
C(64)-H(64B)	0.9900
C(64)-C(65)	1.46(2)
C(65)-H(65A)	0.9900
C(65)-H(65B)	0.9900
C(65)-C(66)	1.55(2)
C(66)-H(66A)	0.9900
C(66)-H(66B)	0.9900
atom(1)-atom(2)-atom(3)	angle/ °
Au(2)-Au(1)-Au(3)	63.245(17)
Au(2)-Au(1)-Au(4)	131.15(2)
Au(2)-Au(1)-Au(5)	90.946(16)
Au(2)-Au(1)-Au(10)	61.120(13)
Au(3)-Au(1)-Au(5)	56.183(12)
Au(3)-Au(1)-Au(10)	59.343(13)
Au(4)-Au(1)-Au(3)	67.905(16)
Au(4)-Au(1)-Au(5)	61.108(16)
Au(4)-Au(1)-Au(10)	93.885(18)
Au(6)-Au(1)-Au(2)	59.228(14)
Au(6)-Au(1)-Au(3)	97.789(18)
Au(6)-Au(1)-Au(4)	130.42(2)

Au(6)-Au(1)-Au(5)	71.447(17)
Au(6)-Au(1)-Au(7)	61.532(17)
Au(6)-Au(1)-Au(10)	120.03(2)
Au(6)-Au(1)-Au(14)	162.61(2)
Au(6)-Au(1)-Au(15)	108.37(2)
Au(7)-Au(1)-Au(2)	56.268(16)
Au(7)-Au(1)-Au(3)	118.30(2)
Au(7)-Au(1)-Au(4)	167.20(2)
Au(7)-Au(1)-Au(5)	131.65(2)
Au(7)-Au(1)-Au(10)	81.212(17)
Au(10)-Au(1)-Au(5)	115.503(19)
Au(14)-Au(1)-Au(2)	129.72(2)
Au(14)-Au(1)-Au(3)	99.597(18)
Au(14)-Au(1)-Au(4)	58.287(16)
Au(14)-Au(1)-Au(5)	119.39(2)
Au(14)-Au(1)-Au(7)	108.94(2)
Au(14)-Au(1)-Au(10)	69.475(17)
Au(14)-Au(1)-Au(15)	61.634(17)
Au(15)-Au(1)-Au(2)	167.47(2)
Au(15)-Au(1)-Au(3)	123.80(2)
Au(15)-Au(1)-Au(4)	57.107(15)
Au(15)-Au(1)-Au(5)	86.129(18)
Au(15)-Au(1)-Au(7)	117.90(2)
Au(15)-Au(1)-Au(10)	130.90(2)
Au(1)-Au(2)-Au(1)#1	117.43(3)
Au(1)-Au(2)-Au(3)	58.713(13)
Au(1)#1-Au(2)-Au(3)	58.714(13)
Au(1)-Au(2)-Au(10)	60.232(15)
Au(1)-Au(2)-Au(10)#1	86.588(17)
Au(1)#1-Au(2)-Au(10)#1	60.232(15)

Au(1)#1-Au(2)-Au(10)	86.588(17)
Au(6)-Au(2)-Au(1)#1	127.184(18)
Au(6)#1-Au(2)-Au(1)	127.183(18)
Au(6)#1-Au(2)-Au(1)#1	57.527(13)
Au(6)-Au(2)-Au(1)	57.530(13)
Au(6)#1-Au(2)-Au(3)	93.725(16)
Au(6)-Au(2)-Au(3)	93.727(16)
Au(6)-Au(2)-Au(6)#1	172.55(3)
Au(6)-Au(2)-Au(10)#1	66.954(14)
Au(6)#1-Au(2)-Au(10)	66.953(14)
Au(6)-Au(2)-Au(10)	117.457(16)
Au(6)#1-Au(2)-Au(10)#1	117.453(16)
Au(7)#1-Au(2)-Au(1)	168.514(15)
Au(7)#1-Au(2)-Au(1)#1	60.414(14)
Au(7)-Au(2)-Au(1)	60.413(14)
Au(7)-Au(2)-Au(1)#1	168.513(15)
Au(7)-Au(2)-Au(3)	117.914(15)
Au(7)#1-Au(2)-Au(3)	117.915(15)
Au(7)#1-Au(2)-Au(6)	113.698(18)
Au(7)-Au(2)-Au(6)#1	113.701(18)
Au(7)#1-Au(2)-Au(6)#1	62.432(15)
Au(7)-Au(2)-Au(6)	62.433(15)
Au(7)-Au(2)-Au(7)#1	124.17(3)
Au(7)-Au(2)-Au(10)	82.791(14)
Au(7)-Au(2)-Au(10)#1	128.807(14)
Au(7)#1-Au(2)-Au(10)#1	82.792(14)
Au(7)#1-Au(2)-Au(10)	128.806(14)
Au(10)-Au(2)-Au(3)	57.635(13)
Au(10)#1-Au(2)-Au(3)	57.634(13)
Au(10)#1-Au(2)-Au(10)	115.27(3)

Au(1)-Au(3)-Au(1)#1	116.08(3)
Au(1)-Au(3)-Au(2)	58.041(13)
Au(1)#1-Au(3)-Au(2)	58.041(13)
Au(1)#1-Au(3)-Au(4)#1	56.012(11)
Au(1)-Au(3)-Au(4)	56.013(11)
Au(1)#1-Au(3)-Au(4)	172.09(2)
Au(1)-Au(3)-Au(4)#1	172.09(2)
Au(1)#1-Au(3)-Au(12)	121.959(13)
Au(1)-Au(3)-Au(12)	121.958(13)
Au(2)-Au(3)-Au(4)	114.054(12)
Au(2)-Au(3)-Au(4)#1	114.053(12)
Au(2)-Au(3)-Au(12)	180.0
Au(4)-Au(3)-Au(4)#1	131.89(2)
Au(5)-Au(3)-Au(1)#1	119.096(17)
Au(5)-Au(3)-Au(1)	63.330(14)
Au(5)#1-Au(3)-Au(1)#1	63.328(14)
Au(5)#1-Au(3)-Au(1)	119.094(17)
Au(5)-Au(3)-Au(2)	92.025(15)
Au(5)#1-Au(3)-Au(2)	92.023(15)
Au(5)-Au(3)-Au(4)	59.038(13)
Au(5)#1-Au(3)-Au(4)#1	59.038(13)
Au(5)-Au(3)-Au(4)#1	119.056(15)
Au(5)#1-Au(3)-Au(4)	119.057(15)
Au(5)-Au(3)-Au(5)#1	175.95(3)
Au(5)-Au(3)-Au(10)	124.088(17)
Au(5)#1-Au(3)-Au(10)#1	124.086(17)
Au(5)-Au(3)-Au(10)#1	58.336(14)
Au(5)#1-Au(3)-Au(10)	58.335(14)
Au(5)#1-Au(3)-Au(11)	60.687(14)
Au(5)-Au(3)-Au(11)#1	60.685(14)

Au(5)#1-Au(3)-Au(11)#1	117.151(17)
Au(5)-Au(3)-Au(11)	117.150(17)
Au(5)-Au(3)-Au(12)	87.975(15)
Au(5)#1-Au(3)-Au(12)	87.977(15)
Au(10)#1-Au(3)-Au(1)#1	60.786(15)
Au(10)-Au(3)-Au(1)	60.786(15)
Au(10)#1-Au(3)-Au(1)	87.475(17)
Au(10)-Au(3)-Au(1)#1	87.474(17)
Au(10)#1-Au(3)-Au(2)	59.823(13)
Au(10)-Au(3)-Au(2)	59.823(13)
Au(10)-Au(3)-Au(4)	87.869(12)
Au(10)#1-Au(3)-Au(4)#1	87.868(13)
Au(10)-Au(3)-Au(4)#1	116.548(13)
Au(10)#1-Au(3)-Au(4)	116.549(13)
Au(10)#1-Au(3)-Au(10)	119.65(3)
Au(10)#1-Au(3)-Au(12)	120.177(13)
Au(10)-Au(3)-Au(12)	120.177(13)
Au(11)#1-Au(3)-Au(1)	123.695(13)
Au(11)-Au(3)-Au(1)#1	123.695(13)
Au(11)#1-Au(3)-Au(1)#1	86.776(13)
Au(11)-Au(3)-Au(1)	86.777(13)
Au(11)-Au(3)-Au(2)	118.096(14)
Au(11)#1-Au(3)-Au(2)	118.094(14)
Au(11)-Au(3)-Au(4)#1	98.043(17)
Au(11)-Au(3)-Au(4)	58.411(14)
Au(11)#1-Au(3)-Au(4)#1	58.411(14)
Au(11)#1-Au(3)-Au(4)	98.043(17)
Au(11)#1-Au(3)-Au(10)#1	58.598(13)
Au(11)#1-Au(3)-Au(10)	173.977(15)
Au(11)-Au(3)-Au(10)	58.600(13)

Au(11)-Au(3)-Au(10)#1	173.978(16)
Au(11)#1-Au(3)-Au(11)	123.81(3)
Au(11)-Au(3)-Au(12)	61.904(14)
Au(11)#1-Au(3)-Au(12)	61.906(14)
Au(12)-Au(3)-Au(4)	65.946(12)
Au(12)-Au(3)-Au(4)#1	65.947(12)
Au(1)-Au(4)-Au(3)	56.082(15)
Au(1)-Au(4)-Au(5)	60.770(15)
Au(1)-Au(4)-Au(11)	83.466(17)
Au(1)-Au(4)-Au(13)	116.41(2)
Au(5)-Au(4)-Au(3)	52.623(12)
Au(5)-Au(4)-Au(13)	171.99(2)
Au(11)-Au(4)-Au(3)	53.002(12)
Au(11)-Au(4)-Au(5)	105.385(18)
Au(11)-Au(4)-Au(13)	66.605(16)
Au(13)-Au(4)-Au(3)	119.378(17)
Au(14)-Au(4)-Au(1)	57.836(16)
Au(14)-Au(4)-Au(3)	91.591(17)
Au(14)-Au(4)-Au(5)	118.61(2)
Au(14)-Au(4)-Au(11)	68.190(17)
Au(14)-Au(4)-Au(13)	59.132(16)
Au(15)-Au(4)-Au(1)	58.806(16)
Au(15)-Au(4)-Au(3)	113.89(2)
Au(15)-Au(4)-Au(5)	86.845(19)
Au(15)-Au(4)-Au(11)	128.24(2)
Au(15)-Au(4)-Au(13)	97.96(2)
Au(15)-Au(4)-Au(14)	62.098(18)
S(7)-Au(4)-Au(1)	140.31(7)
S(7)-Au(4)-Au(3)	91.26(7)
S(7)-Au(4)-Au(5)	82.06(7)

S(7)-Au(4)-Au(11)	94.38(7)
S(7)-Au(4)-Au(13)	98.44(7)
S(7)-Au(4)-Au(14)	155.27(7)
S(7)-Au(4)-Au(15)	137.37(7)
Au(1)-Au(5)-Au(4)	58.122(15)
Au(1)-Au(5)-Au(6)	50.682(14)
Au(3)-Au(5)-Au(1)	60.487(15)
Au(3)-Au(5)-Au(4)	68.339(15)
Au(3)-Au(5)-Au(6)	87.425(18)
Au(3)-Au(5)-Au(11)#1	59.820(14)
Au(4)-Au(5)-Au(6)	107.471(18)
Au(10)#1-Au(5)-Au(1)	88.339(18)
Au(10)#1-Au(5)-Au(3)	62.932(15)
Au(10)#1-Au(5)-Au(4)	130.17(2)
Au(10)#1-Au(5)-Au(6)	61.655(15)
Au(10)#1-Au(5)-Au(11)#1	59.827(16)
Au(11)#1-Au(5)-Au(1)	120.01(2)
Au(11)#1-Au(5)-Au(4)	103.617(19)
Au(11)#1-Au(5)-Au(6)	120.956(19)
S(9)-Au(5)-Au(1)	111.31(8)
S(9)-Au(5)-Au(3)	170.14(9)
S(9)-Au(5)-Au(4)	103.03(9)
S(9)-Au(5)-Au(6)	90.89(8)
S(9)-Au(5)-Au(10)#1	124.36(9)
S(9)-Au(5)-Au(11)#1	128.68(8)
Au(1)-Au(6)-Au(2)	63.242(16)
Au(1)-Au(6)-Au(5)	57.872(15)
Au(1)-Au(6)-Au(7)	60.658(17)
Au(1)-Au(6)-Au(9)#1	137.48(2)
Au(1)-Au(6)-Au(10)#1	85.347(17)

Au(1)-Au(6)-Au(17)	80.241(18)
Au(2)-Au(6)-Au(5)	85.815(19)
Au(2)-Au(6)-Au(7)	57.210(15)
Au(2)-Au(6)-Au(9)#1	74.430(17)
Au(2)-Au(6)-Au(10)#1	59.270(15)
Au(2)-Au(6)-Au(17)	142.28(2)
Au(7)-Au(6)-Au(5)	117.545(19)
Au(7)-Au(6)-Au(9)#1	100.11(2)
Au(7)-Au(6)-Au(10)#1	116.04(2)
Au(7)-Au(6)-Au(17)	97.69(2)
Au(9)#1-Au(6)-Au(5)	117.32(2)
Au(9)#1-Au(6)-Au(10)#1	69.089(16)
Au(9)#1-Au(6)-Au(17)	142.15(2)
Au(10)#1-Au(6)-Au(5)	50.158(14)
Au(10)#1-Au(6)-Au(17)	130.01(2)
Au(17)-Au(6)-Au(5)	82.324(16)
S(10)-Au(6)-Au(1)	123.99(8)
S(10)-Au(6)-Au(2)	170.76(7)
S(10)-Au(6)-Au(5)	93.67(8)
S(10)-Au(6)-Au(7)	130.28(7)
S(10)-Au(6)-Au(9)#1	97.75(7)
S(10)-Au(6)-Au(10)#1	113.68(7)
S(10)-Au(6)-Au(17)	46.44(7)
Au(1)-Au(7)-Au(6)	57.810(16)
Au(1)-Au(7)-Au(8)	132.33(2)
Au(1)-Au(7)-Au(9)	110.54(2)
Au(1)-Au(7)-Au(19)	76.372(17)
Au(2)-Au(7)-Au(1)	63.319(17)
Au(2)-Au(7)-Au(6)	60.356(14)
Au(2)-Au(7)-Au(8)	70.556(19)

Au(2)-Au(7)-Au(9)	72.629(15)
Au(2)-Au(7)-Au(19)	124.56(2)
Au(6)-Au(7)-Au(8)	89.657(17)
Au(6)-Au(7)-Au(9)	131.79(2)
Au(6)-Au(7)-Au(19)	125.38(2)
Au(8)-Au(7)-Au(19)	144.951(19)
Au(9)-Au(7)-Au(8)	63.898(14)
Au(9)-Au(7)-Au(19)	89.139(18)
S(4)-Au(7)-Au(1)	109.25(7)
S(4)-Au(7)-Au(2)	170.64(8)
S(4)-Au(7)-Au(6)	121.66(8)
S(4)-Au(7)-Au(8)	117.77(7)
S(4)-Au(7)-Au(9)	106.47(8)
S(4)-Au(7)-Au(19)	46.23(8)
Au(7)#1-Au(8)-Au(7)	94.72(3)
Au(7)#1-Au(8)-Au(9)#1	56.214(15)
Au(7)-Au(8)-Au(9)	56.214(15)
Au(7)-Au(8)-Au(9)#1	84.084(18)
Au(7)#1-Au(8)-Au(9)	84.084(18)
Au(9)-Au(8)-Au(9)#1	121.78(3)
S(1)#1-Au(8)-Au(7)	87.08(8)
S(1)#1-Au(8)-Au(7)#1	99.72(8)
S(1)-Au(8)-Au(7)	99.72(8)
S(1)-Au(8)-Au(7)#1	87.08(8)
S(1)-Au(8)-Au(9)	44.20(8)
S(1)-Au(8)-Au(9)#1	143.28(8)
S(1)#1-Au(8)-Au(9)	143.29(8)
S(1)#1-Au(8)-Au(9)#1	44.20(8)
S(1)#1-Au(8)-S(1)	170.02(16)
Au(6)#1-Au(9)-Au(7)	99.004(19)

Au(6)#1-Au(9)-Au(8)	85.944(18)
Au(7)-Au(9)-Au(8)	59.888(14)
S(1)-Au(9)-Au(6)#1	86.21(8)
S(1)-Au(9)-Au(7)	102.80(8)
S(1)-Au(9)-Au(8)	43.63(8)
S(2)-Au(9)-Au(6)#1	93.09(7)
S(2)-Au(9)-Au(7)	87.52(7)
S(2)-Au(9)-Au(8)	146.67(7)
S(2)-Au(9)-S(1)	169.65(11)
Au(1)-Au(10)-Au(2)	58.648(13)
Au(1)-Au(10)-Au(6)#1	112.423(19)
Au(1)-Au(10)-Au(14)	52.424(14)
Au(2)-Au(10)-Au(6)#1	53.776(12)
Au(2)-Au(10)-Au(14)	110.481(17)
Au(3)-Au(10)-Au(1)	59.871(13)
Au(3)-Au(10)-Au(2)	62.542(17)
Au(3)-Au(10)-Au(6)#1	88.875(16)
Au(3)-Au(10)-Au(14)	89.305(15)
Au(5)#1-Au(10)-Au(1)	118.58(2)
Au(5)#1-Au(10)-Au(2)	93.961(18)
Au(5)#1-Au(10)-Au(3)	58.732(14)
Au(5)#1-Au(10)-Au(6)#1	68.184(17)
Au(5)#1-Au(10)-Au(11)	60.893(16)
Au(5)#1-Au(10)-Au(14)	124.744(19)
Au(6)#1-Au(10)-Au(14)	162.54(2)
Au(11)-Au(10)-Au(1)	86.357(18)
Au(11)-Au(10)-Au(2)	120.98(2)
Au(11)-Au(10)-Au(3)	58.779(16)
Au(11)-Au(10)-Au(6)#1	128.46(2)
Au(11)-Au(10)-Au(14)	64.035(16)

S(2)-Au(10)-Au(1)	111.42(7)
S(2)-Au(10)-Au(2)	104.74(7)
S(2)-Au(10)-Au(3)	166.79(7)
S(2)-Au(10)-Au(5)#1	129.22(7)
S(2)-Au(10)-Au(6)#1	85.67(7)
S(2)-Au(10)-Au(11)	133.17(7)
S(2)-Au(10)-Au(14)	92.29(7)
Au(3)-Au(11)-Au(4)	68.587(14)
Au(3)-Au(11)-Au(5)#1	59.495(13)
Au(3)-Au(11)-Au(12)	64.447(17)
Au(3)-Au(11)-Au(13)	127.446(18)
Au(3)-Au(11)-Au(14)	91.700(16)
Au(4)-Au(11)-Au(12)	70.286(13)
Au(4)-Au(11)-Au(13)	59.134(15)
Au(4)-Au(11)-Au(14)	52.686(14)
Au(5)#1-Au(11)-Au(4)	128.03(2)
Au(5)#1-Au(11)-Au(12)	88.760(17)
Au(5)#1-Au(11)-Au(13)	170.18(2)
Au(5)#1-Au(11)-Au(14)	124.00(2)
Au(10)-Au(11)-Au(3)	62.621(17)
Au(10)-Au(11)-Au(4)	95.748(18)
Au(10)-Au(11)-Au(5)#1	59.279(16)
Au(10)-Au(11)-Au(12)	126.69(2)
Au(10)-Au(11)-Au(13)	115.89(2)
Au(10)-Au(11)-Au(14)	64.908(16)
Au(12)-Au(11)-Au(13)	100.570(16)
Au(12)-Au(11)-Au(14)	122.968(18)
Au(14)-Au(11)-Au(13)	52.854(14)
S(5)-Au(11)-Au(3)	153.29(8)
S(5)-Au(11)-Au(4)	94.60(8)

S(5)-Au(11)-Au(5)#1	133.92(8)
S(5)-Au(11)-Au(10)	142.40(8)
S(5)-Au(11)-Au(12)	90.79(8)
S(5)-Au(11)-Au(13)	43.83(8)
S(5)-Au(11)-Au(14)	94.04(8)
Au(11)-Au(12)-Au(3)	53.649(13)
Au(11)#1-Au(12)-Au(3)	53.648(13)
Au(11)-Au(12)-Au(11)#1	107.30(3)
S(7)-Au(12)-Au(3)	95.79(7)
S(7)#1-Au(12)-Au(3)	95.79(7)
S(7)-Au(12)-Au(11)#1	93.11(7)
S(7)#1-Au(12)-Au(11)	93.11(7)
S(7)#1-Au(12)-Au(11)#1	93.74(7)
S(7)-Au(12)-Au(11)	93.74(7)
S(7)#1-Au(12)-S(7)	168.43(13)
Au(4)-Au(13)-Au(11)	54.261(14)
Au(14)-Au(13)-Au(4)	53.803(15)
Au(14)-Au(13)-Au(11)	61.022(15)
S(5)-Au(13)-Au(4)	91.71(8)
S(5)-Au(13)-Au(11)	45.56(7)
S(5)-Au(13)-Au(14)	103.49(8)
S(5)-Au(13)-S(6)	174.27(11)
S(6)-Au(13)-Au(4)	93.99(8)
S(6)-Au(13)-Au(11)	139.51(8)
S(6)-Au(13)-Au(14)	80.42(7)
Au(1)-Au(14)-Au(4)	63.877(17)
Au(1)-Au(14)-Au(10)	58.101(15)
Au(1)-Au(14)-Au(11)	81.743(17)
Au(1)-Au(14)-Au(13)	130.19(2)
Au(1)-Au(14)-Au(15)	59.599(17)

Au(1)-Au(14)-Au(19)	79.965(18)
Au(4)-Au(14)-Au(10)	90.487(18)
Au(4)-Au(14)-Au(11)	59.124(15)
Au(4)-Au(14)-Au(13)	67.065(17)
Au(4)-Au(14)-Au(15)	58.246(17)
Au(4)-Au(14)-Au(19)	140.40(2)
Au(11)-Au(14)-Au(10)	51.057(13)
Au(13)-Au(14)-Au(10)	115.35(2)
Au(13)-Au(14)-Au(11)	66.124(16)
Au(13)-Au(14)-Au(19)	149.39(2)
Au(15)-Au(14)-Au(10)	117.54(2)
Au(15)-Au(14)-Au(11)	115.79(2)
Au(15)-Au(14)-Au(13)	100.70(2)
Au(15)-Au(14)-Au(19)	90.429(19)
Au(19)-Au(14)-Au(10)	83.169(17)
Au(19)-Au(14)-Au(11)	133.47(2)
S(3)-Au(14)-Au(1)	124.88(8)
S(3)-Au(14)-Au(4)	170.79(8)
S(3)-Au(14)-Au(10)	92.54(8)
S(3)-Au(14)-Au(11)	116.90(8)
S(3)-Au(14)-Au(13)	103.82(7)
S(3)-Au(14)-Au(15)	127.12(8)
S(3)-Au(14)-Au(19)	48.71(7)
Au(1)-Au(15)-Au(14)	58.768(17)
Au(1)-Au(15)-Au(16)	110.47(2)
Au(1)-Au(15)-Au(17)	81.471(18)
Au(1)-Au(15)-Au(18)	138.17(2)
Au(4)-Au(15)-Au(1)	64.088(17)
Au(4)-Au(15)-Au(14)	59.656(17)
Au(4)-Au(15)-Au(16)	76.177(19)

Au(4)-Au(15)-Au(17)	124.17(2)
Au(4)-Au(15)-Au(18)	75.281(19)
Au(14)-Au(15)-Au(16)	135.03(2)
Au(14)-Au(15)-Au(17)	134.30(2)
Au(14)-Au(15)-Au(18)	92.87(2)
Au(17)-Au(15)-Au(16)	76.863(19)
Au(18)-Au(15)-Au(16)	66.487(19)
Au(18)-Au(15)-Au(17)	132.82(2)
S(11)-Au(15)-Au(1)	123.41(7)
S(11)-Au(15)-Au(4)	160.33(8)
S(11)-Au(15)-Au(14)	139.93(8)
S(11)-Au(15)-Au(16)	84.20(8)
S(11)-Au(15)-Au(17)	47.85(8)
S(11)-Au(15)-Au(18)	98.24(7)
Au(15)-Au(16)-Au(18)	54.970(16)
S(8)-Au(16)-Au(15)	93.64(10)
S(8)-Au(16)-Au(18)	43.57(10)
S(8)-Au(16)-S(9)	171.35(12)
S(9)-Au(16)-Au(15)	94.25(8)
S(9)-Au(16)-Au(18)	145.08(7)
Au(15)-Au(17)-Au(6)	89.036(17)
S(10)-Au(17)-Au(6)	48.03(7)
S(10)-Au(17)-Au(15)	131.33(7)
S(11)-Au(17)-Au(6)	134.01(8)
S(11)-Au(17)-Au(15)	49.18(7)
S(11)-Au(17)-S(10)	176.96(11)
Au(15)-Au(18)-Au(16)	58.543(17)
S(6)-Au(18)-Au(15)	91.49(8)
S(6)-Au(18)-Au(16)	146.26(8)
S(8)-Au(18)-Au(15)	96.88(10)

S(8)-Au(18)-Au(16)	43.48(10)
S(8)-Au(18)-S(6)	170.22(13)
Au(14)-Au(19)-Au(7)	91.316(18)
S(3)-Au(19)-Au(7)	130.55(8)
S(3)-Au(19)-Au(14)	50.59(7)
S(4)-Au(19)-Au(7)	46.99(7)
S(4)-Au(19)-Au(14)	129.10(8)
S(4)-Au(19)-S(3)	176.87(11)
Au(8)-S(1)-Au(9)	92.18(11)
C(1)-S(1)-Au(8)	107.0(5)
C(1)-S(1)-Au(9)	106.1(5)
Au(9)-S(2)-Au(10)	93.92(10)
C(7)-S(2)-Au(9)	100.7(5)
C(7)-S(2)-Au(10)	107.2(5)
Au(19)-S(3)-Au(14)	80.70(10)
C(13)-S(3)-Au(14)	108.3(4)
C(13)-S(3)-Au(19)	107.6(5)
Au(19)-S(4)-Au(7)	86.78(10)
C(19)-S(4)-Au(7)	110.8(5)
C(19)-S(4)-Au(19)	106.8(5)
Au(13)-S(5)-Au(11)	90.61(10)
C(25)-S(5)-Au(11)	111.1(5)
C(25)-S(5)-Au(13)	104.4(5)
Au(18)-S(6)-Au(13)	102.02(13)
C(31)-S(6)-Au(13)	105.7(5)
C(31)-S(6)-Au(18)	104.4(5)
Au(12)-S(7)-Au(4)	93.74(10)
C(37)-S(7)-Au(4)	108.1(4)
C(37)-S(7)-Au(12)	105.6(4)
Au(16)-S(8)-Au(18)	92.95(15)

C(43)-S(8)-Au(16)	102.9(5)
C(43)-S(8)-Au(18)	106.4(5)
Au(16)-S(9)-Au(5)	102.71(12)
C(49)-S(9)-Au(5)	108.5(5)
C(49)-S(9)-Au(16)	101.4(5)
Au(17)-S(10)-Au(6)	85.53(9)
C(55)-S(10)-Au(6)	107.5(4)
C(55)-S(10)-Au(17)	106.5(4)
Au(17)-S(11)-Au(15)	82.97(10)
C(61)-S(11)-Au(15)	104.6(4)
C(61)-S(11)-Au(17)	104.0(4)
S(1)-C(1)-H(1)	110.2
C(2)-C(1)-S(1)	107.2(10)
C(2)-C(1)-H(1)	110.2
C(6)-C(1)-S(1)	109.2(11)
C(6)-C(1)-H(1)	110.2
C(6)-C(1)-C(2)	109.7(12)
C(1)-C(2)-H(2A)	110.1
C(1)-C(2)-H(2B)	110.1
H(2A)-C(2)-H(2B)	108.5
C(3)-C(2)-C(1)	107.8(14)
C(3)-C(2)-H(2A)	110.1
C(3)-C(2)-H(2B)	110.1
C(2)-C(3)-H(3A)	109.1
C(2)-C(3)-H(3B)	109.1
C(2)-C(3)-C(4)	112.5(17)
H(3A)-C(3)-H(3B)	107.8
C(4)-C(3)-H(3A)	109.1
C(4)-C(3)-H(3B)	109.1
C(3)-C(4)-H(4A)	109.3

C(3)-C(4)-H(4B)	109.3
H(4A)-C(4)-H(4B)	107.9
C(5)-C(4)-C(3)	111.8(17)
C(5)-C(4)-H(4A)	109.3
C(5)-C(4)-H(4B)	109.3
C(4)-C(5)-H(5A)	109.6
C(4)-C(5)-H(5B)	109.6
C(4)-C(5)-C(6)	110.4(17)
H(5A)-C(5)-H(5B)	108.1
C(6)-C(5)-H(5A)	109.6
C(6)-C(5)-H(5B)	109.6
C(1)-C(6)-C(5)	112.4(15)
C(1)-C(6)-H(6A)	109.1
C(1)-C(6)-H(6B)	109.1
C(5)-C(6)-H(6A)	109.1
C(5)-C(6)-H(6B)	109.1
H(6A)-C(6)-H(6B)	107.9
S(2)-C(7)-H(7)	107.7
C(8)-C(7)-S(2)	109.9(12)
C(8)-C(7)-H(7)	107.7
C(12)-C(7)-S(2)	114.9(14)
C(12)-C(7)-H(7)	107.7
C(12)-C(7)-C(8)	108.6(17)
C(7)-C(8)-H(8A)	109.1
C(7)-C(8)-H(8B)	109.1
H(8A)-C(8)-H(8B)	107.8
C(9)-C(8)-C(7)	112(2)
C(9)-C(8)-H(8A)	109.1
C(9)-C(8)-H(8B)	109.1
C(8)-C(9)-H(9A)	107.9

C(8)-C(9)-H(9B)	107.9
H(9A)-C(9)-H(9B)	107.2
C(10)-C(9)-C(8)	118(2)
C(10)-C(9)-H(9A)	107.9
C(10)-C(9)-H(9B)	107.9
C(9)-C(10)-H(10A)	109.4
C(9)-C(10)-H(10B)	109.4
C(9)-C(10)-C(11)	111(2)
H(10A)-C(10)-H(10B)	108.0
C(11)-C(10)-H(10A)	109.4
C(11)-C(10)-H(10B)	109.4
C(10)-C(11)-H(11A)	108.9
C(10)-C(11)-H(11B)	108.9
C(10)-C(11)-C(12)	114(2)
H(11A)-C(11)-H(11B)	107.7
C(12)-C(11)-H(11A)	108.9
C(12)-C(11)-H(11B)	108.9
C(7)-C(12)-C(11)	113(2)
C(7)-C(12)-H(12A)	109.0
C(7)-C(12)-H(12B)	109.0
C(11)-C(12)-H(12A)	109.0
C(11)-C(12)-H(12B)	109.0
H(12A)-C(12)-H(12B)	107.8
S(3)-C(13)-H(13)	108.2
C(14)-C(13)-S(3)	110.8(10)
C(14)-C(13)-H(13)	108.2
C(14)-C(13)-C(18)	112.1(12)
C(18)-C(13)-S(3)	109.2(10)
C(18)-C(13)-H(13)	108.2
C(13)-C(14)-H(14A)	110.1

C(13)-C(14)-H(14B)	110.1
C(13)-C(14)-C(15)	108.2(14)
H(14A)-C(14)-H(14B)	108.4
C(15)-C(14)-H(14A)	110.1
C(15)-C(14)-H(14B)	110.1
C(14)-C(15)-H(15A)	109.4
C(14)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0
C(16)-C(15)-C(14)	111.3(18)
C(16)-C(15)-H(15A)	109.4
C(16)-C(15)-H(15B)	109.4
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
C(15)-C(16)-C(17)	110.9(17)
H(16A)-C(16)-H(16B)	108.0
C(17)-C(16)-H(16A)	109.5
C(17)-C(16)-H(16B)	109.5
C(16)-C(17)-H(17A)	109.4
C(16)-C(17)-H(17B)	109.4
C(16)-C(17)-C(18)	111.0(16)
H(17A)-C(17)-H(17B)	108.0
C(18)-C(17)-H(17A)	109.4
C(18)-C(17)-H(17B)	109.4
C(13)-C(18)-C(17)	109.7(13)
C(13)-C(18)-H(18A)	109.7
C(13)-C(18)-H(18B)	109.7
C(17)-C(18)-H(18A)	109.7
C(17)-C(18)-H(18B)	109.7
H(18A)-C(18)-H(18B)	108.2
S(4)-C(19)-H(19)	110.3

C(20)-C(19)-S(4)	108.9(11)
C(20)-C(19)-H(19)	110.3
C(20)-C(19)-C(24)	109.6(12)
C(24)-C(19)-S(4)	107.5(10)
C(24)-C(19)-H(19)	110.3
C(19)-C(20)-H(20A)	109.9
C(19)-C(20)-H(20B)	109.9
H(20A)-C(20)-H(20B)	108.3
C(21)-C(20)-C(19)	108.9(15)
C(21)-C(20)-H(20A)	109.9
C(21)-C(20)-H(20B)	109.9
C(20)-C(21)-H(21A)	109.4
C(20)-C(21)-H(21B)	109.4
C(20)-C(21)-C(22)	111.2(17)
H(21A)-C(21)-H(21B)	108.0
C(22)-C(21)-H(21A)	109.4
C(22)-C(21)-H(21B)	109.4
C(21)-C(22)-H(22A)	110.1
C(21)-C(22)-H(22B)	110.1
H(22A)-C(22)-H(22B)	108.4
C(23)-C(22)-C(21)	108.1(16)
C(23)-C(22)-H(22A)	110.1
C(23)-C(22)-H(22B)	110.1
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	108.1
C(24)-C(23)-C(22)	110.8(14)
C(24)-C(23)-H(23A)	109.5
C(24)-C(23)-H(23B)	109.5
C(19)-C(24)-H(24A)	109.4

C(19)-C(24)-H(24B)	109.4
C(23)-C(24)-C(19)	111.1(13)
C(23)-C(24)-H(24A)	109.4
C(23)-C(24)-H(24B)	109.4
H(24A)-C(24)-H(24B)	108.0
S(5)-C(25)-H(25)	107.6
C(26)-C(25)-S(5)	114.1(13)
C(26)-C(25)-H(25)	107.6
C(26)-C(25)-C(30)	109.6(15)
C(30)-C(25)-S(5)	110.1(12)
C(30)-C(25)-H(25)	107.6
C(25)-C(26)-H(26A)	110.0
C(25)-C(26)-H(26B)	110.0
C(25)-C(26)-C(27)	108(2)
H(26A)-C(26)-H(26B)	108.4
C(27)-C(26)-H(26A)	110.0
C(27)-C(26)-H(26B)	110.0
C(26)-C(27)-H(27A)	109.3
C(26)-C(27)-H(27B)	109.3
H(27A)-C(27)-H(27B)	108.0
C(28)-C(27)-C(26)	112(2)
C(28)-C(27)-H(27A)	109.3
C(28)-C(27)-H(27B)	109.3
C(27)-C(28)-H(28A)	109.7
C(27)-C(28)-H(28B)	109.7
H(28A)-C(28)-H(28B)	108.2
C(29)-C(28)-C(27)	110(2)
C(29)-C(28)-H(28A)	109.7
C(29)-C(28)-H(28B)	109.7
C(28)-C(29)-H(29A)	108.8

C(28)-C(29)-H(29B)	108.8
C(28)-C(29)-C(30)	114(2)
H(29A)-C(29)-H(29B)	107.7
C(30)-C(29)-H(29A)	108.8
C(30)-C(29)-H(29B)	108.8
C(25)-C(30)-H(30A)	109.6
C(25)-C(30)-H(30B)	109.6
C(29)-C(30)-C(25)	110.1(18)
C(29)-C(30)-H(30A)	109.6
C(29)-C(30)-H(30B)	109.6
H(30A)-C(30)-H(30B)	108.2
S(6)-C(31)-H(31)	107.6
C(32)-C(31)-S(6)	113.8(10)
C(32)-C(31)-H(31)	107.6
C(32)-C(31)-C(36)	112.2(12)
C(36)-C(31)-S(6)	107.8(10)
C(36)-C(31)-H(31)	107.6
C(31)-C(32)-H(32A)	109.4
C(31)-C(32)-H(32B)	109.4
H(32A)-C(32)-H(32B)	108.0
C(33)-C(32)-C(31)	111.0(13)
C(33)-C(32)-H(32A)	109.4
C(33)-C(32)-H(32B)	109.4
C(32)-C(33)-H(33A)	109.3
C(32)-C(33)-H(33B)	109.3
C(32)-C(33)-C(34)	111.8(14)
H(33A)-C(33)-H(33B)	107.9
C(34)-C(33)-H(33A)	109.3
C(34)-C(33)-H(33B)	109.3
C(33)-C(34)-H(34A)	109.6

C(33)-C(34)-H(34B)	109.6
H(34A)-C(34)-H(34B)	108.1
C(35)-C(34)-C(33)	110.3(15)
C(35)-C(34)-H(34A)	109.6
C(35)-C(34)-H(34B)	109.6
C(34)-C(35)-H(35A)	109.8
C(34)-C(35)-H(35B)	109.8
C(34)-C(35)-C(36)	109.3(14)
H(35A)-C(35)-H(35B)	108.3
C(36)-C(35)-H(35A)	109.8
C(36)-C(35)-H(35B)	109.8
C(31)-C(36)-H(36A)	109.6
C(31)-C(36)-H(36B)	109.6
C(35)-C(36)-C(31)	110.2(13)
C(35)-C(36)-H(36A)	109.6
C(35)-C(36)-H(36B)	109.6
H(36A)-C(36)-H(36B)	108.1
S(7)-C(37)-H(37)	108.8
C(38)-C(37)-S(7)	113.4(11)
C(38)-C(37)-H(37)	108.8
C(38)-C(37)-C(42)	110.5(13)
C(42)-C(37)-S(7)	106.4(10)
C(42)-C(37)-H(37)	108.8
C(37)-C(38)-H(38A)	109.0
C(37)-C(38)-H(38B)	109.0
C(37)-C(38)-C(39)	112.9(17)
H(38A)-C(38)-H(38B)	107.8
C(39)-C(38)-H(38A)	109.0
C(39)-C(38)-H(38B)	109.0
C(38)-C(39)-H(39A)	109.2

C(38)-C(39)-H(39B)	109.2
H(39A)-C(39)-H(39B)	107.9
C(40)-C(39)-C(38)	112.0(18)
C(40)-C(39)-H(39A)	109.2
C(40)-C(39)-H(39B)	109.2
C(39)-C(40)-H(40A)	109.7
C(39)-C(40)-H(40B)	109.7
C(39)-C(40)-C(41)	109.7(16)
H(40A)-C(40)-H(40B)	108.2
C(41)-C(40)-H(40A)	109.7
C(41)-C(40)-H(40B)	109.7
C(40)-C(41)-H(41A)	108.7
C(40)-C(41)-H(41B)	108.7
C(40)-C(41)-C(42)	114.1(15)
H(41A)-C(41)-H(41B)	107.6
C(42)-C(41)-H(41A)	108.7
C(42)-C(41)-H(41B)	108.7
C(37)-C(42)-H(42A)	109.5
C(37)-C(42)-H(42B)	109.5
C(41)-C(42)-C(37)	110.6(14)
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	108.1
S(8)-C(43)-H(43)	108.2
C(44)-C(43)-S(8)	108.3(12)
C(44)-C(43)-H(43)	108.2
C(48)-C(43)-S(8)	114.5(13)
C(48)-C(43)-H(43)	108.2
C(48)-C(43)-C(44)	109.1(16)
C(43)-C(44)-H(44A)	109.6

C(43)-C(44)-H(44B)	109.6
H(44A)-C(44)-H(44B)	108.1
C(45)-C(44)-C(43)	110.2(19)
C(45)-C(44)-H(44A)	109.6
C(45)-C(44)-H(44B)	109.6
C(44)-C(45)-H(45A)	107.9
C(44)-C(45)-H(45B)	107.9
C(44)-C(45)-C(46)	118(2)
H(45A)-C(45)-H(45B)	107.2
C(46)-C(45)-H(45A)	107.9
C(46)-C(45)-H(45B)	107.9
C(45)-C(46)-H(46A)	108.9
C(45)-C(46)-H(46B)	108.9
C(45)-C(46)-C(47)	113(2)
H(46A)-C(46)-H(46B)	107.7
C(47)-C(46)-H(46A)	108.9
C(47)-C(46)-H(46B)	108.9
C(46)-C(47)-H(47A)	110.7
C(46)-C(47)-H(47B)	110.7
C(46)-C(47)-C(48)	105(2)
H(47A)-C(47)-H(47B)	108.8
C(48)-C(47)-H(47A)	110.7
C(48)-C(47)-H(47B)	110.7
C(43)-C(48)-C(47)	113.8(18)
C(43)-C(48)-H(48A)	108.8
C(43)-C(48)-H(48B)	108.8
C(47)-C(48)-H(48A)	108.8
C(47)-C(48)-H(48B)	108.8
H(48A)-C(48)-H(48B)	107.7
S(9)-C(49)-H(49)	108.2

C(50)-C(49)-S(9)	115.2(10)
C(50)-C(49)-H(49)	108.2
C(50)-C(49)-C(54)	111.9(12)
C(54)-C(49)-S(9)	105.1(10)
C(54)-C(49)-H(49)	108.2
C(49)-C(50)-H(50A)	109.4
C(49)-C(50)-H(50B)	109.4
H(50A)-C(50)-H(50B)	108.0
C(51)-C(50)-C(49)	111.1(14)
C(51)-C(50)-H(50A)	109.4
C(51)-C(50)-H(50B)	109.4
C(50)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51B)	109.5
C(50)-C(51)-C(52)	110.5(16)
H(51A)-C(51)-H(51B)	108.1
C(52)-C(51)-H(51A)	109.5
C(52)-C(51)-H(51B)	109.5
C(51)-C(52)-H(52A)	109.2
C(51)-C(52)-H(52B)	109.2
H(52A)-C(52)-H(52B)	107.9
C(53)-C(52)-C(51)	112.0(18)
C(53)-C(52)-H(52A)	109.2
C(53)-C(52)-H(52B)	109.2
C(52)-C(53)-H(53A)	110.0
C(52)-C(53)-H(53B)	110.0
C(52)-C(53)-C(54)	108.5(16)
H(53A)-C(53)-H(53B)	108.4
C(54)-C(53)-H(53A)	110.0
C(54)-C(53)-H(53B)	110.0
C(49)-C(54)-C(53)	109.7(14)

C(49)-C(54)-H(54A)	109.7
C(49)-C(54)-H(54B)	109.7
C(53)-C(54)-H(54A)	109.7
C(53)-C(54)-H(54B)	109.7
H(54A)-C(54)-H(54B)	108.2
S(10)-C(55)-H(55)	106.8
C(56)-C(55)-S(10)	108.7(9)
C(56)-C(55)-H(55)	106.8
C(60)-C(55)-S(10)	114.5(9)
C(60)-C(55)-H(55)	106.8
C(60)-C(55)-C(56)	112.8(12)
C(55)-C(56)-H(56A)	109.7
C(55)-C(56)-H(56B)	109.7
C(55)-C(56)-C(57)	109.8(13)
H(56A)-C(56)-H(56B)	108.2
C(57)-C(56)-H(56A)	109.7
C(57)-C(56)-H(56B)	109.7
C(56)-C(57)-H(57A)	109.7
C(56)-C(57)-H(57B)	109.7
C(56)-C(57)-C(58)	109.8(15)
H(57A)-C(57)-H(57B)	108.2
C(58)-C(57)-H(57A)	109.7
C(58)-C(57)-H(57B)	109.7
C(57)-C(58)-H(58A)	109.3
C(57)-C(58)-H(58B)	109.3
C(57)-C(58)-C(59)	111.7(15)
H(58A)-C(58)-H(58B)	107.9
C(59)-C(58)-H(58A)	109.3
C(59)-C(58)-H(58B)	109.3
C(58)-C(59)-H(59A)	110.2

C(58)-C(59)-H(59B)	110.2
C(58)-C(59)-C(60)	107.5(14)
H(59A)-C(59)-H(59B)	108.5
C(60)-C(59)-H(59A)	110.2
C(60)-C(59)-H(59B)	110.2
C(55)-C(60)-C(59)	111.7(13)
C(55)-C(60)-H(60A)	109.3
C(55)-C(60)-H(60B)	109.3
C(59)-C(60)-H(60A)	109.3
C(59)-C(60)-H(60B)	109.3
H(60A)-C(60)-H(60B)	107.9
S(11)-C(61)-H(61)	109.9
C(62)-C(61)-S(11)	108.6(9)
C(62)-C(61)-H(61)	109.9
C(62)-C(61)-C(66)	110.9(11)
C(66)-C(61)-S(11)	107.5(9)
C(66)-C(61)-H(61)	109.9
C(61)-C(62)-H(62A)	110.0
C(61)-C(62)-H(62B)	110.0
C(61)-C(62)-C(63)	108.6(13)
H(62A)-C(62)-H(62B)	108.3
C(63)-C(62)-H(62A)	110.0
C(63)-C(62)-H(62B)	110.0
C(62)-C(63)-H(63A)	109.9
C(62)-C(63)-H(63B)	109.9
C(62)-C(63)-C(64)	109.0(15)
H(63A)-C(63)-H(63B)	108.3
C(64)-C(63)-H(63A)	109.9
C(64)-C(63)-H(63B)	109.9
C(63)-C(64)-H(64A)	109.9

C(63)-C(64)-H(64B)	109.9
H(64A)-C(64)-H(64B)	108.3
C(65)-C(64)-C(63)	108.8(15)
C(65)-C(64)-H(64A)	109.9
C(65)-C(64)-H(64B)	109.9
C(64)-C(65)-H(65A)	109.0
C(64)-C(65)-H(65B)	109.0
C(64)-C(65)-C(66)	112.7(14)
H(65A)-C(65)-H(65B)	107.8
C(66)-C(65)-H(65A)	109.0
C(66)-C(65)-H(65B)	109.0
C(61)-C(66)-C(65)	108.7(11)
C(61)-C(66)-H(66A)	109.9
C(61)-C(66)-H(66B)	109.9
C(65)-C(66)-H(66A)	109.9
C(65)-C(66)-H(66B)	109.9
H(66A)-C(66)-H(66B)	108.3

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for$Au_{42}(SC_6H_{11})_{26}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Au(1)	3567	2850	7335	54(1)
Au(2)	4771	2022	7885	51(1)
Au(3)	5942	1239	8432	56(1)
Au(4)	5998	2345	7775	54(1)
Au(5)	4823	3228	7176	52(1)
Au(6)	5793	1734	7061	53(1)
Au(7)	3805	3583	7950	54(1)
Au(8)	3870	4669	7295	58(1)
Au(9)	3423	3970	6662	61(1)
Au(10)	4683	4310	5946	66(1)
Au(11)	5005	4946	6650	71(1)
Au(12)	4654	2532	6516	57(1)
Au(13)	5650	913	6334	64(1)
Au(14)	6879	409	6887	61(1)
Au(15)	5863	533	7648	58(1)
Au(16)	4473	1418	7218	55(1)
Au(17)	3552	1735	7985	57(1)
Au(18)	4652	256	8401	63(1)
Au(19)	2084	2317	7622	63(1)
Au(20)	2267	3563	6964	64(1)
Au(21)	3199	2187	6595	62(1)
Au(22)	5802	2879	6419	58(1)
Au(23)	6231	3417	7177	66(1)
Au(24)	7328	2329	7737	66(1)
Au(25)	8966	1096	7383	74(1)
Au(26)	7001	860	7640	60(1)

Au(27)	6996	1533	6080	67(1)
Au(28)	6365	3001	8498	72(1)
Au(29)	4973	3918	7860	58(1)
Au(30)	3935	4423	8699	67(1)
Au(31)	2707	4160	8576	68(1)
Au(32)	2650	5537	7911	72(1)
Au(33)	2558	4382	7431	64(1)
Au(34)	2522	3266	8106	64(1)
Au(35)	3640	2609	8656	62(1)
Au(36)	5047	2670	8540	58(1)
Au(37)	4818	972	9119	64(1)
Au(38)	7430	1116	8521	64(1)
Au(39)	7029	2022	6990	64(1)
Au(40)	967	4998	8484	131(1)
Au(41)	686	4600	7431	76(1)
Au(42)	8638	-66	6743	76(1)
S(1)	5923	3706	5781	70(2)
S(2)	6263	4366	6605	67(3)
S(3)	3786	5729	6776	80(3)
S(4)	3424	4857	6035	68(3)
S(5)	6260	1297	5706	75(3)
S(6)	7894	1625	6379	67(3)
S(7)	7888	-474	6536	69(3)
S(8)	9472	332	6837	81(3)
S(9)	8540	1878	7908	69(3)
S(10)	5905	4136	8065	98(4)
S(11)	3448	5602	8324	64(2)
S(12)	1748	5610	7522	74(3)
S(13)	1675	4489	9109	143(6)
S(14)	179	5430	7936	101(4)

S(15)	1036	3882	6873	74(3)
S(16)	3777	2698	6040	63(2)
S(17)	5048	361	6859	65(3)
S(18)	5839	-463	8187	65(2)
S(19)	8029	217	8061	62(2)
S(20)	6981	1974	9008	71(3)
S(21)	6059	274	9043	64(2)
S(22)	3604	1734	9278	71(3)
S(23)	3377	804	8519	63(2)
S(24)	2540	1622	7044	62(2)
S(25)	1482	3051	8175	69(3)
S(26)	4428	3313	9157	69(3)
C(1)	5960	3277	5268	76(3)
C(2)	5542	3845	4910	76(4)
C(3)	5649	3543	4485	78(4)
C(4)	6592	3213	4346	80(4)
C(5)	6948	2624	4662	80(4)
C(6)	6811	2912	5099	78(4)
C(7)	6437	5055	6816	90(15)
C(8)	6200	5749	6462	125(18)
C(9)	6355	6420	6592	131(18)
C(10)	7264	5889	6733	190(40)
C(11)	7293	5326	7096	120(20)
C(12)	7126	4783	6980	80(13)
C(13)	3725	6426	7133	90(4)
C(14)	3295	7174	6864	94(5)
C(15)	3261	7817	7055	96(5)
C(16)	4013	7609	7200	96(5)
C(17)	4258	6891	7522	95(5)
C(18)	4419	6180	7361	93(5)

C(19)	3170	4575	5566	55(9)
C(20)	2411	4594	5663	59(9)
C(21)	2232	4431	5233	71(11)
C(22)	2307	4863	4818	120(20)
C(23)	3115	4836	4713	78(12)
C(24)	3212	5077	5135	79(13)
C(25)	6911	422	5465	81(4)
C(26)	6691	-133	5597	83(4)
C(27)	7327	-845	5372	84(5)
C(28)	7389	-697	4902	83(5)
C(29)	7524	-124	4763	83(4)
C(30)	7094	563	4931	83(4)
C(31)	7978	2463	6089	69(11)
C(32)	8507	2264	5664	63(10)
C(33)	8654	2918	5415	82(13)
C(34)	8916	3195	5708	99(17)
C(35)	8454	3349	6160	98(17)
C(36)	8310	2700	6399	70(11)
C(37)	8156	-1439	6851	74(12)
C(38)	7886	-1774	6601	96(16)
C(39)	8146	-2610	6866	101(17)
C(40)	8908	-2964	6876	87(14)
C(41)	9213	-2604	7139	95(16)
C(42)	9058	-1853	6881	107(19)
C(43)	10164	-443	7108	89(15)
C(44)	10861	-346	7124	71(11)
C(45)	11552	-1012	7272	103(18)
C(46)	11320	-1270	7766	83(13)
C(47)	10621	-1476	7782	93(15)
C(48)	10054	-859	7520	120(20)

C(49)	8876	2555	7675	60(9)
C(50)	8419	3281	7888	71(11)
C(51)	8690	3869	7690	95(16)
C(52)	9549	3515	7820	81(13)
C(53)	9947	2822	7628	86(14)
C(54)	9696	2209	7796	71(11)
C(55)	5683	4764	8449	111(5)
C(56)	5327	5573	8252	114(5)
C(57)	5504	6002	8528	117(6)
C(58)	6333	5659	8543	117(6)
C(59)	6588	4901	8822	117(6)
C(60)	5964	4680	8900	114(5)
C(61)	2812	6233	8770	81(13)
C(62)	2350	7016	8542	110(20)
C(63)	1960	7373	8937	140(30)
C(64)	2483	7455	9201	108(19)
C(65)	2930	6784	9367	140(30)
C(66)	3266	6249	9047	150(30)
C(67)	1799	6078	6957	82(13)
C(68)	1398	5978	6642	60(9)
C(69)	1399	6449	6158	109(19)
C(70)	1073	7297	6145	107(19)
C(71)	1522	7304	6525	88(14)
C(72)	1500	6951	6978	75(12)
C(73)	1629	4720	9648	147(7)
C(74)	1747	4243	10107	148(7)
C(75)	2247	4371	10361	149(7)
C(76)	1872	5165	10452	149(8)
C(77)	1838	5671	10007	148(7)
C(78)	1950	5257	9621	148(7)

C(79)	-597	5312	8226	107(5)
C(80)	-894	5272	8719	110(5)
C(81)	-1711	5481	8762	111(5)
C(82)	-2067	6273	8550	111(6)
C(83)	-1798	6364	8061	111(5)
C(84)	-1230	5635	7927	110(5)
C(85)	764	4583	6330	69(11)
C(86)	36	5269	6413	110(20)
C(87)	-575	5057	6589	77(12)
C(88)	-688	4636	6231	90(15)
C(89)	-38	3993	6122	92(15)
C(90)	671	4130	5997	86(14)
C(91)	4195	2107	5583	70(11)
C(92)	3621	1944	5437	58(9)
C(93)	3900	1499	5068	95(16)
C(94)	4150	2050	4615	107(19)
C(95)	4783	2069	4800	87(14)
C(96)	4497	2475	5233	97(16)
C(97)	4415	237	6548	59(9)
C(98)	4055	-171	6879	71(11)
C(99)	3548	-340	6681	76(12)
C(100)	3887	-673	6250	99(17)
C(101)	4290	-225	5896	71(11)
C(102)	4801	-143	6142	75(12)
C(103)	5713	-1070	7858	67(10)
C(104)	5673	-1707	8220	76(12)
C(105)	5534	-2209	7985	80(13)
C(106)	6194	-2509	7558	107(19)
C(107)	6221	-1870	7278	79(13)
C(108)	6348	-1327	7508	59(9)

C(109)	7928	-610	8341	75(12)
C(110)	8577	-1047	8699	61(9)
C(111)	8492	-1785	8964	110(20)
C(112)	8509	-2232	8628	79(13)
C(113)	7925	-1746	8279	86(14)
C(114)	7965	-1060	8042	70(11)
C(115)	7794	2077	9040	72(11)
C(116)	7476	2791	9357	89(15)
C(117)	8127	3007	9367	120(20)
C(118)	8743	2225	9588	140(30)
C(119)	9010	1599	9305	92(15)
C(120)	8440	1399	9282	88(14)
C(121)	6421	492	9534	65(10)
C(122)	5944	415	9962	66(10)
C(123)	6237	535	10369	86(14)
C(124)	7029	8	10390	110(20)
C(125)	7501	39	9972	60(9)
C(126)	7124	41	9555	76(12)
C(127)	3692	2097	9773	66(10)
C(128)	3044	2785	9843	72(11)
C(129)	3134	3085	10253	79(13)
C(130)	3143	2508	10675	84(14)
C(131)	3785	1797	10638	89(14)
C(132)	3795	1498	10201	65(10)
C(133)	3210	223	8212	70(11)
C(134)	2372	452	8232	78(12)
C(135)	2213	16	7952	94(16)
C(136)	2616	-849	8180	81(13)
C(137)	3408	-1024	8130	105(18)
C(138)	3616	-595	8426	79(13)

C(139)	1684	1933	6713	75(12)
C(140)	1377	1408	6932	75(12)
C(141)	633	1661	6729	94(16)
C(142)	894	1448	6218	84(14)
C(143)	1255	2009	5978	120(20)
C(144)	1946	1842	6235	77(12)
C(145)	1584	2405	8727	82(13)
C(146)	1412	2891	9100	75(12)
C(147)	1429	2402	9573	82(13)
C(148)	888	2162	9578	88(14)
C(149)	1011	1711	9217	86(14)
C(150)	977	2207	8766	75(12)
C(151)	5009	3328	9511	87(14)
C(152)	5316	2628	9843	83(13)
C(153)	5813	2605	10174	103(18)
C(154)	5300	3254	10418	110(20)
C(155)	5151	3958	10090	108(19)
C(156)	4652	3986	9763	90(15)

Table S6. Bond lengths [Å] and angles [°] for $Au_{42}(S_C6H_{11})_{26}$

Atom1-Atom2	Length/ Å
Au(1)-Au(2)	2.8569
Au(1)-Au(5)	2.9789
Au(1)-Au(7)	2.8587
Au(1)-Au(9)	2.7056
Au(1)-Au(12)	3.0291
Au(1)-Au(16)	2.7494
Au(1)-Au(17)	2.7334
Au(1)-Au(20)	2.7023
Au(1)-Au(21)	3.2059
Au(1)-Au(33)	2.9361
Au(1)-Au(34)	2.8930
Au(2)-Au(3)	2.7998
Au(2)-Au(4)	2.8570
Au(2)-Au(5)	2.9876
Au(2)-Au(6)	2.9713
Au(2)-Au(7)	2.9501
Au(2)-Au(15)	3.0199
Au(2)-Au(16)	2.8615
Au(2)-Au(17)	2.7981
Au(2)-Au(35)	3.0336
Au(2)-Au(36)	2.8682
Au(3)-Au(4)	2.7556
Au(3)-Au(15)	3.0974
Au(3)-Au(26)	2.9482
Au(3)-Au(36)	2.7361
Au(3)-Au(37)	3.0345
Au(3)-Au(38)	3.0126

Au(3)-S(21)	2.3920
Au(4)-Au(5)	2.9230
Au(4)-Au(6)	2.8950
Au(4)-Au(23)	2.7509
Au(4)-Au(24)	2.7120
Au(4)-Au(26)	2.8854
Au(4)-Au(28)	3.1514
Au(4)-Au(29)	3.0023
Au(4)-Au(36)	2.7668
Au(4)-Au(39)	2.8944
Au(5)-Au(6)	2.8712
Au(5)-Au(7)	2.8615
Au(5)-Au(8)	2.7821
Au(5)-Au(9)	3.0894
Au(5)-Au(12)	2.8437
Au(5)-Au(22)	2.7807
Au(5)-Au(23)	3.1043
Au(5)-Au(29)	2.8777
Au(6)-Au(12)	2.7539
Au(6)-Au(13)	3.1716
Au(6)-Au(14)	2.7203
Au(6)-Au(15)	2.7172
Au(6)-Au(16)	3.0299
Au(6)-Au(22)	2.7600
Au(6)-Au(26)	2.9267
Au(6)-Au(39)	2.8393
Au(7)-Au(8)	2.7277
Au(7)-Au(29)	2.7587
Au(7)-Au(30)	3.2391
Au(7)-Au(31)	2.6861

Au(7)-Au(33)	2.8619
Au(7)-Au(34)	2.9562
Au(7)-Au(35)	2.7311
Au(7)-Au(36)	3.0014
Au(8)-Au(9)	3.0932
Au(8)-Au(11)	2.9964
Au(8)-Au(29)	2.7349
Au(8)-Au(32)	2.9585
Au(8)-Au(33)	2.9772
Au(8)-S(3)	2.3885
Au(9)-Au(10)	3.3540
Au(9)-Au(12)	2.9595
Au(9)-Au(20)	2.8403
Au(9)-Au(33)	2.7275
Au(9)-S(4)	2.3695
Au(10)-Au(11)	3.0234
Au(10)-Au(22)	3.0425
Au(10)-S(1)	2.2937
Au(10)-S(4)	2.3020
Au(11)-Au(23)	3.3028
Au(11)-S(2)	2.2980
Au(11)-S(3)	2.3017
Au(12)-Au(13)	3.1384
Au(12)-Au(16)	2.9311
Au(12)-Au(21)	3.3536
Au(12)-Au(22)	2.7341
Au(12)-S(16)	2.3529
Au(13)-Au(14)	2.9283
Au(13)-Au(16)	3.3040
Au(13)-S(5)	2.3236

Au(13)-S(17)	2.3101
Au(14)-Au(15)	2.8263
Au(14)-Au(26)	2.7245
Au(14)-Au(27)	3.0918
Au(14)-Au(42)	3.2736
Au(14)-S(7)	2.3247
Au(15)-Au(16)	2.9505
Au(15)-Au(18)	3.2800
Au(15)-Au(26)	2.7214
Au(15)-S(18)	2.3806
Au(16)-Au(17)	2.7442
Au(16)-Au(21)	3.0918
Au(16)-S(17)	2.3576
Au(17)-Au(18)	3.0200
Au(17)-Au(19)	3.0025
Au(17)-Au(34)	2.9604
Au(17)-Au(35)	3.0638
Au(17)-S(23)	2.3836
Au(18)-Au(37)	3.0168
Au(18)-S(18)	2.2723
Au(18)-S(23)	2.3357
Au(19)-Au(20)	3.0660
Au(19)-Au(34)	3.1734
Au(19)-S(24)	2.2994
Au(19)-S(25)	2.3029
Au(20)-Au(21)	2.9431
Au(20)-Au(33)	2.7255
Au(20)-Au(41)	3.2526
Au(20)-S(15)	2.3610
Au(21)-S(16)	2.2796

Au(21)-S(24)	2.3040
Au(22)-Au(23)	3.1522
Au(22)-Au(27)	2.9918
Au(22)-Au(39)	2.9345
Au(22)-S(1)	2.3782
Au(23)-Au(24)	2.8491
Au(23)-Au(29)	2.9643
Au(23)-Au(39)	2.7207
Au(23)-S(2)	2.3690
Au(24)-Au(25)	3.3349
Au(24)-Au(28)	2.9179
Au(24)-Au(38)	3.0529
Au(24)-Au(39)	2.7089
Au(24)-S(9)	2.3373
Au(25)-S(8)	2.3088
Au(25)-S(9)	2.2873
Au(26)-Au(38)	3.1627
Au(26)-Au(39)	2.8101
Au(26)-S(19)	2.3455
Au(27)-Au(39)	3.1500
Au(27)-S(5)	2.3021
Au(27)-S(6)	2.2847
Au(28)-Au(29)	3.3012
Au(28)-Au(36)	3.0748
Au(28)-S(10)	2.2969
Au(28)-S(20)	2.3186
Au(29)-Au(30)	3.0716
Au(29)-Au(36)	2.9300
Au(29)-S(10)	2.3624
Au(30)-Au(31)	2.9177

Au(30)-Au(36)	3.3788
Au(30)-S(11)	2.2976
Au(30)-S(26)	2.3012
Au(31)-Au(32)	3.1151
Au(31)-Au(34)	2.7397
Au(31)-Au(35)	2.8748
Au(31)-Au(40)	3.2205
Au(31)-S(13)	2.3729
Au(32)-Au(33)	3.1328
Au(32)-S(11)	2.2873
Au(32)-S(12)	2.2916
Au(33)-Au(34)	2.7887
Au(33)-S(12)	2.3629
Au(34)-Au(35)	2.7210
Au(34)-S(25)	2.3543
Au(35)-Au(36)	2.9243
Au(35)-Au(37)	3.3186
Au(35)-S(22)	2.3601
Au(36)-S(26)	2.3679
Au(37)-S(21)	2.2910
Au(37)-S(22)	2.2987
Au(38)-S(19)	2.3107
Au(38)-S(20)	2.3060
Au(39)-S(6)	2.3463
Au(40)-S(13)	2.3510
Au(40)-S(14)	2.2698
Au(41)-S(14)	2.3019
Au(41)-S(15)	2.2902
Au(42)-S(7)	2.2872
Au(42)-S(8)	2.2977

S(1)-C(1)	1.9195
S(2)-C(7)	1.8693
S(3)-C(13)	1.9245
S(4)-C(19)	1.8729
S(5)-C(25)	1.9013
S(6)-C(31)	1.8558
S(7)-C(37)	1.9027
S(8)-C(43)	1.7441
S(9)-C(49)	1.8168
S(10)-C(55)	1.7766
S(11)-C(61)	1.9585
S(12)-C(67)	1.8085
S(13)-C(73)	1.7730
S(14)-C(79)	1.7950
S(15)-C(85)	1.9335
S(16)-C(91)	1.8725
S(17)-C(97)	1.8594
S(18)-C(103)	1.8819
S(19)-C(109)	1.8418
S(20)-C(115)	1.8055
S(21)-C(121)	1.9814
S(22)-C(127)	1.8795
S(23)-C(133)	1.8377
S(24)-C(139)	1.9513
S(25)-C(145)	1.8995
S(26)-C(151)	1.7472
C(1)-H(1)	1.0000
C(1)-C(2)	1.4730
C(1)-C(6)	1.6015
C(2)-H(2A)	0.9900

C(2)-H(2B)	0.9900
C(2)-C(3)	1.4858
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(3)-C(4)	1.7485
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(4)-C(5)	1.3742
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(5)-C(6)	1.4978
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-H(7)	1.0000
C(7)-C(8)	1.5396
C(7)-C(12)	1.4011
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(8)-C(9)	1.6936
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(9)-C(10)	1.7566
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(10)-C(11)	1.4215
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(11)-C(12)	1.4381
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900

C(13)-H(13)	1.0000
C(13)-C(14)	1.5242
C(13)-C(18)	1.5139
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(14)-C(15)	1.5256
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(15)-C(16)	1.5221
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(16)-C(17)	1.5215
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(17)-C(18)	1.5189
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-H(19)	1.0000
C(19)-C(20)	1.5292
C(19)-C(24)	1.5183
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(20)-C(21)	1.5510
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(21)-C(22)	1.4242
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(22)-C(23)	1.6226
C(23)-H(23A)	0.9900

C(23)-H(23B)	0.9900
C(23)-C(24)	1.5398
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-H(25)	1.0000
C(25)-C(26)	1.3866
C(25)-C(30)	1.6077
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(26)-C(27)	1.6458
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(27)-C(28)	1.3954
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(28)-C(29)	1.3169
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(29)-C(30)	1.4370
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-H(31)	1.0000
C(31)-C(32)	1.5401
C(31)-C(36)	1.5168
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(32)-C(33)	1.5490
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(33)-C(34)	1.4337

C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(34)-C(35)	1.5402
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(35)-C(36)	1.5282
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-H(37)	1.0000
C(37)-C(38)	1.4404
C(37)-C(42)	1.6617
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(38)-C(39)	1.6349
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(39)-C(40)	1.3998
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(40)-C(41)	1.5569
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(41)-C(42)	1.5085
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-H(43)	1.0000
C(43)-C(44)	1.5493
C(43)-C(48)	1.4201
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900

C(44)-C(45)	1.5145
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(45)-C(46)	1.5668
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(46)-C(47)	1.6739
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(47)-C(48)	1.4684
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-H(49)	1.0000
C(49)-C(50)	1.5712
C(49)-C(54)	1.5777
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(50)-C(51)	1.5442
C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900
C(51)-C(52)	1.6579
C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900
C(52)-C(53)	1.4757
C(53)-H(53A)	0.9900
C(53)-H(53B)	0.9900
C(53)-C(54)	1.5510
C(54)-H(54A)	0.9900
C(54)-H(54B)	0.9900
C(55)-C(56)	1.5229

C(55)-C(60)	1.5198
C(56)-H(56A)	0.9900
C(56)-H(56B)	0.9900
C(56)-C(57)	1.5237
C(57)-H(57A)	0.9900
C(57)-H(57B)	0.9900
C(57)-C(58)	1.5264
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
C(58)-C(59)	1.5222
C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(59)-C(60)	1.5235
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900
C(61)-H(61)	1.0000
C(61)-C(62)	1.5390
C(61)-C(66)	1.3714
C(62)-H(62A)	0.9900
C(62)-H(62B)	0.9900
C(62)-C(63)	1.4602
C(63)-H(63A)	0.9900
C(63)-H(63B)	0.9900
C(63)-C(64)	1.5288
C(64)-H(64A)	0.9900
C(64)-H(64B)	0.9900
C(64)-C(65)	1.3159
C(65)-H(65A)	0.9900
C(65)-H(65B)	0.9900
C(65)-C(66)	1.4713

C(66)-H(66A)	0.9900
C(66)-H(66B)	0.9900
C(67)-H(67)	1.0000
C(67)-C(68)	1.4611
C(67)-C(72)	1.6345
C(68)-H(68A)	0.9900
C(68)-H(68B)	0.9900
C(68)-C(69)	1.5934
C(69)-H(69A)	0.9900
C(69)-H(69B)	0.9900
C(69)-C(70)	1.5639
C(70)-H(70A)	0.9900
C(70)-H(70B)	0.9900
C(70)-C(71)	1.5985
C(71)-H(71A)	0.9900
C(71)-H(71B)	0.9900
C(71)-C(72)	1.4259
C(72)-H(72A)	0.9900
C(72)-H(72B)	0.9900
C(73)-H(73)	1.0000
C(73)-C(74)	1.5208
C(73)-C(78)	1.5189
C(74)-H(74A)	0.9900
C(74)-H(74B)	0.9900
C(74)-C(75)	1.5247
C(75)-H(75A)	0.9900
C(75)-H(75B)	0.9900
C(75)-C(76)	1.5260
C(76)-H(76A)	0.9900
C(76)-H(76B)	0.9900

C(76)-C(77)	1.5273
C(77)-H(77A)	0.9900
C(77)-H(77B)	0.9900
C(77)-C(78)	1.5169
C(78)-H(78A)	0.9900
C(78)-H(78B)	0.9900
C(79)-H(79)	1.0000
C(79)-C(80)	1.5271
C(79)-C(84)	1.5193
C(80)-H(80A)	0.9900
C(80)-H(80B)	0.9900
C(80)-C(81)	1.5242
C(81)-H(81A)	0.9900
C(81)-H(81B)	0.9900
C(81)-C(82)	1.5066
C(82)-H(82A)	0.9900
C(82)-H(82B)	0.9900
C(82)-C(83)	1.5062
C(83)-H(83A)	0.9900
C(83)-H(83B)	0.9900
C(83)-C(84)	1.5145
C(84)-H(84A)	0.9900
C(84)-H(84B)	0.9900
C(85)-H(85)	1.0000
C(85)-C(86)	1.5493
C(85)-C(90)	1.5975
C(86)-H(86A)	0.9900
C(86)-H(86B)	0.9900
C(86)-C(87)	1.5066
C(87)-H(87A)	0.9900

C(87)-H(87B)	0.9900
C(87)-C(88)	1.6268
C(88)-H(88A)	0.9900
C(88)-H(88B)	0.9900
C(88)-C(89)	1.4411
C(89)-H(89A)	0.9900
C(89)-H(89B)	0.9900
C(89)-C(90)	1.5892
C(90)-H(90A)	0.9900
C(90)-H(90B)	0.9900
C(91)-H(91)	1.0000
C(91)-C(92)	1.5197
C(91)-C(96)	1.4150
C(92)-H(92A)	0.9900
C(92)-H(92B)	0.9900
C(92)-C(93)	1.4699
C(93)-H(93A)	0.9900
C(93)-H(93B)	0.9900
C(93)-C(94)	1.7746
C(94)-H(94A)	0.9900
C(94)-H(94B)	0.9900
C(94)-C(95)	1.5198
C(95)-H(95A)	0.9900
C(95)-H(95B)	0.9900
C(95)-C(96)	1.5898
C(96)-H(96A)	0.9900
C(96)-H(96B)	0.9900
C(97)-H(97)	1.0000
C(97)-C(98)	1.5098
C(97)-C(102)	1.5104

C(98)-H(98A)	0.9900
C(98)-H(98B)	0.9900
C(98)-C(99)	1.4864
C(99)-H(99A)	0.9900
C(99)-H(99B)	0.9900
C(99)-C(100)	1.5180
C(100)-H(10C)	0.9900
C(100)-H(10D)	0.9900
C(100)-C(101)	1.6525
C(101)-H(10E)	0.9900
C(101)-H(10F)	0.9900
C(101)-C(102)	1.4718
C(102)-H(10G)	0.9900
C(102)-H(10H)	0.9900
C(103)-H(103)	1.0000
C(103)-C(104)	1.5655
C(103)-C(108)	1.5059
C(104)-H(10I)	0.9900
C(104)-H(10J)	0.9900
C(104)-C(105)	1.5227
C(105)-H(10K)	0.9900
C(105)-H(10L)	0.9900
C(105)-C(106)	1.7035
C(106)-H(10M)	0.9900
C(106)-H(10N)	0.9900
C(106)-C(107)	1.4439
C(107)-H(10O)	0.9900
C(107)-H(10P)	0.9900
C(107)-C(108)	1.5712
C(108)-H(10Q)	0.9900

C(108)-H(10R)	0.9900
C(109)-H(109)	1.0000
C(109)-C(110)	1.6593
C(109)-C(114)	1.3973
C(110)-H(11C)	0.9900
C(110)-H(11D)	0.9900
C(110)-C(111)	1.6513
C(111)-H(11E)	0.9900
C(111)-H(11F)	0.9900
C(111)-C(112)	1.4968
C(112)-H(11G)	0.9900
C(112)-H(11H)	0.9900
C(112)-C(113)	1.5674
C(113)-H(11I)	0.9900
C(113)-H(11J)	0.9900
C(113)-C(114)	1.4917
C(114)-H(11K)	0.9900
C(114)-H(11L)	0.9900
C(115)-H(115)	1.0000
C(115)-C(116)	1.7398
C(115)-C(120)	1.5726
C(116)-H(11M)	0.9900
C(116)-H(11N)	0.9900
C(116)-C(117)	1.6039
C(117)-H(11O)	0.9900
C(117)-H(11P)	0.9900
C(117)-C(118)	1.6253
C(118)-H(11Q)	0.9900
C(118)-H(11R)	0.9900
C(118)-C(119)	1.5373

C(119)-H(11S)	0.9900
C(119)-H(11T)	0.9900
C(119)-C(120)	1.4305
C(120)-H(12C)	0.9900
C(120)-H(12D)	0.9900
C(121)-H(121)	1.0000
C(121)-C(122)	1.5272
C(121)-C(126)	1.3204
C(122)-H(12E)	0.9900
C(122)-H(12F)	0.9900
C(122)-C(123)	1.5688
C(123)-H(12G)	0.9900
C(123)-H(12H)	0.9900
C(123)-C(124)	1.4955
C(124)-H(12I)	0.9900
C(124)-H(12J)	0.9900
C(124)-C(125)	1.4807
C(125)-H(12K)	0.9900
C(125)-H(12L)	0.9900
C(125)-C(126)	1.5892
C(126)-H(12M)	0.9900
C(126)-H(12N)	0.9900
C(127)-H(127)	1.0000
C(127)-C(128)	1.4660
C(127)-C(132)	1.5752
C(128)-H(12O)	0.9900
C(128)-H(12P)	0.9900
C(128)-C(129)	1.5699
C(129)-C(130)	1.5649
C(130)-H(13A)	0.9900

C(130)-H(13B)	0.9900
C(130)-C(131)	1.4730
C(131)-H(13C)	0.9900
C(131)-H(13D)	0.9900
C(131)-C(132)	1.5664
C(132)-H(13E)	0.9900
C(132)-H(13F)	0.9900
C(133)-H(133)	1.0000
C(133)-C(134)	1.5631
C(133)-C(138)	1.5591
C(134)-H(13G)	0.9900
C(134)-H(13H)	0.9900
C(134)-C(135)	1.5252
C(135)-H(13I)	0.9900
C(135)-H(13J)	0.9900
C(135)-C(136)	1.6444
C(136)-H(13K)	0.9900
C(136)-H(13L)	0.9900
C(136)-C(137)	1.4905
C(137)-H(13M)	0.9900
C(137)-H(13N)	0.9900
C(137)-C(138)	1.6062
C(138)-H(13O)	0.9900
C(138)-H(13P)	0.9900
C(139)-H(139)	1.0000
C(139)-C(140)	1.4958
C(139)-C(144)	1.4831
C(140)-H(14C)	0.9900
C(140)-H(14D)	0.9900
C(140)-C(141)	1.5641

C(141)-H(14E)	0.9900
C(141)-H(14F)	0.9900
C(141)-C(142)	1.6373
C(142)-H(14G)	0.9900
C(142)-H(14H)	0.9900
C(142)-C(143)	1.6500
C(143)-H(14I)	0.9900
C(143)-H(14J)	0.9900
C(143)-C(144)	1.5987
C(144)-H(14K)	0.9900
C(144)-H(14L)	0.9900
C(145)-H(145)	1.0000
C(145)-C(146)	1.5580
C(145)-C(150)	1.4678
C(146)-H(14M)	0.9900
C(146)-H(14N)	0.9900
C(146)-C(147)	1.5811
C(147)-H(14O)	0.9900
C(147)-H(14P)	0.9900
C(147)-C(148)	1.4131
C(148)-H(14Q)	0.9900
C(148)-H(14R)	0.9900
C(148)-C(149)	1.5015
C(149)-H(14S)	0.9900
C(149)-H(14T)	0.9900
C(149)-C(150)	1.5293
C(150)-H(15C)	0.9900
C(150)-H(15D)	0.9900
C(151)-H(151)	1.0000
C(151)-C(152)	1.5165

C(151)-C(156)	1.5187
C(152)-H(15E)	0.9900
C(152)-H(15F)	0.9900
C(152)-C(153)	1.5255
C(153)-H(15G)	0.9900
C(153)-H(15H)	0.9900
C(153)-C(154)	1.5243
C(154)-H(15I)	0.9900
C(154)-H(15J)	0.9900
C(154)-C(155)	1.5240
C(155)-H(15K)	0.9900
C(155)-H(15L)	0.9900
C(155)-C(156)	1.5171
C(156)-H(15M)	0.9900
C(156)-H(15N)	0.9900
atom(1)-atom(2)-atom(3)	angle/ °
Au(2)-Au(1)-Au(5)	61.5
Au(2)-Au(1)-Au(7)	62.1
Au(2)-Au(1)-Au(12)	88.3
Au(2)-Au(1)-Au(21)	123.3
Au(2)-Au(1)-Au(33)	121.2
Au(2)-Au(1)-Au(34)	92.8
Au(5)-Au(1)-Au(12)	56.5
Au(5)-Au(1)-Au(21)	121.3
Au(7)-Au(1)-Au(5)	58.7
Au(7)-Au(1)-Au(12)	115.1
Au(7)-Au(1)-Au(21)	174.3
Au(7)-Au(1)-Au(33)	59.2
Au(7)-Au(1)-Au(34)	61.9
Au(9)-Au(1)-Au(2)	127.2

Au(9)-Au(1)-Au(5)	65.6
Au(9)-Au(1)-Au(7)	90.9
Au(9)-Au(1)-Au(12)	61.8
Au(9)-Au(1)-Au(16)	121.4
Au(9)-Au(1)-Au(17)	172.8
Au(9)-Au(1)-Au(21)	84.2
Au(9)-Au(1)-Au(33)	57.6
Au(9)-Au(1)-Au(34)	114.4
Au(12)-Au(1)-Au(21)	65.0
Au(16)-Au(1)-Au(2)	61.3
Au(16)-Au(1)-Au(5)	91.7
Au(16)-Au(1)-Au(7)	123.4
Au(16)-Au(1)-Au(12)	60.7
Au(16)-Au(1)-Au(21)	62.0
Au(16)-Au(1)-Au(33)	177.4
Au(16)-Au(1)-Au(34)	123.4
Au(17)-Au(1)-Au(2)	60.0
Au(17)-Au(1)-Au(5)	121.6
Au(17)-Au(1)-Au(7)	93.7
Au(17)-Au(1)-Au(12)	120.6
Au(17)-Au(1)-Au(16)	60.1
Au(17)-Au(1)-Au(21)	90.9
Au(17)-Au(1)-Au(33)	120.6
Au(17)-Au(1)-Au(34)	63.4
Au(20)-Au(1)-Au(2)	168.2
Au(20)-Au(1)-Au(5)	128.6
Au(20)-Au(1)-Au(7)	116.0
Au(20)-Au(1)-Au(9)	63.4
Au(20)-Au(1)-Au(12)	102.5
Au(20)-Au(1)-Au(16)	119.8

Au(20)-Au(1)-Au(17)	109.5
Au(20)-Au(1)-Au(21)	59.0
Au(20)-Au(1)-Au(33)	57.6
Au(20)-Au(1)-Au(34)	76.9
Au(33)-Au(1)-Au(5)	89.9
Au(33)-Au(1)-Au(12)	118.8
Au(33)-Au(1)-Au(21)	115.4
Au(34)-Au(1)-Au(5)	120.5
Au(34)-Au(1)-Au(12)	175.6
Au(34)-Au(1)-Au(21)	117.6
Au(34)-Au(1)-Au(33)	57.2
Au(1)-Au(2)-Au(4)	121.2
Au(1)-Au(2)-Au(5)	61.2
Au(1)-Au(2)-Au(6)	89.8
Au(1)-Au(2)-Au(7)	59.0
Au(1)-Au(2)-Au(15)	117.1
Au(1)-Au(2)-Au(16)	57.5
Au(1)-Au(2)-Au(35)	84.5
Au(1)-Au(2)-Au(36)	121.0
Au(3)-Au(2)-Au(1)	178.7
Au(3)-Au(2)-Au(4)	58.3
Au(3)-Au(2)-Au(5)	118.3
Au(3)-Au(2)-Au(6)	90.9
Au(3)-Au(2)-Au(7)	119.8
Au(3)-Au(2)-Au(15)	64.2
Au(3)-Au(2)-Au(16)	123.8
Au(3)-Au(2)-Au(35)	94.7
Au(3)-Au(2)-Au(36)	57.7
Au(4)-Au(2)-Au(5)	60.0
Au(4)-Au(2)-Au(6)	59.5

Au(4)-Au(2)-Au(7)	88.6
Au(4)-Au(2)-Au(15)	85.5
Au(4)-Au(2)-Au(16)	122.1
Au(4)-Au(2)-Au(35)	116.5
Au(4)-Au(2)-Au(36)	57.8
Au(5)-Au(2)-Au(15)	111.5
Au(5)-Au(2)-Au(35)	111.9
Au(6)-Au(2)-Au(5)	57.6
Au(6)-Au(2)-Au(15)	53.9
Au(6)-Au(2)-Au(35)	169.5
Au(7)-Au(2)-Au(5)	57.6
Au(7)-Au(2)-Au(6)	115.2
Au(7)-Au(2)-Au(15)	169.2
Au(7)-Au(2)-Au(35)	54.3
Au(15)-Au(2)-Au(35)	136.5
Au(16)-Au(2)-Au(5)	89.3
Au(16)-Au(2)-Au(6)	62.6
Au(16)-Au(2)-Au(7)	116.4
Au(16)-Au(2)-Au(15)	60.2
Au(16)-Au(2)-Au(35)	120.5
Au(16)-Au(2)-Au(36)	178.4
Au(17)-Au(2)-Au(1)	57.8
Au(17)-Au(2)-Au(3)	122.7
Au(17)-Au(2)-Au(4)	178.9
Au(17)-Au(2)-Au(5)	119.0
Au(17)-Au(2)-Au(6)	120.5
Au(17)-Au(2)-Au(7)	90.4
Au(17)-Au(2)-Au(15)	95.4
Au(17)-Au(2)-Au(16)	58.0
Au(17)-Au(2)-Au(35)	63.2

Au(17)-Au(2)-Au(36)	122.1
Au(36)-Au(2)-Au(5)	89.3
Au(36)-Au(2)-Au(6)	117.3
Au(36)-Au(2)-Au(7)	62.1
Au(36)-Au(2)-Au(15)	121.2
Au(36)-Au(2)-Au(35)	59.3
Au(2)-Au(3)-Au(15)	61.4
Au(2)-Au(3)-Au(26)	91.5
Au(2)-Au(3)-Au(37)	84.7
Au(2)-Au(3)-Au(38)	139.9
Au(4)-Au(3)-Au(2)	61.9
Au(4)-Au(3)-Au(15)	85.8
Au(4)-Au(3)-Au(26)	60.7
Au(4)-Au(3)-Au(37)	138.0
Au(4)-Au(3)-Au(38)	78.2
Au(26)-Au(3)-Au(15)	53.4
Au(26)-Au(3)-Au(37)	150.9
Au(26)-Au(3)-Au(38)	64.1
Au(36)-Au(3)-Au(2)	62.4
Au(36)-Au(3)-Au(4)	60.5
Au(36)-Au(3)-Au(15)	123.1
Au(36)-Au(3)-Au(26)	121.1
Au(36)-Au(3)-Au(37)	82.4
Au(36)-Au(3)-Au(38)	102.0
Au(37)-Au(3)-Au(15)	100.5
Au(38)-Au(3)-Au(15)	115.0
Au(38)-Au(3)-Au(37)	132.1
S(21)-Au(3)-Au(2)	127.0
S(21)-Au(3)-Au(4)	171.0
S(21)-Au(3)-Au(15)	99.9

S(21)-Au(3)-Au(26)	117.3
S(21)-Au(3)-Au(36)	120.5
S(21)-Au(3)-Au(37)	48.2
S(21)-Au(3)-Au(38)	93.0
Au(2)-Au(4)-Au(5)	62.2
Au(2)-Au(4)-Au(6)	62.2
Au(2)-Au(4)-Au(26)	91.7
Au(2)-Au(4)-Au(28)	123.5
Au(2)-Au(4)-Au(29)	89.5
Au(2)-Au(4)-Au(39)	120.9
Au(3)-Au(4)-Au(2)	59.8
Au(3)-Au(4)-Au(5)	122.1
Au(3)-Au(4)-Au(6)	93.4
Au(3)-Au(4)-Au(26)	63.0
Au(3)-Au(4)-Au(28)	89.7
Au(3)-Au(4)-Au(29)	120.2
Au(3)-Au(4)-Au(36)	59.4
Au(3)-Au(4)-Au(39)	121.1
Au(5)-Au(4)-Au(28)	122.7
Au(5)-Au(4)-Au(29)	58.1
Au(6)-Au(4)-Au(5)	59.1
Au(6)-Au(4)-Au(28)	174.3
Au(6)-Au(4)-Au(29)	117.2
Au(23)-Au(4)-Au(2)	128.5
Au(23)-Au(4)-Au(3)	171.6
Au(23)-Au(4)-Au(5)	66.3
Au(23)-Au(4)-Au(6)	92.4
Au(23)-Au(4)-Au(26)	115.1
Au(23)-Au(4)-Au(28)	84.0
Au(23)-Au(4)-Au(29)	61.8

Au(23)-Au(4)-Au(36)	121.5
Au(23)-Au(4)-Au(39)	57.6
Au(24)-Au(4)-Au(2)	167.3
Au(24)-Au(4)-Au(3)	109.1
Au(24)-Au(4)-Au(5)	128.5
Au(24)-Au(4)-Au(6)	115.3
Au(24)-Au(4)-Au(23)	62.9
Au(24)-Au(4)-Au(26)	76.9
Au(24)-Au(4)-Au(28)	59.1
Au(24)-Au(4)-Au(29)	102.2
Au(24)-Au(4)-Au(36)	120.1
Au(24)-Au(4)-Au(39)	57.7
Au(26)-Au(4)-Au(5)	119.9
Au(26)-Au(4)-Au(6)	60.8
Au(26)-Au(4)-Au(28)	116.8
Au(26)-Au(4)-Au(29)	176.7
Au(26)-Au(4)-Au(39)	58.2
Au(29)-Au(4)-Au(28)	64.8
Au(36)-Au(4)-Au(2)	61.3
Au(36)-Au(4)-Au(5)	92.6
Au(36)-Au(4)-Au(6)	123.5
Au(36)-Au(4)-Au(26)	122.3
Au(36)-Au(4)-Au(28)	62.2
Au(36)-Au(4)-Au(29)	60.9
Au(36)-Au(4)-Au(39)	177.8
Au(39)-Au(4)-Au(5)	88.8
Au(39)-Au(4)-Au(6)	58.7
Au(39)-Au(4)-Au(28)	115.6
Au(39)-Au(4)-Au(29)	118.6
Au(1)-Au(5)-Au(2)	57.2

Au(1)-Au(5)-Au(9)	52.9
Au(1)-Au(5)-Au(23)	169.1
Au(2)-Au(5)-Au(9)	110.1
Au(2)-Au(5)-Au(23)	112.0
Au(4)-Au(5)-Au(1)	115.0
Au(4)-Au(5)-Au(2)	57.8
Au(4)-Au(5)-Au(9)	167.9
Au(4)-Au(5)-Au(23)	54.2
Au(6)-Au(5)-Au(1)	89.3
Au(6)-Au(5)-Au(2)	60.9
Au(6)-Au(5)-Au(4)	59.9
Au(6)-Au(5)-Au(9)	116.5
Au(6)-Au(5)-Au(23)	86.0
Au(6)-Au(5)-Au(29)	122.3
Au(7)-Au(5)-Au(1)	58.6
Au(7)-Au(5)-Au(2)	60.5
Au(7)-Au(5)-Au(4)	89.0
Au(7)-Au(5)-Au(6)	121.4
Au(7)-Au(5)-Au(9)	83.5
Au(7)-Au(5)-Au(23)	116.2
Au(7)-Au(5)-Au(29)	57.5
Au(8)-Au(5)-Au(1)	89.9
Au(8)-Au(5)-Au(2)	118.3
Au(8)-Au(5)-Au(4)	120.1
Au(8)-Au(5)-Au(6)	179.2
Au(8)-Au(5)-Au(7)	57.8
Au(8)-Au(5)-Au(9)	63.3
Au(8)-Au(5)-Au(12)	122.3
Au(8)-Au(5)-Au(23)	94.7
Au(8)-Au(5)-Au(29)	57.8

Au(9)-Au(5)-Au(23)	137.8
Au(12)-Au(5)-Au(1)	62.6
Au(12)-Au(5)-Au(2)	89.3
Au(12)-Au(5)-Au(4)	117.5
Au(12)-Au(5)-Au(6)	57.6
Au(12)-Au(5)-Au(7)	121.2
Au(12)-Au(5)-Au(9)	59.7
Au(12)-Au(5)-Au(23)	122.0
Au(12)-Au(5)-Au(29)	178.5
Au(22)-Au(5)-Au(1)	120.8
Au(22)-Au(5)-Au(2)	119.3
Au(22)-Au(5)-Au(4)	91.4
Au(22)-Au(5)-Au(6)	58.4
Au(22)-Au(5)-Au(7)	179.3
Au(22)-Au(5)-Au(8)	122.3
Au(22)-Au(5)-Au(9)	96.0
Au(22)-Au(5)-Au(12)	58.2
Au(22)-Au(5)-Au(23)	64.5
Au(22)-Au(5)-Au(29)	123.2
Au(29)-Au(5)-Au(1)	116.0
Au(29)-Au(5)-Au(2)	89.4
Au(29)-Au(5)-Au(4)	62.3
Au(29)-Au(5)-Au(9)	120.1
Au(29)-Au(5)-Au(23)	59.3
Au(2)-Au(6)-Au(13)	121.0
Au(2)-Au(6)-Au(16)	56.9
Au(4)-Au(6)-Au(2)	58.3
Au(4)-Au(6)-Au(13)	174.4
Au(4)-Au(6)-Au(16)	115.2
Au(4)-Au(6)-Au(26)	59.4

Au(5)-Au(6)-Au(2)	61.5
Au(5)-Au(6)-Au(4)	60.9
Au(5)-Au(6)-Au(13)	124.2
Au(5)-Au(6)-Au(16)	88.3
Au(5)-Au(6)-Au(26)	120.3
Au(12)-Au(6)-Au(2)	91.4
Au(12)-Au(6)-Au(4)	121.5
Au(12)-Au(6)-Au(5)	60.7
Au(12)-Au(6)-Au(13)	63.5
Au(12)-Au(6)-Au(16)	60.7
Au(12)-Au(6)-Au(22)	59.5
Au(12)-Au(6)-Au(26)	178.8
Au(12)-Au(6)-Au(39)	122.6
Au(14)-Au(6)-Au(2)	126.2
Au(14)-Au(6)-Au(4)	116.4
Au(14)-Au(6)-Au(5)	170.3
Au(14)-Au(6)-Au(12)	121.6
Au(14)-Au(6)-Au(13)	59.0
Au(14)-Au(6)-Au(16)	101.0
Au(14)-Au(6)-Au(22)	112.9
Au(14)-Au(6)-Au(26)	57.6
Au(14)-Au(6)-Au(39)	80.0
Au(15)-Au(6)-Au(2)	63.9
Au(15)-Au(6)-Au(4)	90.6
Au(15)-Au(6)-Au(5)	125.4
Au(15)-Au(6)-Au(12)	121.5
Au(15)-Au(6)-Au(13)	84.4
Au(15)-Au(6)-Au(14)	62.6
Au(15)-Au(6)-Au(16)	61.5
Au(15)-Au(6)-Au(22)	175.4

Au(15)-Au(6)-Au(26)	57.5
Au(15)-Au(6)-Au(39)	115.6
Au(16)-Au(6)-Au(13)	64.3
Au(22)-Au(6)-Au(2)	120.6
Au(22)-Au(6)-Au(4)	92.4
Au(22)-Au(6)-Au(5)	59.1
Au(22)-Au(6)-Au(13)	92.5
Au(22)-Au(6)-Au(16)	120.0
Au(22)-Au(6)-Au(26)	121.5
Au(22)-Au(6)-Au(39)	63.2
Au(26)-Au(6)-Au(2)	88.6
Au(26)-Au(6)-Au(13)	115.5
Au(26)-Au(6)-Au(16)	118.4
Au(39)-Au(6)-Au(2)	118.9
Au(39)-Au(6)-Au(4)	60.6
Au(39)-Au(6)-Au(5)	90.9
Au(39)-Au(6)-Au(13)	119.6
Au(39)-Au(6)-Au(16)	175.4
Au(39)-Au(6)-Au(26)	58.3
Au(1)-Au(7)-Au(2)	58.9
Au(1)-Au(7)-Au(5)	62.8
Au(1)-Au(7)-Au(30)	174.7
Au(1)-Au(7)-Au(33)	61.8
Au(1)-Au(7)-Au(34)	59.6
Au(1)-Au(7)-Au(36)	116.5
Au(2)-Au(7)-Au(30)	123.0
Au(2)-Au(7)-Au(34)	89.6
Au(2)-Au(7)-Au(36)	57.6
Au(5)-Au(7)-Au(2)	61.8
Au(5)-Au(7)-Au(30)	122.5

Au(5)-Au(7)-Au(33)	93.8
Au(5)-Au(7)-Au(34)	122.4
Au(5)-Au(7)-Au(36)	89.1
Au(8)-Au(7)-Au(1)	93.6
Au(8)-Au(7)-Au(2)	121.5
Au(8)-Au(7)-Au(5)	59.6
Au(8)-Au(7)-Au(29)	59.8
Au(8)-Au(7)-Au(30)	89.3
Au(8)-Au(7)-Au(33)	64.3
Au(8)-Au(7)-Au(34)	121.6
Au(8)-Au(7)-Au(35)	174.1
Au(8)-Au(7)-Au(36)	120.6
Au(29)-Au(7)-Au(1)	124.3
Au(29)-Au(7)-Au(2)	92.5
Au(29)-Au(7)-Au(5)	61.6
Au(29)-Au(7)-Au(30)	61.0
Au(29)-Au(7)-Au(33)	124.0
Au(29)-Au(7)-Au(34)	176.1
Au(29)-Au(7)-Au(36)	61.0
Au(31)-Au(7)-Au(1)	116.7
Au(31)-Au(7)-Au(2)	128.3
Au(31)-Au(7)-Au(5)	168.9
Au(31)-Au(7)-Au(8)	110.1
Au(31)-Au(7)-Au(29)	118.3
Au(31)-Au(7)-Au(30)	58.1
Au(31)-Au(7)-Au(33)	77.1
Au(31)-Au(7)-Au(34)	57.9
Au(31)-Au(7)-Au(35)	64.1
Au(31)-Au(7)-Au(36)	100.4
Au(33)-Au(7)-Au(2)	120.6

Au(33)-Au(7)-Au(30)	115.9
Au(33)-Au(7)-Au(34)	57.3
Au(33)-Au(7)-Au(36)	175.0
Au(34)-Au(7)-Au(30)	115.1
Au(34)-Au(7)-Au(36)	117.8
Au(35)-Au(7)-Au(1)	90.3
Au(35)-Au(7)-Au(2)	64.4
Au(35)-Au(7)-Au(5)	126.3
Au(35)-Au(7)-Au(29)	121.2
Au(35)-Au(7)-Au(30)	86.5
Au(35)-Au(7)-Au(33)	113.9
Au(35)-Au(7)-Au(34)	57.0
Au(35)-Au(7)-Au(36)	61.1
Au(36)-Au(7)-Au(30)	65.4
Au(5)-Au(8)-Au(9)	63.2
Au(5)-Au(8)-Au(11)	81.1
Au(5)-Au(8)-Au(32)	141.6
Au(5)-Au(8)-Au(33)	93.0
Au(7)-Au(8)-Au(5)	62.6
Au(7)-Au(8)-Au(9)	85.7
Au(7)-Au(8)-Au(11)	137.9
Au(7)-Au(8)-Au(29)	60.7
Au(7)-Au(8)-Au(32)	79.1
Au(7)-Au(8)-Au(33)	60.0
Au(11)-Au(8)-Au(9)	96.8
Au(29)-Au(8)-Au(5)	62.9
Au(29)-Au(8)-Au(9)	125.0
Au(29)-Au(8)-Au(11)	84.9
Au(29)-Au(8)-Au(32)	101.5
Au(29)-Au(8)-Au(33)	120.6

Au(32)-Au(8)-Au(9)	114.0
Au(32)-Au(8)-Au(11)	134.9
Au(32)-Au(8)-Au(33)	63.7
Au(33)-Au(8)-Au(9)	53.4
Au(33)-Au(8)-Au(11)	147.9
S(3)-Au(8)-Au(5)	125.0
S(3)-Au(8)-Au(7)	172.3
S(3)-Au(8)-Au(9)	97.1
S(3)-Au(8)-Au(11)	49.0
S(3)-Au(8)-Au(29)	122.2
S(3)-Au(8)-Au(32)	93.2
S(3)-Au(8)-Au(33)	116.2
Au(1)-Au(9)-Au(5)	61.4
Au(1)-Au(9)-Au(8)	89.0
Au(1)-Au(9)-Au(10)	130.9
Au(1)-Au(9)-Au(12)	64.5
Au(1)-Au(9)-Au(20)	58.3
Au(1)-Au(9)-Au(33)	65.4
Au(5)-Au(9)-Au(8)	53.5
Au(5)-Au(9)-Au(10)	75.1
Au(8)-Au(9)-Au(10)	82.4
Au(12)-Au(9)-Au(5)	56.0
Au(12)-Au(9)-Au(8)	109.0
Au(12)-Au(9)-Au(10)	73.0
Au(20)-Au(9)-Au(5)	119.4
Au(20)-Au(9)-Au(8)	118.9
Au(20)-Au(9)-Au(10)	158.4
Au(20)-Au(9)-Au(12)	100.9
Au(33)-Au(9)-Au(5)	91.7
Au(33)-Au(9)-Au(8)	61.1

Au(33)-Au(9)-Au(10)	141.1
Au(33)-Au(9)-Au(12)	129.0
Au(33)-Au(9)-Au(20)	58.6
S(4)-Au(9)-Au(1)	173.5
S(4)-Au(9)-Au(5)	114.8
S(4)-Au(9)-Au(8)	92.6
S(4)-Au(9)-Au(10)	43.3
S(4)-Au(9)-Au(12)	109.1
S(4)-Au(9)-Au(20)	125.8
S(4)-Au(9)-Au(33)	120.8
Au(11)-Au(10)-Au(9)	91.0
Au(11)-Au(10)-Au(22)	82.3
Au(22)-Au(10)-Au(9)	85.9
S(1)-Au(10)-Au(9)	136.3
S(1)-Au(10)-Au(11)	87.6
S(1)-Au(10)-Au(22)	50.6
S(1)-Au(10)-S(4)	172.7
S(4)-Au(10)-Au(9)	44.9
S(4)-Au(10)-Au(11)	99.7
S(4)-Au(10)-Au(22)	130.7
Au(8)-Au(11)-Au(10)	89.8
Au(8)-Au(11)-Au(23)	86.8
Au(10)-Au(11)-Au(23)	99.2
S(2)-Au(11)-Au(8)	132.3
S(2)-Au(11)-Au(10)	101.4
S(2)-Au(11)-Au(23)	45.8
S(2)-Au(11)-S(3)	165.7
S(3)-Au(11)-Au(8)	51.6
S(3)-Au(11)-Au(10)	92.0
S(3)-Au(11)-Au(23)	137.0

Au(1)-Au(12)-Au(13)	120.7
Au(1)-Au(12)-Au(21)	60.0
Au(5)-Au(12)-Au(1)	60.9
Au(5)-Au(12)-Au(9)	64.3
Au(5)-Au(12)-Au(13)	126.4
Au(5)-Au(12)-Au(16)	90.8
Au(5)-Au(12)-Au(21)	120.7
Au(6)-Au(12)-Au(1)	90.6
Au(6)-Au(12)-Au(5)	61.7
Au(6)-Au(12)-Au(9)	125.0
Au(6)-Au(12)-Au(13)	64.7
Au(6)-Au(12)-Au(16)	64.3
Au(6)-Au(12)-Au(21)	122.7
Au(9)-Au(12)-Au(1)	53.7
Au(9)-Au(12)-Au(13)	166.0
Au(9)-Au(12)-Au(21)	77.9
Au(13)-Au(12)-Au(21)	88.3
Au(16)-Au(12)-Au(1)	54.9
Au(16)-Au(12)-Au(9)	107.7
Au(16)-Au(12)-Au(13)	65.9
Au(16)-Au(12)-Au(21)	58.5
Au(22)-Au(12)-Au(1)	120.6
Au(22)-Au(12)-Au(5)	59.8
Au(22)-Au(12)-Au(6)	60.4
Au(22)-Au(12)-Au(9)	100.1
Au(22)-Au(12)-Au(13)	93.7
Au(22)-Au(12)-Au(16)	124.5
Au(22)-Au(12)-Au(21)	176.9
S(16)-Au(12)-Au(1)	93.6
S(16)-Au(12)-Au(5)	139.9

S(16)-Au(12)-Au(6)	155.5
S(16)-Au(12)-Au(9)	75.7
S(16)-Au(12)-Au(13)	92.6
S(16)-Au(12)-Au(16)	98.8
S(16)-Au(12)-Au(21)	42.8
S(16)-Au(12)-Au(22)	134.6
Au(6)-Au(13)-Au(16)	55.7
Au(12)-Au(13)-Au(6)	51.8
Au(12)-Au(13)-Au(16)	54.1
Au(14)-Au(13)-Au(6)	52.8
Au(14)-Au(13)-Au(12)	103.9
Au(14)-Au(13)-Au(16)	90.7
S(5)-Au(13)-Au(6)	100.5
S(5)-Au(13)-Au(12)	91.8
S(5)-Au(13)-Au(14)	92.5
S(5)-Au(13)-Au(16)	145.4
S(17)-Au(13)-Au(6)	91.9
S(17)-Au(13)-Au(12)	97.4
S(17)-Au(13)-Au(14)	93.5
S(17)-Au(13)-Au(16)	45.5
S(17)-Au(13)-S(5)	167.5
Au(6)-Au(14)-Au(13)	68.2
Au(6)-Au(14)-Au(15)	58.6
Au(6)-Au(14)-Au(26)	65.0
Au(6)-Au(14)-Au(27)	74.3
Au(6)-Au(14)-Au(42)	127.0
Au(13)-Au(14)-Au(27)	70.7
Au(13)-Au(14)-Au(42)	138.3
Au(15)-Au(14)-Au(13)	87.2
Au(15)-Au(14)-Au(27)	132.7

Au(15)-Au(14)-Au(42)	134.5
Au(26)-Au(14)-Au(13)	131.7
Au(26)-Au(14)-Au(15)	58.7
Au(26)-Au(14)-Au(27)	106.5
Au(26)-Au(14)-Au(42)	82.2
Au(27)-Au(14)-Au(42)	77.0
S(7)-Au(14)-Au(6)	160.8
S(7)-Au(14)-Au(13)	107.0
S(7)-Au(14)-Au(15)	140.5
S(7)-Au(14)-Au(26)	121.1
S(7)-Au(14)-Au(27)	86.6
S(7)-Au(14)-Au(42)	44.3
Au(2)-Au(15)-Au(3)	54.5
Au(2)-Au(15)-Au(18)	73.7
Au(3)-Au(15)-Au(18)	78.7
Au(6)-Au(15)-Au(2)	62.1
Au(6)-Au(15)-Au(3)	89.8
Au(6)-Au(15)-Au(14)	58.7
Au(6)-Au(15)-Au(16)	64.5
Au(6)-Au(15)-Au(18)	132.0
Au(6)-Au(15)-Au(26)	65.1
Au(14)-Au(15)-Au(2)	120.5
Au(14)-Au(15)-Au(3)	118.8
Au(14)-Au(15)-Au(16)	100.5
Au(14)-Au(15)-Au(18)	161.4
Au(16)-Au(15)-Au(2)	57.3
Au(16)-Au(15)-Au(3)	111.3
Au(16)-Au(15)-Au(18)	76.6
Au(26)-Au(15)-Au(2)	91.6
Au(26)-Au(15)-Au(3)	60.5

Au(26)-Au(15)-Au(14)	58.8
Au(26)-Au(15)-Au(16)	128.9
Au(26)-Au(15)-Au(18)	136.9
S(18)-Au(15)-Au(2)	113.8
S(18)-Au(15)-Au(3)	88.4
S(18)-Au(15)-Au(6)	175.8
S(18)-Au(15)-Au(14)	125.4
S(18)-Au(15)-Au(16)	112.7
S(18)-Au(15)-Au(18)	43.9
S(18)-Au(15)-Au(26)	117.1
Au(1)-Au(16)-Au(2)	61.2
Au(1)-Au(16)-Au(6)	90.6
Au(1)-Au(16)-Au(12)	64.4
Au(1)-Au(16)-Au(13)	124.4
Au(1)-Au(16)-Au(15)	123.1
Au(1)-Au(16)-Au(21)	66.3
Au(2)-Au(16)-Au(6)	60.5
Au(2)-Au(16)-Au(12)	90.1
Au(2)-Au(16)-Au(13)	120.1
Au(2)-Au(16)-Au(15)	62.6
Au(2)-Au(16)-Au(21)	127.4
Au(6)-Au(16)-Au(13)	59.9
Au(6)-Au(16)-Au(21)	122.5
Au(12)-Au(16)-Au(6)	55.0
Au(12)-Au(16)-Au(13)	60.1
Au(12)-Au(16)-Au(15)	108.5
Au(12)-Au(16)-Au(21)	67.6
Au(15)-Au(16)-Au(6)	54.0
Au(15)-Au(16)-Au(13)	78.5
Au(15)-Au(16)-Au(21)	168.1

Au(17)-Au(16)-Au(1)	59.7
Au(17)-Au(16)-Au(2)	59.8
Au(17)-Au(16)-Au(6)	120.3
Au(17)-Au(16)-Au(12)	123.9
Au(17)-Au(16)-Au(13)	175.8
Au(17)-Au(16)-Au(15)	98.2
Au(17)-Au(16)-Au(21)	93.1
Au(21)-Au(16)-Au(13)	90.0
S(17)-Au(16)-Au(1)	158.5
S(17)-Au(16)-Au(2)	138.5
S(17)-Au(16)-Au(6)	94.6
S(17)-Au(16)-Au(12)	102.1
S(17)-Au(16)-Au(13)	44.4
S(17)-Au(16)-Au(15)	76.0
S(17)-Au(16)-Au(17)	132.4
S(17)-Au(16)-Au(21)	93.6
Au(1)-Au(17)-Au(2)	62.2
Au(1)-Au(17)-Au(16)	60.3
Au(1)-Au(17)-Au(18)	137.2
Au(1)-Au(17)-Au(19)	78.5
Au(1)-Au(17)-Au(34)	60.9
Au(1)-Au(17)-Au(35)	86.1
Au(2)-Au(17)-Au(18)	81.1
Au(2)-Au(17)-Au(19)	140.6
Au(2)-Au(17)-Au(34)	92.6
Au(2)-Au(17)-Au(35)	62.1
Au(16)-Au(17)-Au(2)	62.2
Au(16)-Au(17)-Au(18)	84.3
Au(16)-Au(17)-Au(19)	101.4
Au(16)-Au(17)-Au(34)	121.1

Au(16)-Au(17)-Au(35)	123.5
Au(18)-Au(17)-Au(35)	96.0
Au(19)-Au(17)-Au(18)	135.6
Au(19)-Au(17)-Au(35)	115.5
Au(34)-Au(17)-Au(18)	147.2
Au(34)-Au(17)-Au(19)	64.3
Au(34)-Au(17)-Au(35)	53.7
S(23)-Au(17)-Au(1)	172.1
S(23)-Au(17)-Au(2)	125.7
S(23)-Au(17)-Au(16)	121.9
S(23)-Au(17)-Au(18)	49.5
S(23)-Au(17)-Au(19)	93.6
S(23)-Au(17)-Au(34)	116.0
S(23)-Au(17)-Au(35)	97.8
Au(17)-Au(18)-Au(15)	86.1
Au(37)-Au(18)-Au(15)	96.8
Au(37)-Au(18)-Au(17)	89.6
S(18)-Au(18)-Au(15)	46.5
S(18)-Au(18)-Au(17)	132.0
S(18)-Au(18)-Au(37)	101.7
S(18)-Au(18)-S(23)	165.1
S(23)-Au(18)-Au(15)	135.9
S(23)-Au(18)-Au(17)	50.9
S(23)-Au(18)-Au(37)	92.7
Au(17)-Au(19)-Au(20)	94.0
Au(17)-Au(19)-Au(34)	57.2
Au(20)-Au(19)-Au(34)	67.8
S(24)-Au(19)-Au(17)	93.8
S(24)-Au(19)-Au(20)	87.9
S(24)-Au(19)-Au(34)	138.6

S(24)-Au(19)-S(25)	172.7
S(25)-Au(19)-Au(17)	93.5
S(25)-Au(19)-Au(20)	92.8
S(25)-Au(19)-Au(34)	47.7
Au(1)-Au(20)-Au(9)	58.4
Au(1)-Au(20)-Au(19)	77.8
Au(1)-Au(20)-Au(21)	69.1
Au(1)-Au(20)-Au(33)	65.5
Au(1)-Au(20)-Au(41)	127.8
Au(9)-Au(20)-Au(19)	135.9
Au(9)-Au(20)-Au(21)	86.9
Au(9)-Au(20)-Au(41)	125.1
Au(19)-Au(20)-Au(41)	84.2
Au(21)-Au(20)-Au(19)	72.3
Au(21)-Au(20)-Au(41)	147.8
Au(33)-Au(20)-Au(9)	58.6
Au(33)-Au(20)-Au(19)	109.1
Au(33)-Au(20)-Au(21)	132.7
Au(33)-Au(20)-Au(41)	75.3
S(15)-Au(20)-Au(1)	157.8
S(15)-Au(20)-Au(9)	143.6
S(15)-Au(20)-Au(19)	80.4
S(15)-Au(20)-Au(21)	108.1
S(15)-Au(20)-Au(33)	118.8
S(15)-Au(20)-Au(41)	44.7
Au(1)-Au(21)-Au(12)	54.9
Au(16)-Au(21)-Au(1)	51.7
Au(16)-Au(21)-Au(12)	53.9
Au(20)-Au(21)-Au(1)	51.9
Au(20)-Au(21)-Au(12)	90.3

Au(20)-Au(21)-Au(16)	102.8
S(16)-Au(21)-Au(1)	90.5
S(16)-Au(21)-Au(12)	44.5
S(16)-Au(21)-Au(16)	96.1
S(16)-Au(21)-Au(20)	94.5
S(16)-Au(21)-S(24)	169.1
S(24)-Au(21)-Au(1)	100.3
S(24)-Au(21)-Au(12)	145.2
S(24)-Au(21)-Au(16)	92.1
S(24)-Au(21)-Au(20)	90.8
Au(5)-Au(22)-Au(10)	84.8
Au(5)-Au(22)-Au(23)	62.7
Au(5)-Au(22)-Au(27)	137.7
Au(5)-Au(22)-Au(39)	90.8
Au(6)-Au(22)-Au(5)	62.4
Au(6)-Au(22)-Au(10)	137.5
Au(6)-Au(22)-Au(23)	86.9
Au(6)-Au(22)-Au(27)	75.4
Au(6)-Au(22)-Au(39)	59.7
Au(10)-Au(22)-Au(23)	102.1
Au(12)-Au(22)-Au(5)	62.1
Au(12)-Au(22)-Au(6)	60.2
Au(12)-Au(22)-Au(10)	81.3
Au(12)-Au(22)-Au(23)	124.1
Au(12)-Au(22)-Au(27)	100.0
Au(12)-Au(22)-Au(39)	119.9
Au(27)-Au(22)-Au(10)	132.7
Au(27)-Au(22)-Au(23)	114.7
Au(39)-Au(22)-Au(10)	153.0
Au(39)-Au(22)-Au(23)	53.0

Au(39)-Au(22)-Au(27)	64.2
S(1)-Au(22)-Au(5)	127.2
S(1)-Au(22)-Au(6)	170.0
S(1)-Au(22)-Au(10)	48.2
S(1)-Au(22)-Au(12)	119.7
S(1)-Au(22)-Au(23)	100.2
S(1)-Au(22)-Au(27)	95.1
S(1)-Au(22)-Au(39)	119.3
Au(4)-Au(23)-Au(5)	59.5
Au(4)-Au(23)-Au(11)	128.1
Au(4)-Au(23)-Au(22)	87.3
Au(4)-Au(23)-Au(24)	57.9
Au(4)-Au(23)-Au(29)	63.2
Au(5)-Au(23)-Au(11)	71.8
Au(5)-Au(23)-Au(22)	52.8
Au(22)-Au(23)-Au(11)	76.4
Au(24)-Au(23)-Au(5)	117.0
Au(24)-Au(23)-Au(11)	166.6
Au(24)-Au(23)-Au(22)	116.9
Au(24)-Au(23)-Au(29)	99.9
Au(29)-Au(23)-Au(5)	56.6
Au(29)-Au(23)-Au(11)	76.1
Au(29)-Au(23)-Au(22)	108.9
Au(39)-Au(23)-Au(4)	63.9
Au(39)-Au(23)-Au(5)	88.4
Au(39)-Au(23)-Au(11)	134.4
Au(39)-Au(23)-Au(22)	59.4
Au(39)-Au(23)-Au(24)	58.1
Au(39)-Au(23)-Au(29)	126.2
S(2)-Au(23)-Au(4)	170.5

S(2)-Au(23)-Au(5)	111.1
S(2)-Au(23)-Au(11)	44.1
S(2)-Au(23)-Au(22)	85.2
S(2)-Au(23)-Au(24)	131.1
S(2)-Au(23)-Au(29)	113.9
S(2)-Au(23)-Au(39)	116.5
Au(4)-Au(24)-Au(23)	59.2
Au(4)-Au(24)-Au(25)	129.4
Au(4)-Au(24)-Au(28)	68.0
Au(4)-Au(24)-Au(38)	78.1
Au(23)-Au(24)-Au(25)	125.9
Au(23)-Au(24)-Au(28)	86.7
Au(23)-Au(24)-Au(38)	137.0
Au(28)-Au(24)-Au(25)	147.1
Au(28)-Au(24)-Au(38)	71.5
Au(38)-Au(24)-Au(25)	84.4
Au(39)-Au(24)-Au(4)	64.5
Au(39)-Au(24)-Au(23)	58.6
Au(39)-Au(24)-Au(25)	77.8
Au(39)-Au(24)-Au(28)	130.8
Au(39)-Au(24)-Au(38)	109.5
S(9)-Au(24)-Au(4)	156.4
S(9)-Au(24)-Au(23)	144.2
S(9)-Au(24)-Au(25)	43.3
S(9)-Au(24)-Au(28)	108.3
S(9)-Au(24)-Au(38)	78.7
S(9)-Au(24)-Au(39)	120.3
S(8)-Au(25)-Au(24)	138.9
S(9)-Au(25)-Au(24)	44.4
S(9)-Au(25)-S(8)	175.4

Au(3)-Au(26)-Au(38)	58.9
Au(4)-Au(26)-Au(3)	56.4
Au(4)-Au(26)-Au(6)	59.7
Au(4)-Au(26)-Au(38)	73.9
Au(6)-Au(26)-Au(3)	88.9
Au(6)-Au(26)-Au(38)	133.3
Au(14)-Au(26)-Au(3)	128.1
Au(14)-Au(26)-Au(4)	116.6
Au(14)-Au(26)-Au(6)	57.4
Au(14)-Au(26)-Au(38)	169.2
Au(14)-Au(26)-Au(39)	80.5
Au(15)-Au(26)-Au(3)	66.1
Au(15)-Au(26)-Au(4)	90.7
Au(15)-Au(26)-Au(6)	57.4
Au(15)-Au(26)-Au(14)	62.5
Au(15)-Au(26)-Au(38)	122.1
Au(15)-Au(26)-Au(39)	116.5
Au(39)-Au(26)-Au(3)	117.4
Au(39)-Au(26)-Au(4)	61.1
Au(39)-Au(26)-Au(6)	59.3
Au(39)-Au(26)-Au(38)	103.9
S(19)-Au(26)-Au(3)	94.7
S(19)-Au(26)-Au(4)	119.2
S(19)-Au(26)-Au(6)	174.6
S(19)-Au(26)-Au(14)	122.4
S(19)-Au(26)-Au(15)	127.9
S(19)-Au(26)-Au(38)	46.8
S(19)-Au(26)-Au(39)	115.4
Au(14)-Au(27)-Au(39)	69.9
Au(22)-Au(27)-Au(14)	97.3

Au(22)-Au(27)-Au(39)	57.0
S(5)-Au(27)-Au(14)	88.8
S(5)-Au(27)-Au(22)	96.1
S(5)-Au(27)-Au(39)	141.2
S(6)-Au(27)-Au(14)	92.4
S(6)-Au(27)-Au(22)	93.7
S(6)-Au(27)-Au(39)	48.0
S(6)-Au(27)-S(5)	169.9
Au(4)-Au(28)-Au(29)	55.4
Au(24)-Au(28)-Au(4)	52.9
Au(24)-Au(28)-Au(29)	91.2
Au(24)-Au(28)-Au(36)	104.8
Au(36)-Au(28)-Au(4)	52.8
Au(36)-Au(28)-Au(29)	54.6
S(10)-Au(28)-Au(4)	90.1
S(10)-Au(28)-Au(24)	91.4
S(10)-Au(28)-Au(29)	45.7
S(10)-Au(28)-Au(36)	98.6
S(10)-Au(28)-S(20)	166.0
S(20)-Au(28)-Au(4)	102.9
S(20)-Au(28)-Au(24)	92.3
S(20)-Au(28)-Au(29)	147.7
S(20)-Au(28)-Au(36)	93.6
Au(4)-Au(29)-Au(28)	59.8
Au(4)-Au(29)-Au(30)	124.0
Au(5)-Au(29)-Au(4)	59.6
Au(5)-Au(29)-Au(23)	64.2
Au(5)-Au(29)-Au(28)	119.2
Au(5)-Au(29)-Au(30)	128.2
Au(5)-Au(29)-Au(36)	90.2

Au(7)-Au(29)-Au(4)	89.4
Au(7)-Au(29)-Au(5)	61.0
Au(7)-Au(29)-Au(23)	124.5
Au(7)-Au(29)-Au(28)	122.4
Au(7)-Au(29)-Au(30)	67.3
Au(7)-Au(29)-Au(36)	63.6
Au(8)-Au(29)-Au(4)	118.9
Au(8)-Au(29)-Au(5)	59.4
Au(8)-Au(29)-Au(7)	59.5
Au(8)-Au(29)-Au(23)	99.0
Au(8)-Au(29)-Au(28)	177.1
Au(8)-Au(29)-Au(30)	92.7
Au(8)-Au(29)-Au(36)	123.0
Au(23)-Au(29)-Au(4)	54.9
Au(23)-Au(29)-Au(28)	78.2
Au(23)-Au(29)-Au(30)	166.7
Au(30)-Au(29)-Au(28)	90.1
Au(36)-Au(29)-Au(4)	55.6
Au(36)-Au(29)-Au(23)	109.6
Au(36)-Au(29)-Au(28)	58.8
Au(36)-Au(29)-Au(30)	68.5
S(10)-Au(29)-Au(4)	92.6
S(10)-Au(29)-Au(5)	136.2
S(10)-Au(29)-Au(7)	159.5
S(10)-Au(29)-Au(8)	134.8
S(10)-Au(29)-Au(23)	72.1
S(10)-Au(29)-Au(28)	44.1
S(10)-Au(29)-Au(30)	95.1
S(10)-Au(29)-Au(36)	101.1
Au(7)-Au(30)-Au(36)	53.9

Au(29)-Au(30)-Au(7)	51.8
Au(29)-Au(30)-Au(36)	53.8
Au(31)-Au(30)-Au(7)	51.4
Au(31)-Au(30)-Au(29)	102.6
Au(31)-Au(30)-Au(36)	87.7
S(11)-Au(30)-Au(7)	99.3
S(11)-Au(30)-Au(29)	89.3
S(11)-Au(30)-Au(31)	94.2
S(11)-Au(30)-Au(36)	142.3
S(11)-Au(30)-S(26)	172.0
S(26)-Au(30)-Au(7)	88.7
S(26)-Au(30)-Au(29)	96.2
S(26)-Au(30)-Au(31)	90.2
S(26)-Au(30)-Au(36)	44.4
Au(7)-Au(31)-Au(30)	70.5
Au(7)-Au(31)-Au(32)	77.0
Au(7)-Au(31)-Au(34)	66.0
Au(7)-Au(31)-Au(35)	58.7
Au(7)-Au(31)-Au(40)	129.5
Au(30)-Au(31)-Au(32)	70.9
Au(30)-Au(31)-Au(40)	141.5
Au(32)-Au(31)-Au(40)	81.7
Au(34)-Au(31)-Au(30)	135.1
Au(34)-Au(31)-Au(32)	108.4
Au(34)-Au(31)-Au(35)	57.9
Au(34)-Au(31)-Au(40)	78.6
Au(35)-Au(31)-Au(30)	90.3
Au(35)-Au(31)-Au(32)	135.6
Au(35)-Au(31)-Au(40)	127.9
S(13)-Au(31)-Au(7)	168.8

S(13)-Au(31)-Au(30)	119.3
S(13)-Au(31)-Au(32)	110.5
S(13)-Au(31)-Au(34)	103.2
S(13)-Au(31)-Au(35)	113.7
S(13)-Au(31)-Au(40)	46.7
Au(8)-Au(32)-Au(31)	93.8
Au(8)-Au(32)-Au(33)	58.4
Au(31)-Au(32)-Au(33)	67.2
S(11)-Au(32)-Au(8)	91.3
S(11)-Au(32)-Au(31)	89.4
S(11)-Au(32)-Au(33)	138.4
S(11)-Au(32)-S(12)	172.9
S(12)-Au(32)-Au(8)	94.9
S(12)-Au(32)-Au(31)	93.8
S(12)-Au(32)-Au(33)	48.7
Au(1)-Au(33)-Au(8)	87.1
Au(1)-Au(33)-Au(32)	132.6
Au(7)-Au(33)-Au(1)	59.1
Au(7)-Au(33)-Au(8)	55.7
Au(7)-Au(33)-Au(32)	74.3
Au(8)-Au(33)-Au(32)	57.9
Au(9)-Au(33)-Au(1)	56.9
Au(9)-Au(33)-Au(7)	90.4
Au(9)-Au(33)-Au(8)	65.5
Au(9)-Au(33)-Au(32)	119.9
Au(9)-Au(33)-Au(34)	117.1
Au(20)-Au(33)-Au(1)	56.9
Au(20)-Au(33)-Au(7)	115.2
Au(20)-Au(33)-Au(8)	127.4
Au(20)-Au(33)-Au(9)	62.8

Au(20)-Au(33)-Au(32)	170.5
Au(20)-Au(33)-Au(34)	78.3
Au(34)-Au(33)-Au(1)	60.6
Au(34)-Au(33)-Au(7)	63.1
Au(34)-Au(33)-Au(8)	118.7
Au(34)-Au(33)-Au(32)	106.6
S(12)-Au(33)-Au(1)	179.0
S(12)-Au(33)-Au(7)	120.1
S(12)-Au(33)-Au(8)	92.9
S(12)-Au(33)-Au(9)	124.0
S(12)-Au(33)-Au(20)	123.8
S(12)-Au(33)-Au(32)	46.7
S(12)-Au(33)-Au(34)	118.5
Au(1)-Au(34)-Au(7)	58.5
Au(1)-Au(34)-Au(17)	55.7
Au(1)-Au(34)-Au(19)	73.4
Au(7)-Au(34)-Au(17)	87.2
Au(7)-Au(34)-Au(19)	131.5
Au(17)-Au(34)-Au(19)	58.5
Au(31)-Au(34)-Au(1)	113.8
Au(31)-Au(34)-Au(7)	56.1
Au(31)-Au(34)-Au(17)	127.5
Au(31)-Au(34)-Au(19)	172.2
Au(31)-Au(34)-Au(33)	77.5
Au(33)-Au(34)-Au(1)	62.2
Au(33)-Au(34)-Au(7)	59.7
Au(33)-Au(34)-Au(17)	117.9
Au(33)-Au(34)-Au(19)	104.6
Au(35)-Au(34)-Au(1)	89.8
Au(35)-Au(34)-Au(7)	57.3

Au(35)-Au(34)-Au(17)	65.1
Au(35)-Au(34)-Au(19)	120.8
Au(35)-Au(34)-Au(31)	63.5
Au(35)-Au(34)-Au(33)	116.7
S(25)-Au(34)-Au(1)	118.7
S(25)-Au(34)-Au(7)	175.8
S(25)-Au(34)-Au(17)	93.5
S(25)-Au(34)-Au(19)	46.4
S(25)-Au(34)-Au(31)	125.9
S(25)-Au(34)-Au(33)	116.5
S(25)-Au(34)-Au(35)	126.6
Au(2)-Au(35)-Au(17)	54.6
Au(2)-Au(35)-Au(37)	76.4
Au(7)-Au(35)-Au(2)	61.3
Au(7)-Au(35)-Au(17)	89.3
Au(7)-Au(35)-Au(31)	57.2
Au(7)-Au(35)-Au(36)	64.0
Au(7)-Au(35)-Au(37)	131.9
Au(17)-Au(35)-Au(37)	83.5
Au(31)-Au(35)-Au(2)	118.3
Au(31)-Au(35)-Au(17)	118.8
Au(31)-Au(35)-Au(36)	97.9
Au(31)-Au(35)-Au(37)	157.4
Au(34)-Au(35)-Au(2)	92.5
Au(34)-Au(35)-Au(7)	65.7
Au(34)-Au(35)-Au(17)	61.2
Au(34)-Au(35)-Au(31)	58.6
Au(34)-Au(35)-Au(36)	129.2
Au(34)-Au(35)-Au(37)	142.0
Au(36)-Au(35)-Au(2)	57.5

Au(36)-Au(35)-Au(17)	111.8
Au(36)-Au(35)-Au(37)	74.9
S(22)-Au(35)-Au(2)	116.3
S(22)-Au(35)-Au(7)	175.0
S(22)-Au(35)-Au(17)	92.4
S(22)-Au(35)-Au(31)	125.5
S(22)-Au(35)-Au(34)	119.2
S(22)-Au(35)-Au(36)	111.0
S(22)-Au(35)-Au(37)	43.8
Au(2)-Au(36)-Au(7)	60.3
Au(2)-Au(36)-Au(28)	125.9
Au(2)-Au(36)-Au(29)	90.7
Au(2)-Au(36)-Au(30)	120.9
Au(2)-Au(36)-Au(35)	63.2
Au(3)-Au(36)-Au(2)	59.9
Au(3)-Au(36)-Au(4)	60.1
Au(3)-Au(36)-Au(7)	120.1
Au(3)-Au(36)-Au(28)	91.7
Au(3)-Au(36)-Au(29)	123.6
Au(3)-Au(36)-Au(30)	178.7
Au(3)-Au(36)-Au(35)	98.6
Au(4)-Au(36)-Au(2)	60.9
Au(4)-Au(36)-Au(7)	89.3
Au(4)-Au(36)-Au(28)	65.0
Au(4)-Au(36)-Au(29)	63.5
Au(4)-Au(36)-Au(30)	121.2
Au(4)-Au(36)-Au(35)	123.3
Au(7)-Au(36)-Au(28)	122.0
Au(7)-Au(36)-Au(30)	60.7
Au(28)-Au(36)-Au(30)	88.6

Au(29)-Au(36)-Au(7)	55.4
Au(29)-Au(36)-Au(28)	66.7
Au(29)-Au(36)-Au(30)	57.7
Au(35)-Au(36)-Au(7)	54.9
Au(35)-Au(36)-Au(28)	169.1
Au(35)-Au(36)-Au(29)	109.6
Au(35)-Au(36)-Au(30)	81.0
S(26)-Au(36)-Au(2)	139.5
S(26)-Au(36)-Au(3)	135.8
S(26)-Au(36)-Au(4)	155.8
S(26)-Au(36)-Au(7)	93.3
S(26)-Au(36)-Au(28)	93.6
S(26)-Au(36)-Au(29)	98.6
S(26)-Au(36)-Au(30)	42.9
S(26)-Au(36)-Au(35)	76.7
Au(3)-Au(37)-Au(35)	84.9
Au(18)-Au(37)-Au(3)	84.0
Au(18)-Au(37)-Au(35)	90.9
S(21)-Au(37)-Au(3)	51.1
S(21)-Au(37)-Au(18)	89.3
S(21)-Au(37)-Au(35)	135.7
S(21)-Au(37)-S(22)	171.8
S(22)-Au(37)-Au(3)	130.0
S(22)-Au(37)-Au(18)	98.9
S(22)-Au(37)-Au(35)	45.3
Au(3)-Au(38)-Au(24)	94.5
Au(3)-Au(38)-Au(26)	57.0
Au(24)-Au(38)-Au(26)	68.2
S(19)-Au(38)-Au(3)	93.8
S(19)-Au(38)-Au(24)	92.0

S(19)-Au(38)-Au(26)	47.7
S(20)-Au(38)-Au(3)	93.5
S(20)-Au(38)-Au(24)	89.1
S(20)-Au(38)-Au(26)	139.1
S(20)-Au(38)-S(19)	172.5
Au(4)-Au(39)-Au(22)	88.9
Au(4)-Au(39)-Au(27)	132.1
Au(6)-Au(39)-Au(4)	60.6
Au(6)-Au(39)-Au(22)	57.1
Au(6)-Au(39)-Au(27)	71.8
Au(22)-Au(39)-Au(27)	58.8
Au(23)-Au(39)-Au(4)	58.6
Au(23)-Au(39)-Au(6)	94.3
Au(23)-Au(39)-Au(22)	67.6
Au(23)-Au(39)-Au(26)	118.7
Au(23)-Au(39)-Au(27)	123.4
Au(24)-Au(39)-Au(4)	57.8
Au(24)-Au(39)-Au(6)	117.3
Au(24)-Au(39)-Au(22)	130.0
Au(24)-Au(39)-Au(23)	63.3
Au(24)-Au(39)-Au(26)	78.3
Au(24)-Au(39)-Au(27)	169.4
Au(26)-Au(39)-Au(4)	60.7
Au(26)-Au(39)-Au(6)	62.4
Au(26)-Au(39)-Au(22)	119.5
Au(26)-Au(39)-Au(27)	102.9
S(6)-Au(39)-Au(4)	173.7
S(6)-Au(39)-Au(6)	116.5
S(6)-Au(39)-Au(22)	93.9
S(6)-Au(39)-Au(23)	127.7

S(6)-Au(39)-Au(24)	123.4
S(6)-Au(39)-Au(26)	113.0
S(6)-Au(39)-Au(27)	46.3
S(13)-Au(40)-Au(31)	47.3
S(14)-Au(40)-Au(31)	138.6
S(14)-Au(40)-S(13)	172.2
S(14)-Au(41)-Au(20)	140.6
S(15)-Au(41)-Au(20)	46.5
S(15)-Au(41)-S(14)	171.4
S(7)-Au(42)-Au(14)	45.2
S(7)-Au(42)-S(8)	171.0
S(8)-Au(42)-Au(14)	140.6
Au(10)-S(1)-Au(22)	81.2
C(1)-S(1)-Au(10)	101.0
C(1)-S(1)-Au(22)	105.2
Au(11)-S(2)-Au(23)	90.1
C(7)-S(2)-Au(11)	99.3
C(7)-S(2)-Au(23)	113.2
Au(11)-S(3)-Au(8)	79.4
C(13)-S(3)-Au(8)	106.1
C(13)-S(3)-Au(11)	107.6
Au(10)-S(4)-Au(9)	91.8
C(19)-S(4)-Au(9)	103.7
C(19)-S(4)-Au(10)	102.7
Au(27)-S(5)-Au(13)	97.9
C(25)-S(5)-Au(13)	104.4
C(25)-S(5)-Au(27)	104.1
Au(27)-S(6)-Au(39)	85.7
C(31)-S(6)-Au(27)	109.1
C(31)-S(6)-Au(39)	104.2

Au(42)-S(7)-Au(14)	90.4
C(37)-S(7)-Au(14)	112.8
C(37)-S(7)-Au(42)	106.5
Au(42)-S(8)-Au(25)	107.7
C(43)-S(8)-Au(25)	102.8
C(43)-S(8)-Au(42)	104.0
Au(25)-S(9)-Au(24)	92.3
C(49)-S(9)-Au(24)	109.6
C(49)-S(9)-Au(25)	103.7
Au(28)-S(10)-Au(29)	90.2
C(55)-S(10)-Au(28)	104.6
C(55)-S(10)-Au(29)	119.6
Au(32)-S(11)-Au(30)	99.7
C(61)-S(11)-Au(30)	106.6
C(61)-S(11)-Au(32)	104.0
Au(32)-S(12)-Au(33)	84.6
C(67)-S(12)-Au(32)	109.3
C(67)-S(12)-Au(33)	101.4
Au(40)-S(13)-Au(31)	86.0
C(73)-S(13)-Au(31)	126.2
C(73)-S(13)-Au(40)	136.6
Au(40)-S(14)-Au(41)	106.1
C(79)-S(14)-Au(40)	102.4
C(79)-S(14)-Au(41)	106.1
Au(41)-S(15)-Au(20)	88.7
C(85)-S(15)-Au(20)	107.5
C(85)-S(15)-Au(41)	103.8
Au(21)-S(16)-Au(12)	92.7
C(91)-S(16)-Au(12)	111.9
C(91)-S(16)-Au(21)	109.7

Au(13)-S(17)-Au(16)	90.1
C(97)-S(17)-Au(13)	106.6
C(97)-S(17)-Au(16)	113.3
Au(18)-S(18)-Au(15)	89.6
C(103)-S(18)-Au(15)	105.4
C(103)-S(18)-Au(18)	100.2
Au(38)-S(19)-Au(26)	85.6
C(109)-S(19)-Au(26)	103.0
C(109)-S(19)-Au(38)	108.3
Au(38)-S(20)-Au(28)	98.0
C(115)-S(20)-Au(28)	100.5
C(115)-S(20)-Au(38)	100.1
Au(37)-S(21)-Au(3)	80.7
C(121)-S(21)-Au(3)	105.4
C(121)-S(21)-Au(37)	103.7
Au(37)-S(22)-Au(35)	90.8
C(127)-S(22)-Au(35)	103.8
C(127)-S(22)-Au(37)	99.1
Au(18)-S(23)-Au(17)	79.6
C(133)-S(23)-Au(17)	108.3
C(133)-S(23)-Au(18)	97.3
Au(19)-S(24)-Au(21)	100.7
C(139)-S(24)-Au(19)	103.4
C(139)-S(24)-Au(21)	103.7
Au(19)-S(25)-Au(34)	85.9
C(145)-S(25)-Au(19)	106.1
C(145)-S(25)-Au(34)	102.9
Au(30)-S(26)-Au(36)	92.7
C(151)-S(26)-Au(30)	109.6
C(151)-S(26)-Au(36)	114.1

S(1)-C(1)-H(1)	110.7
C(2)-C(1)-S(1)	110.9
C(2)-C(1)-H(1)	110.7
C(2)-C(1)-C(6)	109.6
C(6)-C(1)-S(1)	104.1
C(6)-C(1)-H(1)	110.7
C(1)-C(2)-H(2A)	109.2
C(1)-C(2)-H(2B)	109.2
C(1)-C(2)-C(3)	111.8
H(2A)-C(2)-H(2B)	107.9
C(3)-C(2)-H(2A)	109.2
C(3)-C(2)-H(2B)	109.2
C(2)-C(3)-H(3A)	111.1
C(2)-C(3)-H(3B)	111.1
C(2)-C(3)-C(4)	103.2
H(3A)-C(3)-H(3B)	109.1
C(4)-C(3)-H(3A)	111.1
C(4)-C(3)-H(3B)	111.1
C(3)-C(4)-H(4A)	110.0
C(3)-C(4)-H(4B)	110.0
H(4A)-C(4)-H(4B)	108.4
C(5)-C(4)-C(3)	108.4
C(5)-C(4)-H(4A)	110.0
C(5)-C(4)-H(4B)	110.0
C(4)-C(5)-H(5A)	110.3
C(4)-C(5)-H(5B)	110.3
C(4)-C(5)-C(6)	107.0
H(5A)-C(5)-H(5B)	108.6
C(6)-C(5)-H(5A)	110.3
C(6)-C(5)-H(5B)	110.3

C(1)-C(6)-H(6A)	109.1
C(1)-C(6)-H(6B)	109.1
C(5)-C(6)-C(1)	112.5
C(5)-C(6)-H(6A)	109.1
C(5)-C(6)-H(6B)	109.1
H(6A)-C(6)-H(6B)	107.8
S(2)-C(7)-H(7)	105.2
C(8)-C(7)-S(2)	107.6
C(8)-C(7)-H(7)	105.2
C(12)-C(7)-S(2)	115.1
C(12)-C(7)-H(7)	105.2
C(12)-C(7)-C(8)	117.5
C(7)-C(8)-H(8A)	108.8
C(7)-C(8)-H(8B)	108.8
C(7)-C(8)-C(9)	113.7
H(8A)-C(8)-H(8B)	107.7
C(9)-C(8)-H(8A)	108.8
C(9)-C(8)-H(8B)	108.8
C(8)-C(9)-H(9A)	112.1
C(8)-C(9)-H(9B)	112.0
C(8)-C(9)-C(10)	98.6
H(9A)-C(9)-H(9B)	109.7
C(10)-C(9)-H(9A)	112.0
C(10)-C(9)-H(9B)	112.0
C(9)-C(10)-H(10A)	109.8
C(9)-C(10)-H(10B)	109.8
H(10A)-C(10)-H(10B)	108.3
C(11)-C(10)-C(9)	109.3
C(11)-C(10)-H(10A)	109.8
C(11)-C(10)-H(10B)	109.8

C(10)-C(11)-H(11A)	108.8
C(10)-C(11)-H(11B)	108.8
C(10)-C(11)-C(12)	114.0
H(11A)-C(11)-H(11B)	107.7
C(12)-C(11)-H(11A)	108.8
C(12)-C(11)-H(11B)	108.8
C(7)-C(12)-C(11)	115.1
C(7)-C(12)-H(12A)	108.5
C(7)-C(12)-H(12B)	108.5
C(11)-C(12)-H(12A)	108.5
C(11)-C(12)-H(12B)	108.5
H(12A)-C(12)-H(12B)	107.5
S(3)-C(13)-H(13)	103.0
C(14)-C(13)-S(3)	104.9
C(14)-C(13)-H(13)	103.0
C(18)-C(13)-S(3)	113.0
C(18)-C(13)-H(13)	103.0
C(18)-C(13)-C(14)	126.9
C(13)-C(14)-H(14A)	108.7
C(13)-C(14)-H(14B)	108.7
C(13)-C(14)-C(15)	114.3
H(14A)-C(14)-H(14B)	107.6
C(15)-C(14)-H(14A)	108.7
C(15)-C(14)-H(14B)	108.7
C(14)-C(15)-H(15A)	110.0
C(14)-C(15)-H(15B)	110.0
H(15A)-C(15)-H(15B)	108.4
C(16)-C(15)-C(14)	108.6
C(16)-C(15)-H(15A)	110.0
C(16)-C(15)-H(15B)	110.0

C(15)-C(16)-H(16A)	109.9
C(15)-C(16)-H(16B)	109.9
H(16A)-C(16)-H(16B)	108.3
C(17)-C(16)-C(15)	109.1
C(17)-C(16)-H(16A)	109.9
C(17)-C(16)-H(16B)	109.9
C(16)-C(17)-H(17A)	107.1
C(16)-C(17)-H(17B)	107.1
H(17A)-C(17)-H(17B)	106.8
C(18)-C(17)-C(16)	120.9
C(18)-C(17)-H(17A)	107.1
C(18)-C(17)-H(17B)	107.1
C(13)-C(18)-C(17)	99.7
C(13)-C(18)-H(18A)	111.8
C(13)-C(18)-H(18B)	111.8
C(17)-C(18)-H(18A)	111.8
C(17)-C(18)-H(18B)	111.8
H(18A)-C(18)-H(18B)	109.5
S(4)-C(19)-H(19)	108.4
C(20)-C(19)-S(4)	112.0
C(20)-C(19)-H(19)	108.4
C(24)-C(19)-S(4)	108.1
C(24)-C(19)-H(19)	108.4
C(24)-C(19)-C(20)	111.3
C(19)-C(20)-H(20A)	110.3
C(19)-C(20)-H(20B)	110.3
C(19)-C(20)-C(21)	107.0
H(20A)-C(20)-H(20B)	108.6
C(21)-C(20)-H(20A)	110.3
C(21)-C(20)-H(20B)	110.3

C(20)-C(21)-H(21A)	108.0
C(20)-C(21)-H(21B)	108.0
H(21A)-C(21)-H(21B)	107.3
C(22)-C(21)-C(20)	117.1
C(22)-C(21)-H(21A)	108.0
C(22)-C(21)-H(21B)	108.0
C(21)-C(22)-H(22A)	109.0
C(21)-C(22)-H(22B)	109.0
C(21)-C(22)-C(23)	113.0
H(22A)-C(22)-H(22B)	107.8
C(23)-C(22)-H(22A)	109.0
C(23)-C(22)-H(22B)	109.0
C(22)-C(23)-H(23A)	111.2
C(22)-C(23)-H(23B)	111.2
H(23A)-C(23)-H(23B)	109.1
C(24)-C(23)-C(22)	103.0
C(24)-C(23)-H(23A)	111.2
C(24)-C(23)-H(23B)	111.2
C(19)-C(24)-C(23)	113.0
C(19)-C(24)-H(24A)	109.0
C(19)-C(24)-H(24B)	109.0
C(23)-C(24)-H(24A)	109.0
C(23)-C(24)-H(24B)	109.0
H(24A)-C(24)-H(24B)	107.8
S(5)-C(25)-H(25)	105.8
C(26)-C(25)-S(5)	112.7
C(26)-C(25)-H(25)	105.8
C(26)-C(25)-C(30)	113.2
C(30)-C(25)-S(5)	112.8
C(30)-C(25)-H(25)	105.8

C(25)-C(26)-H(26A)	110.6
C(25)-C(26)-H(26B)	110.6
C(25)-C(26)-C(27)	105.7
H(26A)-C(26)-H(26B)	108.7
C(27)-C(26)-H(26A)	110.6
C(27)-C(26)-H(26B)	110.6
C(26)-C(27)-H(27A)	109.2
C(26)-C(27)-H(27B)	109.2
H(27A)-C(27)-H(27B)	107.9
C(28)-C(27)-C(26)	111.9
C(28)-C(27)-H(27A)	109.2
C(28)-C(27)-H(27B)	109.2
C(27)-C(28)-H(28A)	109.3
C(27)-C(28)-H(28B)	109.3
H(28A)-C(28)-H(28B)	108.0
C(29)-C(28)-C(27)	111.6
C(29)-C(28)-H(28A)	109.3
C(29)-C(28)-H(28B)	109.3
C(28)-C(29)-H(29A)	106.7
C(28)-C(29)-H(29B)	106.7
C(28)-C(29)-C(30)	122.4
H(29A)-C(29)-H(29B)	106.6
C(30)-C(29)-H(29A)	106.7
C(30)-C(29)-H(29B)	106.7
C(25)-C(30)-H(30A)	109.7
C(25)-C(30)-H(30B)	109.7
C(29)-C(30)-C(25)	110.0
C(29)-C(30)-H(30A)	109.7
C(29)-C(30)-H(30B)	109.7
H(30A)-C(30)-H(30B)	108.2

S(6)-C(31)-H(31)	110.6
C(32)-C(31)-S(6)	108.0
C(32)-C(31)-H(31)	110.6
C(36)-C(31)-S(6)	108.6
C(36)-C(31)-H(31)	110.6
C(36)-C(31)-C(32)	108.3
C(31)-C(32)-H(32A)	109.2
C(31)-C(32)-H(32B)	109.2
C(31)-C(32)-C(33)	111.8
H(32A)-C(32)-H(32B)	107.9
C(33)-C(32)-H(32A)	109.2
C(33)-C(32)-H(32B)	109.2
C(32)-C(33)-H(33A)	109.3
C(32)-C(33)-H(33B)	109.3
H(33A)-C(33)-H(33B)	108.0
C(34)-C(33)-C(32)	111.6
C(34)-C(33)-H(33A)	109.3
C(34)-C(33)-H(33B)	109.3
C(33)-C(34)-H(34A)	108.6
C(33)-C(34)-H(34B)	108.6
C(33)-C(34)-C(35)	114.5
H(34A)-C(34)-H(34B)	107.6
C(35)-C(34)-H(34A)	108.6
C(35)-C(34)-H(34B)	108.6
C(34)-C(35)-H(35A)	109.1
C(34)-C(35)-H(35B)	109.1
H(35A)-C(35)-H(35B)	107.9
C(36)-C(35)-C(34)	112.3
C(36)-C(35)-H(35A)	109.1
C(36)-C(35)-H(35B)	109.1

C(31)-C(36)-C(35)	110.7
C(31)-C(36)-H(36A)	109.5
C(31)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	108.1
S(7)-C(37)-H(37)	109.6
C(38)-C(37)-S(7)	104.9
C(38)-C(37)-H(37)	109.6
C(38)-C(37)-C(42)	114.6
C(42)-C(37)-S(7)	108.4
C(42)-C(37)-H(37)	109.6
C(37)-C(38)-H(38A)	110.9
C(37)-C(38)-H(38B)	110.9
C(37)-C(38)-C(39)	104.3
H(38A)-C(38)-H(38B)	108.9
C(39)-C(38)-H(38A)	110.9
C(39)-C(38)-H(38B)	110.9
C(38)-C(39)-H(39A)	109.7
C(38)-C(39)-H(39B)	109.7
H(39A)-C(39)-H(39B)	108.2
C(40)-C(39)-C(38)	109.9
C(40)-C(39)-H(39A)	109.7
C(40)-C(39)-H(39B)	109.7
C(39)-C(40)-H(40A)	108.8
C(39)-C(40)-H(40B)	108.8
C(39)-C(40)-C(41)	113.9
H(40A)-C(40)-H(40B)	107.7
C(41)-C(40)-H(40A)	108.8
C(41)-C(40)-H(40B)	108.8

C(40)-C(41)-H(41A)	110.3
C(40)-C(41)-H(41B)	110.3
H(41A)-C(41)-H(41B)	108.6
C(42)-C(41)-C(40)	107.1
C(42)-C(41)-H(41A)	110.3
C(42)-C(41)-H(41B)	110.3
C(37)-C(42)-H(42A)	110.9
C(37)-C(42)-H(42B)	110.9
C(41)-C(42)-C(37)	104.3
C(41)-C(42)-H(42A)	110.9
C(41)-C(42)-H(42B)	110.9
H(42A)-C(42)-H(42B)	108.9
S(8)-C(43)-H(43)	102.5
C(44)-C(43)-S(8)	113.0
C(44)-C(43)-H(43)	102.5
C(48)-C(43)-S(8)	124.6
C(48)-C(43)-H(43)	102.5
C(48)-C(43)-C(44)	108.6
C(43)-C(44)-H(44A)	107.6
C(43)-C(44)-H(44B)	107.6
H(44A)-C(44)-H(44B)	107.0
C(45)-C(44)-C(43)	118.8
C(45)-C(44)-H(44A)	107.6
C(45)-C(44)-H(44B)	107.6
C(44)-C(45)-H(45A)	111.2
C(44)-C(45)-H(45B)	111.2
C(44)-C(45)-C(46)	102.9
H(45A)-C(45)-H(45B)	109.1
C(46)-C(45)-H(45A)	111.2
C(46)-C(45)-H(45B)	111.2

C(45)-C(46)-H(46A)	109.3
C(45)-C(46)-H(46B)	109.3
C(45)-C(46)-C(47)	111.4
H(46A)-C(46)-H(46B)	108.0
C(47)-C(46)-H(46A)	109.3
C(47)-C(46)-H(46B)	109.3
C(46)-C(47)-H(47A)	110.2
C(46)-C(47)-H(47B)	110.2
H(47A)-C(47)-H(47B)	108.5
C(48)-C(47)-C(46)	107.5
C(48)-C(47)-H(47A)	110.2
C(48)-C(47)-H(47B)	110.2
C(43)-C(48)-C(47)	126.9
C(43)-C(48)-H(48A)	105.6
C(43)-C(48)-H(48B)	105.6
C(47)-C(48)-H(48A)	105.6
C(47)-C(48)-H(48B)	105.6
H(48A)-C(48)-H(48B)	106.1
S(9)-C(49)-H(49)	109.9
C(50)-C(49)-S(9)	111.0
C(50)-C(49)-H(49)	109.9
C(50)-C(49)-C(54)	109.3
C(54)-C(49)-S(9)	106.7
C(54)-C(49)-H(49)	109.9
C(49)-C(50)-H(50A)	109.2
C(49)-C(50)-H(50B)	109.2
H(50A)-C(50)-H(50B)	107.9
C(51)-C(50)-C(49)	111.9
C(51)-C(50)-H(50A)	109.2
C(51)-C(50)-H(50B)	109.2

C(50)-C(51)-H(51A)	110.5
C(50)-C(51)-H(51B)	110.5
C(50)-C(51)-C(52)	106.1
H(51A)-C(51)-H(51B)	108.7
C(52)-C(51)-H(51A)	110.5
C(52)-C(51)-H(51B)	110.5
C(51)-C(52)-H(52A)	110.4
C(51)-C(52)-H(52B)	110.4
H(52A)-C(52)-H(52B)	108.6
C(53)-C(52)-C(51)	106.5
C(53)-C(52)-H(52A)	110.4
C(53)-C(52)-H(52B)	110.4
C(52)-C(53)-H(53A)	107.8
C(52)-C(53)-H(53B)	107.8
C(52)-C(53)-C(54)	118.2
H(53A)-C(53)-H(53B)	107.1
C(54)-C(53)-H(53A)	107.8
C(54)-C(53)-H(53B)	107.8
C(49)-C(54)-H(54A)	110.7
C(49)-C(54)-H(54B)	110.7
C(53)-C(54)-C(49)	105.4
C(53)-C(54)-H(54A)	110.7
C(53)-C(54)-H(54B)	110.7
H(54A)-C(54)-H(54B)	108.8
C(56)-C(55)-S(10)	115.7
C(60)-C(55)-S(10)	132.2
C(60)-C(55)-C(56)	109.3
C(55)-C(56)-H(56A)	109.9
C(55)-C(56)-H(56B)	109.9
C(55)-C(56)-C(57)	108.8

H(56A)-C(56)-H(56B)	108.3
C(57)-C(56)-H(56A)	109.9
C(57)-C(56)-H(56B)	109.9
C(56)-C(57)-H(57A)	110.1
C(56)-C(57)-H(57B)	110.1
C(56)-C(57)-C(58)	108.2
H(57A)-C(57)-H(57B)	108.4
C(58)-C(57)-H(57A)	110.1
C(58)-C(57)-H(57B)	110.1
C(57)-C(58)-H(58A)	109.9
C(57)-C(58)-H(58B)	109.9
H(58A)-C(58)-H(58B)	108.3
C(59)-C(58)-C(57)	108.9
C(59)-C(58)-H(58A)	109.9
C(59)-C(58)-H(58B)	109.9
C(58)-C(59)-H(59A)	109.9
C(58)-C(59)-H(59B)	109.9
C(58)-C(59)-C(60)	109.0
H(59A)-C(59)-H(59B)	108.3
C(60)-C(59)-H(59A)	109.9
C(60)-C(59)-H(59B)	109.9
C(55)-C(60)-C(59)	109.1
C(55)-C(60)-H(60A)	109.9
C(55)-C(60)-H(60B)	109.9
C(59)-C(60)-H(60A)	109.9
C(59)-C(60)-H(60B)	109.9
H(60A)-C(60)-H(60B)	108.3
S(11)-C(61)-H(61)	110.0
C(62)-C(61)-S(11)	111.1
C(62)-C(61)-H(61)	110.0

C(66)-C(61)-S(11)	106.3
C(66)-C(61)-H(61)	110.0
C(66)-C(61)-C(62)	109.3
C(61)-C(62)-H(62A)	111.7
C(61)-C(62)-H(62B)	111.7
H(62A)-C(62)-H(62B)	109.5
C(63)-C(62)-C(61)	100.4
C(63)-C(62)-H(62A)	111.7
C(63)-C(62)-H(62B)	111.7
C(62)-C(63)-H(63A)	109.5
C(62)-C(63)-H(63B)	109.5
C(62)-C(63)-C(64)	110.7
H(63A)-C(63)-H(63B)	108.1
C(64)-C(63)-H(63A)	109.5
C(64)-C(63)-H(63B)	109.5
C(63)-C(64)-H(64A)	110.6
C(63)-C(64)-H(64B)	110.6
H(64A)-C(64)-H(64B)	108.7
C(65)-C(64)-C(63)	105.7
C(65)-C(64)-H(64A)	110.6
C(65)-C(64)-H(64B)	110.6
C(64)-C(65)-H(65A)	108.3
C(64)-C(65)-H(65B)	108.3
C(64)-C(65)-C(66)	116.1
H(65A)-C(65)-H(65B)	107.4
C(66)-C(65)-H(65A)	108.3
C(66)-C(65)-H(65B)	108.3
C(61)-C(66)-C(65)	117.1
C(61)-C(66)-H(66A)	108.0
C(61)-C(66)-H(66B)	108.0

C(65)-C(66)-H(66A)	108.0
C(65)-C(66)-H(66B)	108.0
H(66A)-C(66)-H(66B)	107.3
S(12)-C(67)-H(67)	107.9
C(68)-C(67)-S(12)	114.0
C(68)-C(67)-H(67)	107.9
C(68)-C(67)-C(72)	110.1
C(72)-C(67)-S(12)	109.0
C(72)-C(67)-H(67)	107.9
C(67)-C(68)-H(68A)	109.0
C(67)-C(68)-H(68B)	109.0
C(67)-C(68)-C(69)	112.8
H(68A)-C(68)-H(68B)	107.8
C(69)-C(68)-H(68A)	109.0
C(69)-C(68)-H(68B)	109.0
C(68)-C(69)-H(69A)	108.2
C(68)-C(69)-H(69B)	108.2
H(69A)-C(69)-H(69B)	107.3
C(70)-C(69)-C(68)	116.4
C(70)-C(69)-H(69A)	108.2
C(70)-C(69)-H(69B)	108.2
C(69)-C(70)-H(70A)	112.0
C(69)-C(70)-H(70B)	112.0
C(69)-C(70)-C(71)	98.7
H(70A)-C(70)-H(70B)	109.7
C(71)-C(70)-H(70A)	112.0
C(71)-C(70)-H(70B)	112.0
C(70)-C(71)-H(71A)	106.5
C(70)-C(71)-H(71B)	106.5
H(71A)-C(71)-H(71B)	106.5

C(72)-C(71)-C(70)	123.4
C(72)-C(71)-H(71A)	106.5
C(72)-C(71)-H(71B)	106.5
C(67)-C(72)-H(72A)	110.3
C(67)-C(72)-H(72B)	110.3
C(71)-C(72)-C(67)	107.2
C(71)-C(72)-H(72A)	110.3
C(71)-C(72)-H(72B)	110.3
H(72A)-C(72)-H(72B)	108.5
S(13)-C(73)-H(73)	100.4
C(74)-C(73)-S(13)	130.0
C(74)-C(73)-H(73)	100.4
C(78)-C(73)-S(13)	111.0
C(78)-C(73)-H(73)	100.4
C(78)-C(73)-C(74)	109.2
C(73)-C(74)-H(74A)	109.6
C(73)-C(74)-H(74B)	109.6
C(73)-C(74)-C(75)	110.4
H(74A)-C(74)-H(74B)	108.1
C(75)-C(74)-H(74A)	109.6
C(75)-C(74)-H(74B)	109.6
C(74)-C(75)-H(75A)	109.9
C(74)-C(75)-H(75B)	109.9
C(74)-C(75)-C(76)	109.0
H(75A)-C(75)-H(75B)	108.3
C(76)-C(75)-H(75A)	109.9
C(76)-C(75)-H(75B)	109.9
C(75)-C(76)-H(76A)	109.9
C(75)-C(76)-H(76B)	109.9
C(75)-C(76)-C(77)	109.0

H(76A)-C(76)-H(76B)	108.3
C(77)-C(76)-H(76A)	109.9
C(77)-C(76)-H(76B)	109.9
C(76)-C(77)-H(77A)	109.9
C(76)-C(77)-H(77B)	109.9
H(77A)-C(77)-H(77B)	108.3
C(78)-C(77)-C(76)	109.1
C(78)-C(77)-H(77A)	109.9
C(78)-C(77)-H(77B)	109.9
C(73)-C(78)-H(78A)	106.8
C(73)-C(78)-H(78B)	106.8
C(77)-C(78)-C(73)	122.1
C(77)-C(78)-H(78A)	106.8
C(77)-C(78)-H(78B)	106.8
H(78A)-C(78)-H(78B)	106.7
S(14)-C(79)-H(79)	97.8
C(80)-C(79)-S(14)	133.7
C(80)-C(79)-H(79)	97.8
C(84)-C(79)-S(14)	111.3
C(84)-C(79)-H(79)	97.8
C(84)-C(79)-C(80)	109.2
C(79)-C(80)-H(80A)	109.4
C(79)-C(80)-H(80B)	109.4
H(80A)-C(80)-H(80B)	108.0
C(81)-C(80)-C(79)	111.2
C(81)-C(80)-H(80A)	109.4
C(81)-C(80)-H(80B)	109.4
C(80)-C(81)-H(81A)	110.7
C(80)-C(81)-H(81B)	110.7
H(81A)-C(81)-H(81B)	108.8

C(82)-C(81)-C(80)	105.1
C(82)-C(81)-H(81A)	110.7
C(82)-C(81)-H(81B)	110.7
C(81)-C(82)-H(82A)	109.4
C(81)-C(82)-H(82B)	109.4
H(82A)-C(82)-H(82B)	108.0
C(83)-C(82)-C(81)	111.1
C(83)-C(82)-H(82A)	109.4
C(83)-C(82)-H(82B)	109.4
C(82)-C(83)-H(83A)	109.5
C(82)-C(83)-H(83B)	109.5
C(82)-C(83)-C(84)	110.7
H(83A)-C(83)-H(83B)	108.1
C(84)-C(83)-H(83A)	109.5
C(84)-C(83)-H(83B)	109.5
C(79)-C(84)-H(84A)	109.8
C(79)-C(84)-H(84B)	109.8
C(83)-C(84)-C(79)	109.5
C(83)-C(84)-H(84A)	109.8
C(83)-C(84)-H(84B)	109.8
H(84A)-C(84)-H(84B)	108.2
S(15)-C(85)-H(85)	110.5
C(86)-C(85)-S(15)	111.6
C(86)-C(85)-H(85)	110.5
C(86)-C(85)-C(90)	110.9
C(90)-C(85)-S(15)	102.8
C(90)-C(85)-H(85)	110.5
C(85)-C(86)-H(86A)	109.5
C(85)-C(86)-H(86B)	109.5
H(86A)-C(86)-H(86B)	108.0

C(87)-C(86)-C(85)	110.9
C(87)-C(86)-H(86A)	109.5
C(87)-C(86)-H(86B)	109.5
C(86)-C(87)-H(87A)	109.6
C(86)-C(87)-H(87B)	109.6
C(86)-C(87)-C(88)	110.2
H(87A)-C(87)-H(87B)	108.1
C(88)-C(87)-H(87A)	109.6
C(88)-C(87)-H(87B)	109.6
C(87)-C(88)-H(88A)	108.8
C(87)-C(88)-H(88B)	108.8
H(88A)-C(88)-H(88B)	107.7
C(89)-C(88)-C(87)	113.8
C(89)-C(88)-H(88A)	108.8
C(89)-C(88)-H(88B)	108.8
C(88)-C(89)-H(89A)	108.9
C(88)-C(89)-H(89B)	108.9
C(88)-C(89)-C(90)	113.3
H(89A)-C(89)-H(89B)	107.7
C(90)-C(89)-H(89A)	108.9
C(90)-C(89)-H(89B)	108.9
C(85)-C(90)-H(90A)	108.8
C(85)-C(90)-H(90B)	108.8
C(89)-C(90)-C(85)	114.0
C(89)-C(90)-H(90A)	108.8
C(89)-C(90)-H(90B)	108.8
H(90A)-C(90)-H(90B)	107.7
S(16)-C(91)-H(91)	108.6
C(92)-C(91)-S(16)	109.5
C(92)-C(91)-H(91)	108.6

C(96)-C(91)-S(16)	107.4
C(96)-C(91)-H(91)	108.6
C(96)-C(91)-C(92)	114.1
C(91)-C(92)-H(92A)	109.0
C(91)-C(92)-H(92B)	109.0
H(92A)-C(92)-H(92B)	107.8
C(93)-C(92)-C(91)	112.9
C(93)-C(92)-H(92A)	109.0
C(93)-C(92)-H(92B)	109.0
C(92)-C(93)-H(93A)	110.9
C(92)-C(93)-H(93B)	110.9
C(92)-C(93)-C(94)	104.3
H(93A)-C(93)-H(93B)	108.9
C(94)-C(93)-H(93A)	110.9
C(94)-C(93)-H(93B)	110.9
C(93)-C(94)-H(94A)	111.6
C(93)-C(94)-H(94B)	111.6
H(94A)-C(94)-H(94B)	109.4
C(95)-C(94)-C(93)	101.0
C(95)-C(94)-H(94A)	111.6
C(95)-C(94)-H(94B)	111.6
C(94)-C(95)-H(95A)	109.7
C(94)-C(95)-H(95B)	109.7
C(94)-C(95)-C(96)	110.0
H(95A)-C(95)-H(95B)	108.2
C(96)-C(95)-H(95A)	109.7
C(96)-C(95)-H(95B)	109.7
C(91)-C(96)-C(95)	111.7
C(91)-C(96)-H(96A)	109.3
C(91)-C(96)-H(96B)	109.3

C(95)-C(96)-H(96A)	109.3
C(95)-C(96)-H(96B)	109.3
H(96A)-C(96)-H(96B)	107.9
S(17)-C(97)-H(97)	108.1
C(98)-C(97)-S(17)	107.5
C(98)-C(97)-H(97)	108.1
C(98)-C(97)-C(102)	112.7
C(102)-C(97)-S(17)	112.2
C(102)-C(97)-H(97)	108.1
C(97)-C(98)-H(98A)	108.6
C(97)-C(98)-H(98B)	108.6
H(98A)-C(98)-H(98B)	107.6
C(99)-C(98)-C(97)	114.5
C(99)-C(98)-H(98A)	108.6
C(99)-C(98)-H(98B)	108.6
C(98)-C(99)-H(99A)	109.2
C(98)-C(99)-H(99B)	109.2
C(98)-C(99)-C(100)	112.1
H(99A)-C(99)-H(99B)	107.9
C(100)-C(99)-H(99A)	109.2
C(100)-C(99)-H(99B)	109.2
C(99)-C(100)-H(10C)	108.9
C(99)-C(100)-H(10D)	108.9
C(99)-C(100)-C(101)	113.3
H(10C)-C(100)-H(10D)	107.7
C(101)-C(100)-H(10C)	108.9
C(101)-C(100)-H(10D)	108.9
C(100)-C(101)-H(10E)	110.0
C(100)-C(101)-H(10F)	110.0
H(10E)-C(101)-H(10F)	108.4

C(102)-C(101)-C(100)	108.4
C(102)-C(101)-H(10E)	110.0
C(102)-C(101)-H(10F)	110.0
C(97)-C(102)-H(10G)	109.4
C(97)-C(102)-H(10H)	109.4
C(101)-C(102)-C(97)	111.4
C(101)-C(102)-H(10G)	109.4
C(101)-C(102)-H(10H)	109.4
H(10G)-C(102)-H(10H)	108.0
S(18)-C(103)-H(103)	109.9
C(104)-C(103)-S(18)	104.6
C(104)-C(103)-H(103)	109.9
C(108)-C(103)-S(18)	108.8
C(108)-C(103)-H(103)	109.9
C(108)-C(103)-C(104)	113.5
C(103)-C(104)-H(10I)	110.0
C(103)-C(104)-H(10J)	110.0
H(10I)-C(104)-H(10J)	108.4
C(105)-C(104)-C(103)	108.3
C(105)-C(104)-H(10I)	110.0
C(105)-C(104)-H(10J)	110.0
C(104)-C(105)-H(10K)	109.7
C(104)-C(105)-H(10L)	109.7
C(104)-C(105)-C(106)	109.8
H(10K)-C(105)-H(10L)	108.2
C(106)-C(105)-H(10K)	109.7
C(106)-C(105)-H(10L)	109.7
C(105)-C(106)-H(10M)	110.2
C(105)-C(106)-H(10N)	110.2
H(10M)-C(106)-H(10N)	108.5

C(107)-C(106)-C(105)	107.3
C(107)-C(106)-H(10M)	110.2
C(107)-C(106)-H(10N)	110.2
C(106)-C(107)-H(10O)	107.8
C(106)-C(107)-H(10P)	107.8
C(106)-C(107)-C(108)	118.0
H(10O)-C(107)-H(10P)	107.1
C(108)-C(107)-H(10O)	107.8
C(108)-C(107)-H(10P)	107.8
C(103)-C(108)-C(107)	104.8
C(103)-C(108)-H(10Q)	110.8
C(103)-C(108)-H(10R)	110.8
C(107)-C(108)-H(10Q)	110.8
C(107)-C(108)-H(10R)	110.8
H(10Q)-C(108)-H(10R)	108.9
S(19)-C(109)-H(109)	108.3
C(110)-C(109)-S(19)	106.2
C(110)-C(109)-H(109)	108.3
C(114)-C(109)-S(19)	113.8
C(114)-C(109)-H(109)	108.3
C(114)-C(109)-C(110)	111.9
C(109)-C(110)-H(11C)	110.2
C(109)-C(110)-H(11D)	110.2
H(11C)-C(110)-H(11D)	108.5
C(111)-C(110)-C(109)	107.5
C(111)-C(110)-H(11C)	110.2
C(111)-C(110)-H(11D)	110.2
C(110)-C(111)-H(11E)	109.7
C(110)-C(111)-H(11F)	109.7
H(11E)-C(111)-H(11F)	108.2

C(112)-C(111)-C(110)	109.9
C(112)-C(111)-H(11E)	109.7
C(112)-C(111)-H(11F)	109.7
C(111)-C(112)-H(11G)	109.6
C(111)-C(112)-H(11H)	109.6
C(111)-C(112)-C(113)	110.4
H(11G)-C(112)-H(11H)	108.1
C(113)-C(112)-H(11G)	109.6
C(113)-C(112)-H(11H)	109.6
C(112)-C(113)-H(11I)	108.3
C(112)-C(113)-H(11J)	108.3
H(11I)-C(113)-H(11J)	107.4
C(114)-C(113)-C(112)	116.0
C(114)-C(113)-H(11I)	108.3
C(114)-C(113)-H(11J)	108.3
C(109)-C(114)-C(113)	112.7
C(109)-C(114)-H(11K)	109.1
C(109)-C(114)-H(11L)	109.1
C(113)-C(114)-H(11K)	109.1
C(113)-C(114)-H(11L)	109.1
H(11K)-C(114)-H(11L)	107.8
S(20)-C(115)-H(115)	109.6
C(116)-C(115)-S(20)	102.9
C(116)-C(115)-H(115)	109.6
C(120)-C(115)-S(20)	116.7
C(120)-C(115)-H(115)	109.6
C(120)-C(115)-C(116)	108.0
C(115)-C(116)-H(11M)	110.0
C(115)-C(116)-H(11N)	110.0
H(11M)-C(116)-H(11N)	108.4

C(117)-C(116)-C(115)	108.6
C(117)-C(116)-H(11M)	110.0
C(117)-C(116)-H(11N)	110.0
C(116)-C(117)-H(11O)	111.7
C(116)-C(117)-H(11P)	111.7
C(116)-C(117)-C(118)	100.3
H(11O)-C(117)-H(11P)	109.5
C(118)-C(117)-H(11O)	111.7
C(118)-C(117)-H(11P)	111.7
C(117)-C(118)-H(11Q)	108.6
C(117)-C(118)-H(11R)	108.6
H(11Q)-C(118)-H(11R)	107.5
C(119)-C(118)-C(117)	114.8
C(119)-C(118)-H(11Q)	108.6
C(119)-C(118)-H(11R)	108.6
C(118)-C(119)-H(11S)	109.4
C(118)-C(119)-H(11T)	109.4
H(11S)-C(119)-H(11T)	108.0
C(120)-C(119)-C(118)	111.3
C(120)-C(119)-H(11S)	109.4
C(120)-C(119)-H(11T)	109.4
C(115)-C(120)-H(12C)	109.9
C(115)-C(120)-H(12D)	109.9
C(119)-C(120)-C(115)	108.8
C(119)-C(120)-H(12C)	109.9
C(119)-C(120)-H(12D)	109.9
H(12C)-C(120)-H(12D)	108.3
S(21)-C(121)-H(121)	109.2
C(122)-C(121)-S(21)	106.5
C(122)-C(121)-H(121)	109.2

C(126)-C(121)-S(21)	108.1
C(126)-C(121)-H(121)	109.2
C(126)-C(121)-C(122)	114.4
C(121)-C(122)-H(12E)	109.9
C(121)-C(122)-H(12F)	109.9
C(121)-C(122)-C(123)	108.8
H(12E)-C(122)-H(12F)	108.3
C(123)-C(122)-H(12E)	109.9
C(123)-C(122)-H(12F)	109.9
C(122)-C(123)-H(12G)	110.0
C(122)-C(123)-H(12H)	110.0
H(12G)-C(123)-H(12H)	108.4
C(124)-C(123)-C(122)	108.4
C(124)-C(123)-H(12G)	110.0
C(124)-C(123)-H(12H)	110.0
C(123)-C(124)-H(12I)	108.4
C(123)-C(124)-H(12J)	108.4
H(12I)-C(124)-H(12J)	107.4
C(125)-C(124)-C(123)	115.6
C(125)-C(124)-H(12I)	108.4
C(125)-C(124)-H(12J)	108.4
C(124)-C(125)-H(12K)	109.8
C(124)-C(125)-H(12L)	109.8
C(124)-C(125)-C(126)	109.3
H(12K)-C(125)-H(12L)	108.3
C(126)-C(125)-H(12K)	109.8
C(126)-C(125)-H(12L)	109.8
C(121)-C(126)-C(125)	116.6
C(121)-C(126)-H(12M)	108.2
C(121)-C(126)-H(12N)	108.2

C(125)-C(126)-H(12M)	108.2
C(125)-C(126)-H(12N)	108.2
H(12M)-C(126)-H(12N)	107.3
S(22)-C(127)-H(127)	109.0
C(128)-C(127)-S(22)	110.3
C(128)-C(127)-H(127)	109.0
C(128)-C(127)-C(132)	111.0
C(132)-C(127)-S(22)	108.5
C(132)-C(127)-H(127)	109.0
C(127)-C(128)-H(12O)	109.8
C(127)-C(128)-H(12P)	109.8
C(127)-C(128)-C(129)	109.5
H(12O)-C(128)-H(12P)	108.2
C(129)-C(128)-H(12O)	109.8
C(129)-C(128)-H(12P)	109.8
C(130)-C(129)-C(128)	105.5
C(129)-C(130)-H(13A)	109.4
C(129)-C(130)-H(13B)	109.4
H(13A)-C(130)-H(13B)	108.0
C(131)-C(130)-C(129)	111.0
C(131)-C(130)-H(13A)	109.4
C(131)-C(130)-H(13B)	109.4
C(130)-C(131)-H(13C)	109.4
C(130)-C(131)-H(13D)	109.4
C(130)-C(131)-C(132)	111.0
H(13C)-C(131)-H(13D)	108.0
C(132)-C(131)-H(13C)	109.4
C(132)-C(131)-H(13D)	109.4
C(127)-C(132)-H(13E)	109.4
C(127)-C(132)-H(13F)	109.4

C(131)-C(132)-C(127)	111.3
C(131)-C(132)-H(13E)	109.4
C(131)-C(132)-H(13F)	109.4
H(13E)-C(132)-H(13F)	108.0
S(23)-C(133)-H(133)	109.2
C(134)-C(133)-S(23)	110.4
C(134)-C(133)-H(133)	109.2
C(138)-C(133)-S(23)	109.5
C(138)-C(133)-H(133)	109.2
C(138)-C(133)-C(134)	109.4
C(133)-C(134)-H(13G)	109.3
C(133)-C(134)-H(13H)	109.3
H(13G)-C(134)-H(13H)	108.0
C(135)-C(134)-C(133)	111.5
C(135)-C(134)-H(13G)	109.3
C(135)-C(134)-H(13H)	109.3
C(134)-C(135)-H(13I)	110.4
C(134)-C(135)-H(13J)	110.4
C(134)-C(135)-C(136)	106.6
H(13I)-C(135)-H(13J)	108.6
C(136)-C(135)-H(13I)	110.4
C(136)-C(135)-H(13J)	110.4
C(135)-C(136)-H(13K)	111.0
C(135)-C(136)-H(13L)	111.0
H(13K)-C(136)-H(13L)	109.0
C(137)-C(136)-C(135)	103.9
C(137)-C(136)-H(13K)	111.0
C(137)-C(136)-H(13L)	111.0
C(136)-C(137)-H(13M)	108.8
C(136)-C(137)-H(13N)	108.8

C(136)-C(137)-C(138)	113.9
H(13M)-C(137)-H(13N)	107.7
C(138)-C(137)-H(13M)	108.8
C(138)-C(137)-H(13N)	108.8
C(133)-C(138)-C(137)	103.5
C(133)-C(138)-H(13O)	111.1
C(133)-C(138)-H(13P)	111.1
C(137)-C(138)-H(13O)	111.1
C(137)-C(138)-H(13P)	111.1
H(13O)-C(138)-H(13P)	109.0
S(24)-C(139)-H(139)	111.3
C(140)-C(139)-S(24)	103.1
C(140)-C(139)-H(139)	111.3
C(144)-C(139)-S(24)	107.6
C(144)-C(139)-H(139)	111.3
C(144)-C(139)-C(140)	111.8
C(139)-C(140)-H(14C)	110.2
C(139)-C(140)-H(14D)	110.2
C(139)-C(140)-C(141)	107.6
H(14C)-C(140)-H(14D)	108.5
C(141)-C(140)-H(14C)	110.2
C(141)-C(140)-H(14D)	110.2
C(140)-C(141)-H(14E)	111.2
C(140)-C(141)-H(14F)	111.2
C(140)-C(141)-C(142)	102.7
H(14E)-C(141)-H(14F)	109.1
C(142)-C(141)-H(14E)	111.2
C(142)-C(141)-H(14F)	111.2
C(141)-C(142)-H(14G)	111.2
C(141)-C(142)-H(14H)	111.2

C(141)-C(142)-C(143)	103.0
H(14G)-C(142)-H(14H)	109.1
C(143)-C(142)-H(14G)	111.2
C(143)-C(142)-H(14H)	111.2
C(142)-C(143)-H(14I)	109.7
C(142)-C(143)-H(14J)	109.7
H(14I)-C(143)-H(14J)	108.2
C(144)-C(143)-C(142)	109.7
C(144)-C(143)-H(14I)	109.7
C(144)-C(143)-H(14J)	109.7
C(139)-C(144)-C(143)	107.2
C(139)-C(144)-H(14K)	110.3
C(139)-C(144)-H(14L)	110.3
C(143)-C(144)-H(14K)	110.3
C(143)-C(144)-H(14L)	110.3
H(14K)-C(144)-H(14L)	108.5
S(25)-C(145)-H(145)	113.2
C(146)-C(145)-S(25)	105.0
C(146)-C(145)-H(145)	113.2
C(150)-C(145)-S(25)	104.8
C(150)-C(145)-H(145)	113.2
C(150)-C(145)-C(146)	106.5
C(145)-C(146)-H(14M)	110.1
C(145)-C(146)-H(14N)	110.1
C(145)-C(146)-C(147)	107.9
H(14M)-C(146)-H(14N)	108.4
C(147)-C(146)-H(14M)	110.1
C(147)-C(146)-H(14N)	110.1
C(146)-C(147)-H(14O)	110.6
C(146)-C(147)-H(14P)	110.6

H(14O)-C(147)-H(14P)	108.8
C(148)-C(147)-C(146)	105.5
C(148)-C(147)-H(14O)	110.6
C(148)-C(147)-H(14P)	110.6
C(147)-C(148)-H(14Q)	108.6
C(147)-C(148)-H(14R)	108.6
C(147)-C(148)-C(149)	114.8
H(14Q)-C(148)-H(14R)	107.5
C(149)-C(148)-H(14Q)	108.6
C(149)-C(148)-H(14R)	108.6
C(148)-C(149)-H(14S)	110.4
C(148)-C(149)-H(14T)	110.4
C(148)-C(149)-C(150)	106.6
H(14S)-C(149)-H(14T)	108.6
C(150)-C(149)-H(14S)	110.4
C(150)-C(149)-H(14T)	110.4
C(145)-C(150)-C(149)	107.3
C(145)-C(150)-H(15C)	110.3
C(145)-C(150)-H(15D)	110.3
C(149)-C(150)-H(15C)	110.3
C(149)-C(150)-H(15D)	110.3
H(15C)-C(150)-H(15D)	108.5
S(26)-C(151)-H(151)	107.1
C(152)-C(151)-S(26)	112.3
C(152)-C(151)-H(151)	107.1
C(152)-C(151)-C(156)	109.7
C(156)-C(151)-S(26)	113.1
C(156)-C(151)-H(151)	107.1
C(151)-C(152)-H(15E)	108.4
C(151)-C(152)-H(15F)	108.4

C(151)-C(152)-C(153)	115.6
H(15E)-C(152)-H(15F)	107.4
C(153)-C(152)-H(15E)	108.4
C(153)-C(152)-H(15F)	108.4
C(152)-C(153)-H(15G)	111.4
C(152)-C(153)-H(15H)	111.4
H(15G)-C(153)-H(15H)	109.3
C(154)-C(153)-C(152)	101.7
C(154)-C(153)-H(15G)	111.4
C(154)-C(153)-H(15H)	111.4
C(153)-C(154)-H(15I)	110.0
C(153)-C(154)-H(15J)	110.0
H(15I)-C(154)-H(15J)	108.4
C(155)-C(154)-C(153)	108.3
C(155)-C(154)-H(15I)	110.0
C(155)-C(154)-H(15J)	110.0
C(154)-C(155)-H(15K)	110.7
C(154)-C(155)-H(15L)	110.7
H(15K)-C(155)-H(15L)	108.8
C(156)-C(155)-C(154)	105.2
C(156)-C(155)-H(15K)	110.7
C(156)-C(155)-H(15L)	110.7
C(151)-C(156)-H(15M)	109.2
C(151)-C(156)-H(15N)	109.2
C(155)-C(156)-C(151)	111.9
C(155)-C(156)-H(15M)	109.2
C(155)-C(156)-H(15N)	109.2
H(15M)-C(156)-H(15N)	107.9