

Supporting information

Structure of Chiral Au₄₄(2,4-DMBT)₂₆ Nanocluster with an 18-electron Shell Closure

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1. Experimental

1.1 Materials.

Tetraoctylammonium bromide (TOAB, ≥ 98.0 %), Tetrachloroauric (III) acid (HAuCl₄·4H₂O, > 99.9 % metals basis), 2,4-Dimethylbenzenethiol (2,4-DMBT, 99 %, shanghai chemical reagent co., Ltd.), 4-tert-Butylbenzenethiol (TBBTH, 99 %, Sigma-Aldrich), Sodium borohydride (NaBH₄, 99.8 %, shanghai chemical reagent co., Ltd.), 20-25 nm Au nanoparticles (Sigma-Aldrich). Solvents: DCM, toluene, acetonitrile, petroleum ether and methanol were purchased from Shanghai chemical reagent co., Ltd. All chemicals were used as received. The water used in all experiments was ultrapure (resistivity 18.2 MΩ cm), produced by a Milli-Q NANO pure water system. Au₄₄(TBBT)₂₈ was synthesized by a method reported by Jin's group.¹⁻²

1.2 Synthesis of Au₄₄(2,4-DMBT)₂₆.

HAuCl₄·4H₂O (100 mg, 0.2428 mmol) dissolved in 2 mL water was added to 15 mL of CH₂Cl₂ solution containing TOAB (154 mg, 0.2816 mmol). The mixture was vigorously stirred for ~ 30 min until the phase transfer was completed. The water layer was removed using a separatory funnel, and three equivalents of 2,4-DMBT (0.7284 mmol) were added to the organic layer. After continuously stirring for ~ 3 h, 3 mL of aqueous solution containing 47 mg of NaBH₄ was quickly added to the cooled reaction mixture (0 °C) at once. The reduction was allowed to proceed overnight. A rotary evaporator was employed to remove the solvent under reduced pressure, and then a large amount of methanol was used to clean the product to remove excess TBBTH and TOAB. Next, 100 μL of 2,4-DMBT was added to the precursor under 40 °C for subsequent etching. The crude products dissolved in 1 mL of DCM were pipetted onto four pieces of PTLC plate (10 cm × 20 cm), and the separation was conducted in a developing tank (solvent: DCM/petroleum ether = 10/25 v/v) for ~ 30 min. A knife was used to cut the bands of Au₄₄(2,4-DMBT)₂₆ in the PTLC plate,

which were extracted by pure DCM. Single crystals of $\text{Au}_{44}(\text{2,4-DMBT})_{26}$ were formed by vapor diffusion of acetonitrile into the toluene solution of $\text{Au}_{44}(\text{2,4-DMBT})_{26}$ over 1 month.

1.3 Characterization.

The single crystal X-ray diffraction data were collected on a Bruker D8 VENTURE CMOS photon 100 diffractometer with helios mx multilayer monochromator Cu $K\alpha$ radiation ($\lambda = 1.54178 \text{ \AA}$). All UV-Vis adsorption spectra were acquired in the range of 190–900 nm using a UV2550 spectrophotometer. Elemental analysis was performed on an Elementar vario EL cube (Elementar, Germany). 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 ($\sim 0.5 \text{ g/L}$), 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 $5 \mu\text{L/min}$. The source temperature was maintained at $70 \text{ }^\circ\text{C}$, the spray voltage was 2.20 kV and the cone voltage was adjusted to 60 V. Thermal gravimetric analysis (TGA) ($\sim 3 \text{ mg}$ sample used) was conducted in an N_2 atmosphere (flow rate $\sim 50 \text{ mL/min}$) on a TG/DTA 6300 analyzer (Seiko Instruments, Inc.) at a heating rate of $10 \text{ }^\circ\text{C/min}$. X-ray Photoelectron Spectroscopy (XPS) measurements were conducted on an ESCALAB 250Xi XPS spectrometer (Thermo Scientific, America) using a monochromatized Al $K\alpha$ source and equipped with an Ar^+ ion sputtering gun. All binding energies were calibrated using the C (1s) carbon peak (284.8 eV).

References:

- (1) Zeng, C.; Chen, Y.; Li, G.; Jin, R., *Chem. Commun.* **2014**, 50, 55.
- (2) Zeng, C.; Chen, Y.; Iida, K.; Nobusada, K.; Kirschbaum, K.; Lambright, K. J.; Jin, R., *J. Am. Chem. Soc.* **2016**, 138, 3950.

2. Supporting figures

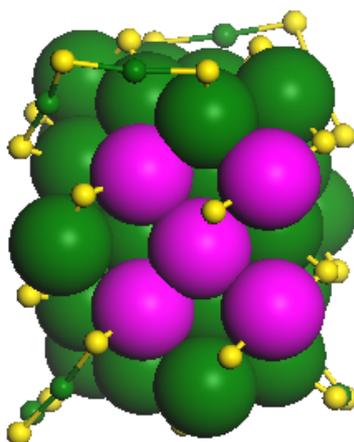


Figure S1. The structure of $\text{Au}_{44}(\text{TBBT})_{28}$ nanocluster. For clarity, C and H atoms are omitted. Color labels: yellow = S; others = Au.

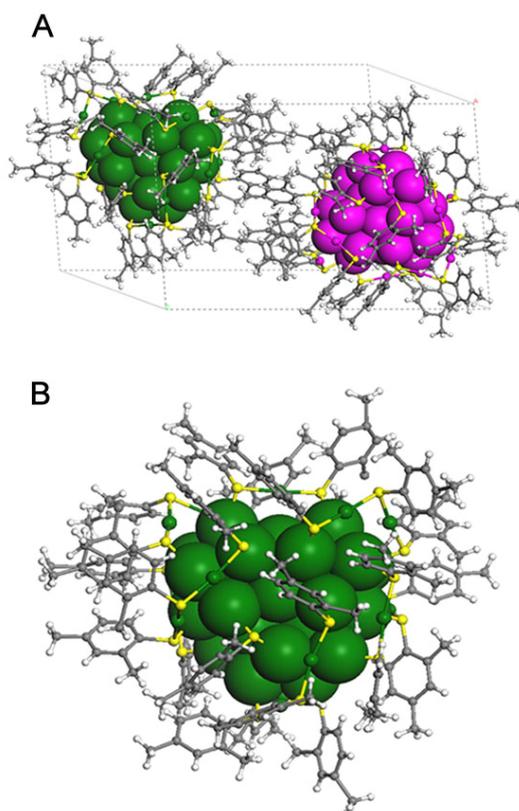


Figure S2. Total structure of the Au₄₄(2,4-DMBT)₂₆ nanocluster. The unit cell contains a pair of enantiomers (A). Color labels: yellow = S; gray = C or H; others = Au.

3. Single crystal data of Au₄₄(2,4-DMBT)₂₆

Table S1. Crystal data and structure refinement for Au₄₄(2,4-DMBT)₂₆.

Identification code	160421anhui2_0m	
Empirical formula	C ₂₀₈ H ₂₃₄ Au ₄₄ S ₂₆	
Formula weight	12234.03	
Temperature	150.0 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 19.0970(10) Å	α = 88.620(2)°.
	b = 24.0131(13) Å	β = 89.464(2)°.
	c = 29.8101(15) Å	γ = 71.411(2)°.
Volume	12953.3(12) Å ³	
Z	1	
Density (calculated)	3.137 Mg/m ³	
Absorption coefficient	47.736 mm ⁻¹	
F(000)	10748	
Crystal size	0.15 × 0.10 × 0.20 mm ³	

Theta range for data collection	2.417 to 66.878°.
Index ranges	-22<=h<=22, -28<=k<=28, -35<=l<=35
Reflections collected	232123
Independent reflections	45135 [R(int) = 0.0953]
Completeness to theta = 66.878°	98.0%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.1643 and 0.0268
Refinement method	Full-matrix-block least-squares on F ²
Data / restraints / parameters	45135 / 1973 / 2234
Goodness-of-fit on F ²	1.644
Final R indices [I>2sigma(I)]	R1 = 0.1398, wR2 = 0.3650
R indices (all data)	R1 = 0.1666, wR2 = 0.4009
Extinction coefficient	n/a
Largest diff. peak and hole	11.107 and -7.718 e.Å ⁻³

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for Au₄₄(2,4-DMBT)₂₆. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Au(1)	5936	6926	7988	43(1)
Au(2)	6169	7994	7406	43(1)
Au(3)	5844	6057	7404	43(1)
Au(4)	7227	5976	7848	46(1)
Au(5)	6981	6710	8668	49(1)
Au(6)	6401	7857	8305	42(1)
Au(7)	4956	8113	8016	44(1)
Au(8)	5089	7418	7207	41(1)
Au(9)	4329	7133	7929	45(1)
Au(10)	3436	8509	7912	51(1)
Au(11)	3555	7746	7189	47(1)
Au(12)	4368	6613	7076	44(1)
Au(13)	4158	5968	7867	49(1)
Au(14)	2705	7358	7971	54(1)
Au(15)	2809	9218	7026	59(1)
Au(16)	4258	9952	7233	58(1)
Au(17)	4340	8680	7241	49(1)
Au(18)	4153	9285	8069	52(1)

Au(19)	5788	8988	7920	48(1)
Au(20)	5186	9879	8690	60(1)
Au(21)	6894	8723	8650	52(1)
Au(22)	5269	8640	8785	50(1)
Au(23)	6530	7718	9226	54(1)
Au(24)	7867	8269	9454	59(1)
Au(25)	4987	7960	9707	64(1)
Au(26)	6229	6631	9620	78(1)
Au(27)	5422	7397	8827	48(1)
Au(28)	7135	5714	6809	45(1)
Au(29)	5723	6593	6515	43(1)
Au(30)	7054	6849	6259	49(1)
Au(31)	5729	7486	5645	52(1)
Au(32)	5913	7791	6538	44(1)
Au(33)	7049	8120	6004	56(1)
Au(34)	8497	5534	6278	53(1)
Au(35)	8154	6236	7130	47(1)
Au(36)	7521	7047	7831	44(1)
Au(37)	7527	7499	6949	48(1)
Au(38)	7367	8264	7770	47(1)
Au(39)	6638	6815	7154	40(1)
Au(40)	8519	8544	8397	59(1)
Au(41)	9097	6505	8003	58(1)
Au(42)	8435	4938	7334	60(1)
Au(43)	5585	5410	6621	47(1)
Au(44)	7851	7589	8619	48(1)
S(1)	8209	8813	7648	60(2)
S(2)	8865	6720	8753	61(2)
S(3)	7908	8195	6528	55(2)
S(4)	9389	6223	7275	60(2)
S(5)	6349	8106	5378	61(2)
S(6)	8086	6368	5824	50(2)
S(7)	9110	4673	6679	61(2)
S(8)	7829	4977	8008	62(3)
S(9)	6826	4855	6625	47(2)
S(10)	4978	6938	5862	49(2)
S(11)	4337	5879	6557	48(2)
S(12)	5407	5546	8000	50(2)

S(13)	7333	6089	9313	70(3)
S(14)	5117	7032	9975	85(4)
S(15)	2920	6410	7719	54(2)
S(16)	4239	7271	8723	71(3)
S(17)	2479	8275	8292	58(2)
S(18)	4814	8937	9519	53(2)
S(19)	2388	8412	6980	54(2)
S(20)	3946	10101	8542	62(3)
S(21)	3050	10104	6994	70(3)
S(22)	6387	9685	8930	59(2)
S(23)	5361	9943	7550	59(2)
S(24)	5058	8759	6601	55(2)
S(25)	8926	8378	9134	68(3)
S(26)	6851	8185	9832	69(3)
C(1)	9041	8429	7348	69(5)
C(2)	9310	7819	7344	69(5)
C(3)	9929	7537	7089	69(5)
C(4)	10279	7865	6837	71(5)
C(5)	10011	8476	6841	71(5)
C(6)	9392	8758	7096	71(5)
C(7)	9015	9370	7073	79(7)
C(8)	11006	7567	6492	78(7)
C(9)	9654	6832	9037	158(12)
C(10)	10191	6937	8760	158(12)
C(11)	10785	7064	8946	159(12)
C(12)	10843	7087	9409	159(12)
C(13)	10306	6983	9686	159(12)
C(14)	9712	6856	9500	158(12)
C(15)	9161	6571	9694	158(13)
C(17)	8720	7884	6186	87(6)
C(18)	9037	7276	6194	87(6)
C(19)	9643	7013	5923	87(6)
C(20)	9932	7358	5644	88(6)
C(21)	9616	7965	5636	88(6)
C(22)	9010	8229	5907	88(6)
C(23)	8645	8855	5831	91(8)
C(24)	10682	7051	5332	93(8)
C(25)	9975	5484	7324	51(8)

C(26)	9915	5123	7684	58(9)
C(27)	10331	4531	7690	52(8)
C(28)	10808	4300	7336	77(13)
C(29)	10868	4662	6977	93(16)
C(30)	10451	5254	6971	51(8)
C(31)	10436	5616	6540	120(30)
C(32)	11174	3558	7411	98(18)
C(33)	7011	7718	4954	85(15)
C(34)	7757	7634	5022	70(11)
C(35)	8271	7371	4695	73(12)
C(36)	8038	7191	4299	75(13)
C(37)	7292	7275	4230	70(12)
C(38)	6779	7538	4558	77(13)
C(39)	5869	7682	4370	160(40)
C(40)	8540	6854	3938	93(16)
C(41)	7873	6103	5301	42(7)
C(42)	7149	6204	5163	55(9)
C(43)	7009	6020	4744	79(13)
C(44)	7593	5735	4464	80(14)
C(45)	8317	5634	4602	76(13)
C(46)	8457	5818	5021	67(11)
C(47)	9305	5699	5138	87(15)
C(48)	7458	5572	3968	87(15)
C(49)	8820	4047	6503	58(9)
C(50)	8497	3737	6793	65(11)
C(51)	8361	3235	6649	56(9)
C(52)	8547	3043	6214	96(17)
C(53)	8870	3353	5924	75(12)
C(54)	9006	3855	6068	39(6)
C(55)	9272	4179	5676	110(20)
C(56)	8299	2448	6132	93(17)
C(57)	8524	4787	8395	64(4)
C(58)	8762	5254	8639	63(4)
C(59)	9247	5124	8941	63(4)
C(60)	9590	4540	9096	65(4)
C(61)	9395	4096	8884	66(4)
C(62)	8897	4182	8550	66(4)
C(63)	8722	3611	8334	76(7)

C(64)	10154	4408	9507	69(6)
C(65)	6971	4635	6020	56(9)
C(66)	7343	4895	5761	63(10)
C(67)	7451	4707	5297	67(11)
C(68)	7267	4157	5199	67(11)
C(69)	6967	3916	5535	45(7)
C(70)	6787	4109	5955	49(8)
C(71)	6455	3775	6288	52(8)
C(72)	7395	3872	4719	72(12)
C(73)	5146	6425	5400	49(8)
C(78)	4805	6629	4991	42(7)
C(77)	4889	6246	4637	79(13)
C(76)	5315	5659	4692	69(11)
C(75)	5656	5456	5101	71(12)
C(74)	5571	5838	5455	78(13)
C(79)	4258	7223	4939	47(8)
C(80)	5417	5281	4265	46(8)
C(81)	3859	5412	6830	54(4)
C(82)	4278	4934	7088	55(4)
C(83)	3934	4592	7330	58(4)
C(84)	3170	4728	7313	59(4)
C(85)	2751	5206	7055	57(4)
C(86)	3096	5548	6813	55(4)
C(87)	2679	6072	6495	56(6)
C(88)	2741	4473	7668	70(6)
C(89)	5692	4772	7916	92(6)
C(90)	6317	4528	7655	91(6)
C(91)	6639	3921	7644	93(6)
C(92)	6335	3558	7893	93(6)
C(93)	5709	3802	8154	93(6)
C(94)	5388	4409	8165	92(6)
C(95)	4719	4648	8476	93(8)
C(96)	6683	2928	7742	98(8)
C(97)	7255	5375	9258	71(12)
C(98)	6824	5234	8934	69(11)
C(99)	6818	4659	8902	100(18)
C(100)	7242	4225	9194	97(17)
C(101)	7673	4366	9518	103(19)

C(102)	7680	4941	9550	126(19)
C(103)	8137	4967	9984	129(19)
C(104)	7143	3627	9100	140(30)
C(105)	5313	7073	10582	117(9)
C(106)	5797	6590	10805	117(9)
C(107)	5924	6614	11262	117(9)
C(108)	5567	7121	11495	117(9)
C(109)	5083	7604	11272	117(9)
C(110)	4956	7580	10816	117(9)
C(113)	2436	6043	8086	51(8)
C(114)	2737	5770	8489	69(11)
C(115)	2344	5495	8759	91(16)
C(116)	1649	5492	8627	65(11)
C(117)	1348	5764	8225	63(10)
C(118)	1741	6040	7954	73(12)
C(119)	1353	6433	7567	74(12)
C(120)	1186	5248	8879	110(20)
C(121)	4239	6647	9038	150(13)
C(122)	4787	6103	9040	150(13)
C(123)	4710	5644	9307	150(13)
C(124)	4084	5729	9573	151(13)
C(125)	3536	6273	9572	151(13)
C(126)	3613	6732	9304	151(13)
C(129)	1637	8849	8158	103(8)
C(130)	1648	9424	8132	105(8)
C(131)	1003	9882	8039	105(8)
C(132)	345	9763	7972	105(8)
C(133)	333	9188	7998	104(8)
C(134)	979	8730	8091	104(8)
C(135)	948	8058	8000	110(20)
C(136)	-456	10257	8135	110(20)
C(137)	3839	9297	9493	78(5)
C(138)	3390	9023	9287	80(5)
C(139)	2637	9315	9243	82(5)
C(140)	2334	9880	9403	81(5)
C(141)	2783	10154	9608	79(5)
C(142)	3536	9863	9653	77(5)
C(143)	4030	10125	9852	70(7)

C(144)	1516	10197	9323	81(7)
C(145)	2245	8321	6385	66(11)
C(146)	2661	7799	6190	80(14)
C(147)	2539	7693	5746	54(9)
C(148)	2001	8109	5496	120(20)
C(149)	1584	8631	5691	86(15)
C(150)	1706	8737	6135	61(10)
C(151)	1242	9281	6343	83(14)
C(152)	1824	8079	4996	150(40)
C(153)	3596	10772	8216	87(6)
C(158)	2860	10966	8085	88(6)
C(157)	2590	11475	7822	89(6)
C(156)	3057	11791	7691	89(6)
C(155)	3793	11597	7823	89(6)
C(154)	4063	11088	8086	87(6)
C(159)	2361	10626	8155	87(8)
C(160)	2687	12367	7480	91(8)
C(161)	3054	10300	6402	94(6)
C(162)	2856	9933	6110	92(6)
C(163)	2708	10103	5663	93(6)
C(164)	2758	10639	5508	95(6)
C(165)	2956	11006	5800	95(6)
C(166)	3104	10836	6247	95(6)
C(167)	3335	11247	6626	98(8)
C(169)	6708	10186	8606	111(8)
C(170)	7043	10027	8191	111(8)
C(171)	7352	10402	7960	111(8)
C(172)	7325	10935	8143	112(8)
C(173)	6990	11094	8557	112(8)
C(174)	6681	10719	8789	111(8)
C(175)	6237	10868	9209	111(9)
C(176)	7750	11348	7850	115(9)
C(177)	5991	10054	7139	82(6)
C(182)	6058	10614	7122	83(5)
C(181)	6542	10745	6818	83(5)
C(180)	6960	10317	6531	84(5)
C(179)	6893	9757	6548	84(6)
C(178)	6409	9625	6852	83(6)

C(183)	5780	11114	7497	82(7)
C(184)	7573	10393	6263	86(7)
C(185)	4560	8873	6060	69(11)
C(186)	4058	8579	5973	45(7)
C(187)	3733	8632	5552	85(15)
C(188)	3911	8979	5218	76(13)
C(189)	4413	9273	5305	74(12)
C(190)	4738	9220	5726	55(9)
C(191)	5177	9589	5809	52(8)
C(192)	3550	8906	4729	110(20)
C(193)	8970	9080	9299	122(9)
C(194)	8332	9561	9320	122(9)
C(195)	8380	10120	9380	123(9)
C(196)	9068	10197	9420	123(9)
C(197)	9707	9715	9399	122(9)
C(198)	9658	9157	9338	122(9)
C(199)	10223	8563	9233	124(10)
C(200)	9258	10861	9452	123(10)
C(201)	7183	7670	10299	97(7)
C(206)	7042	7844	10741	99(7)
C(205)	7284	7435	11090	100(7)
C(204)	7667	6852	10998	100(7)
C(203)	7809	6678	10556	98(7)
C(202)	7567	7087	10206	97(7)
C(208)	7972	6548	11403	102(8)
C(112)	5492	7191	11988	150(30)
C(207)	6473	8520	10794	102(8)
C(168)	2781	10780	5027	96(8)
C(16)	11676	6959	9427	162(13)

Table S3. Bond lengths [\AA] and angles [$^\circ$] for $\text{Au}_{44}(\text{2,4-DMBT})_{26}$.

Au(1)-Au(2)	3.2077	S(25)-Au(24)-Au(23)	140.3
Au(1)-Au(3)	2.7981	S(25)-Au(24)-Au(44)	83.4
Au(1)-Au(4)	2.8099	S(26)-Au(24)-Au(21)	88.4
Au(1)-Au(5)	2.7785	S(26)-Au(24)-Au(23)	44.8
Au(1)-Au(6)	2.8394	S(26)-Au(24)-Au(44)	101.6
Au(1)-Au(7)	2.8708	S(26)-Au(24)-S(25)	174.7

Au(1)-Au(8)	2.8554	Au(22)-Au(25)-Au(26)	102.6
Au(1)-Au(9)	2.9549	Au(23)-Au(25)-Au(22)	55.3
Au(1)-Au(27)	2.8069	Au(23)-Au(25)-Au(26)	56.1
Au(1)-Au(36)	3.1614	Au(27)-Au(25)-Au(22)	55
Au(1)-Au(39)	2.7914	Au(27)-Au(25)-Au(23)	53.5
Au(2)-Au(6)	2.7174	Au(27)-Au(25)-Au(26)	57.9
Au(2)-Au(7)	2.8772	S(14)-Au(25)-Au(22)	140.2
Au(2)-Au(8)	2.8975	S(14)-Au(25)-Au(23)	99.3
Au(2)-Au(19)	2.7605	S(14)-Au(25)-Au(26)	43.5
Au(2)-Au(32)	2.721	S(14)-Au(25)-Au(27)	85.4
Au(2)-Au(36)	3.1034	S(18)-Au(25)-Au(22)	46.5
Au(2)-Au(37)	2.8366	S(18)-Au(25)-Au(23)	85
Au(2)-Au(38)	2.8049	S(18)-Au(25)-Au(26)	141
Au(2)-Au(39)	2.8037	S(18)-Au(25)-Au(27)	101.3
Au(3)-Au(4)	2.9152	Au(5)-Au(26)-Au(25)	102.9
Au(3)-Au(8)	3.1665	Au(23)-Au(26)-Au(5)	54.5
Au(3)-Au(12)	2.876	Au(23)-Au(26)-Au(25)	59
Au(3)-Au(28)	2.9329	Au(23)-Au(26)-Au(27)	53.7
Au(3)-Au(29)	2.8958	Au(27)-Au(26)-Au(5)	56.1
Au(3)-Au(39)	2.7995	Au(27)-Au(26)-Au(25)	55.1
Au(3)-Au(43)	2.9654	S(13)-Au(26)-Au(5)	47.8
Au(3)-S(12)	2.4236	S(13)-Au(26)-Au(23)	87.1
Au(4)-Au(5)	2.992	S(13)-Au(26)-Au(25)	146
Au(4)-Au(28)	3.1943	S(13)-Au(26)-Au(27)	103.2
Au(4)-Au(35)	2.9446	S(13)-Au(26)-S(14)	170.7
Au(4)-Au(36)	2.7999	S(14)-Au(26)-Au(5)	139.2
Au(4)-Au(39)	2.8287	S(14)-Au(26)-Au(23)	102.2
Au(4)-Au(42)	3.2159	S(14)-Au(26)-Au(25)	43.4
Au(4)-S(8)	2.346	S(14)-Au(26)-Au(27)	83.1
Au(5)-Au(6)	2.8124	Au(1)-Au(27)-Au(5)	57.7
Au(5)-Au(23)	2.8638	Au(1)-Au(27)-Au(6)	59.8
Au(5)-Au(26)	3.1967	Au(1)-Au(27)-Au(7)	60.3
Au(5)-Au(27)	2.9473	Au(1)-Au(27)-Au(22)	107.7
Au(5)-Au(36)	2.886	Au(1)-Au(27)-Au(25)	174.2
Au(5)-Au(44)	3.0747	Au(1)-Au(27)-Au(26)	113.4
Au(5)-S(13)	2.3715	Au(5)-Au(27)-Au(25)	119.2
Au(6)-Au(7)	2.7715	Au(5)-Au(27)-Au(26)	64.2
Au(6)-Au(19)	2.8136	Au(6)-Au(27)-Au(5)	57.7
Au(6)-Au(21)	2.7651	Au(6)-Au(27)-Au(7)	57.2
Au(6)-Au(22)	2.7818	Au(6)-Au(27)-Au(22)	57.4
Au(6)-Au(23)	2.7612	Au(6)-Au(27)-Au(25)	114.5
Au(6)-Au(27)	2.8842	Au(6)-Au(27)-Au(26)	111.4
Au(6)-Au(36)	2.7887	Au(7)-Au(27)-Au(5)	105
Au(6)-Au(38)	2.8159	Au(7)-Au(27)-Au(25)	118.3

Au(6)-Au(44)	2.7994	Au(7)-Au(27)-Au(26)	168.3
Au(7)-Au(8)	2.9268	Au(22)-Au(27)-Au(5)	108.9
Au(7)-Au(9)	2.9785	Au(22)-Au(27)-Au(7)	57.7
Au(7)-Au(10)	2.7693	Au(22)-Au(27)-Au(25)	68.1
Au(7)-Au(17)	2.7297	Au(22)-Au(27)-Au(26)	119.8
Au(7)-Au(18)	2.7505	Au(23)-Au(27)-Au(1)	108.1
Au(7)-Au(19)	3.0192	Au(23)-Au(27)-Au(5)	60.1
Au(7)-Au(22)	2.8051	Au(23)-Au(27)-Au(6)	58.5
Au(7)-Au(27)	2.9093	Au(23)-Au(27)-Au(7)	108.5
Au(8)-Au(9)	2.7772	Au(23)-Au(27)-Au(22)	63.7
Au(8)-Au(11)	2.78	Au(23)-Au(27)-Au(25)	66.7
Au(8)-Au(12)	2.7448	Au(23)-Au(27)-Au(26)	62.9
Au(8)-Au(17)	2.9131	Au(25)-Au(27)-Au(26)	67
Au(8)-Au(29)	2.8759	S(16)-Au(27)-Au(1)	92.6
Au(8)-Au(32)	2.8313	S(16)-Au(27)-Au(5)	136.9
Au(8)-Au(39)	2.8545	S(16)-Au(27)-Au(6)	136.6
Au(9)-Au(10)	3.1989	S(16)-Au(27)-Au(7)	80.5
Au(9)-Au(11)	2.7827	S(16)-Au(27)-Au(22)	109.7
Au(9)-Au(12)	2.8502	S(16)-Au(27)-Au(23)	159.3
Au(9)-Au(13)	2.9274	S(16)-Au(27)-Au(25)	92.6
Au(9)-Au(14)	2.9751	S(16)-Au(27)-Au(26)	110.3
Au(9)-S(16)	2.3931	Au(3)-Au(28)-Au(4)	56.6
Au(10)-Au(11)	2.8232	Au(3)-Au(28)-Au(29)	58.8
Au(10)-Au(15)	3.1369	Au(3)-Au(28)-Au(30)	105
Au(10)-Au(17)	2.7385	Au(3)-Au(28)-Au(34)	170.4
Au(10)-Au(18)	2.694	Au(3)-Au(28)-Au(42)	108.5
Au(10)-S(17)	2.3512	Au(3)-Au(28)-Au(43)	56.2
Au(11)-Au(12)	2.6956	Au(4)-Au(28)-Au(43)	109.2
Au(11)-Au(14)	3.1194	Au(29)-Au(28)-Au(4)	103.5
Au(11)-Au(17)	3.0773	Au(29)-Au(28)-Au(30)	56.8
Au(11)-S(19)	2.3705	Au(29)-Au(28)-Au(42)	165.7
Au(12)-Au(13)	2.8853	Au(29)-Au(28)-Au(43)	55.5
Au(12)-Au(29)	3.056	Au(30)-Au(28)-Au(4)	108.2
Au(12)-S(11)	2.3869	Au(30)-Au(28)-Au(43)	107.5
Au(13)-S(12)	2.3088	Au(34)-Au(28)-Au(4)	116.5
Au(13)-S(15)	2.3036	Au(34)-Au(28)-Au(29)	120.7
Au(14)-S(15)	2.3237	Au(34)-Au(28)-Au(30)	69.8
Au(14)-S(17)	2.333	Au(34)-Au(28)-Au(42)	70.6
Au(15)-Au(17)	2.8661	Au(34)-Au(28)-Au(43)	132.6
Au(15)-S(19)	2.3254	Au(35)-Au(28)-Au(3)	107.3
Au(15)-S(21)	2.3178	Au(35)-Au(28)-Au(4)	58.3
Au(16)-Au(17)	3.0074	Au(35)-Au(28)-Au(29)	112.8
Au(16)-Au(18)	2.969	Au(35)-Au(28)-Au(30)	68.9
Au(16)-S(21)	2.3336	Au(35)-Au(28)-Au(34)	63.4

Au(16)-S(23)	2.309	Au(35)-Au(28)-Au(42)	62.7
Au(17)-Au(18)	2.8569	Au(35)-Au(28)-Au(43)	162.5
Au(17)-S(24)	2.3772	Au(39)-Au(28)-Au(3)	59.1
Au(18)-Au(19)	3.0039	Au(39)-Au(28)-Au(4)	56.4
Au(18)-Au(20)	3.3671	Au(39)-Au(28)-Au(29)	57.9
Au(18)-Au(22)	3.0515	Au(39)-Au(28)-Au(30)	56.5
Au(18)-S(20)	2.3686	Au(39)-Au(28)-Au(34)	111.8
Au(19)-Au(20)	3.1291	Au(39)-Au(28)-Au(35)	60.3
Au(19)-Au(21)	2.9617	Au(39)-Au(28)-Au(42)	111.1
Au(19)-Au(22)	2.951	Au(39)-Au(28)-Au(43)	103
Au(19)-Au(38)	2.9975	Au(42)-Au(28)-Au(4)	62.3
Au(19)-S(23)	2.4176	Au(42)-Au(28)-Au(30)	127.1
Au(20)-Au(22)	2.9354	Au(42)-Au(28)-Au(43)	125
Au(20)-S(20)	2.2995	S(9)-Au(28)-Au(3)	88.7
Au(20)-S(22)	2.3059	S(9)-Au(28)-Au(4)	117.3
Au(21)-Au(22)	3.1947	S(9)-Au(28)-Au(29)	97
Au(21)-Au(23)	3.1807	S(9)-Au(28)-Au(30)	132
Au(21)-Au(24)	3.0066	S(9)-Au(28)-Au(34)	100.8
Au(21)-Au(38)	2.8944	S(9)-Au(28)-Au(35)	150.2
Au(21)-Au(40)	3.0815	S(9)-Au(28)-Au(39)	145.9
Au(21)-Au(44)	2.7579	S(9)-Au(28)-Au(42)	88.7
Au(21)-S(22)	2.3706	S(9)-Au(28)-Au(43)	44.3
Au(22)-Au(23)	2.9921	Au(3)-Au(29)-Au(12)	57.7
Au(22)-Au(25)	3.2899	Au(3)-Au(29)-Au(28)	60
Au(22)-Au(27)	2.9056	Au(3)-Au(29)-Au(31)	164
Au(22)-S(18)	2.3872	Au(3)-Au(29)-Au(32)	111.4
Au(23)-Au(24)	3.3112	Au(3)-Au(29)-Au(43)	61
Au(23)-Au(25)	3.153	Au(8)-Au(29)-Au(3)	66.5
Au(23)-Au(26)	3.0509	Au(8)-Au(29)-Au(12)	55
Au(23)-Au(27)	2.7598	Au(8)-Au(29)-Au(28)	111.6
Au(23)-Au(44)	3.0313	Au(8)-Au(29)-Au(30)	104.1
Au(23)-S(26)	2.3357	Au(8)-Au(29)-Au(31)	101.6
Au(24)-Au(44)	3.0155	Au(8)-Au(29)-Au(32)	57.4
Au(24)-S(25)	2.3157	Au(8)-Au(29)-Au(43)	117.1
Au(24)-S(26)	2.2968	Au(12)-Au(29)-Au(31)	125.3
Au(25)-Au(26)	3.329	Au(28)-Au(29)-Au(12)	115.5
Au(25)-Au(27)	2.9685	Au(28)-Au(29)-Au(31)	119.2
Au(25)-S(14)	2.2891	Au(28)-Au(29)-Au(32)	107.8
Au(25)-S(18)	2.3178	Au(30)-Au(29)-Au(3)	111.8
Au(26)-Au(27)	3.0645	Au(30)-Au(29)-Au(12)	158.4
Au(26)-S(13)	2.2899	Au(30)-Au(29)-Au(28)	64
Au(26)-S(14)	2.2932	Au(30)-Au(29)-Au(31)	59.2
Au(27)-S(16)	2.3967	Au(30)-Au(29)-Au(32)	55.1
Au(28)-Au(29)	2.9684	Au(30)-Au(29)-Au(43)	125.5

Au(28)-Au(30)	3.1073	Au(32)-Au(29)-Au(12)	108.6
Au(28)-Au(34)	2.9489	Au(32)-Au(29)-Au(31)	52.8
Au(28)-Au(35)	2.8136	Au(39)-Au(29)-Au(3)	59.2
Au(28)-Au(39)	2.7298	Au(39)-Au(29)-Au(8)	60.7
Au(28)-Au(42)	3.0111	Au(39)-Au(29)-Au(12)	101.7
Au(28)-Au(43)	3.323	Au(39)-Au(29)-Au(28)	56.7
Au(28)-S(9)	2.398	Au(39)-Au(29)-Au(30)	58.9
Au(29)-Au(30)	2.891	Au(39)-Au(29)-Au(31)	106.2
Au(29)-Au(31)	3.3291	Au(39)-Au(29)-Au(32)	60.6
Au(29)-Au(32)	3.015	Au(39)-Au(29)-Au(43)	112.6
Au(29)-Au(39)	2.7681	Au(43)-Au(29)-Au(12)	68.6
Au(29)-Au(43)	2.9445	Au(43)-Au(29)-Au(28)	68.4
Au(29)-S(10)	2.3945	Au(43)-Au(29)-Au(31)	134.8
Au(30)-Au(31)	3.095	Au(43)-Au(29)-Au(32)	172.4
Au(30)-Au(32)	2.7335	S(10)-Au(29)-Au(3)	147.3
Au(30)-Au(33)	3.1255	S(10)-Au(29)-Au(8)	106.2
Au(30)-Au(35)	3.3591	S(10)-Au(29)-Au(12)	91.4
Au(30)-Au(37)	2.9284	S(10)-Au(29)-Au(28)	141.6
Au(30)-Au(39)	2.7849	S(10)-Au(29)-Au(30)	100.9
Au(30)-S(6)	2.3371	S(10)-Au(29)-Au(31)	44
Au(31)-Au(32)	2.8333	S(10)-Au(29)-Au(32)	86.9
Au(31)-S(5)	2.3022	S(10)-Au(29)-Au(39)	147.3
Au(31)-S(10)	2.3139	S(10)-Au(29)-Au(43)	100.1
Au(32)-Au(33)	2.9723	Au(28)-Au(30)-Au(33)	162
Au(32)-Au(37)	3.1852	Au(28)-Au(30)-Au(35)	51.4
Au(32)-Au(39)	2.9254	Au(29)-Au(30)-Au(28)	59.2
Au(32)-S(24)	2.3871	Au(29)-Au(30)-Au(31)	67.5
Au(33)-Au(37)	3.1591	Au(29)-Au(30)-Au(33)	122.2
Au(33)-S(3)	2.328	Au(29)-Au(30)-Au(35)	100.5
Au(33)-S(5)	2.3126	Au(29)-Au(30)-Au(37)	112
Au(34)-Au(35)	3.0321	Au(31)-Au(30)-Au(28)	122.4
Au(34)-S(6)	2.3107	Au(31)-Au(30)-Au(33)	69
Au(34)-S(7)	2.3328	Au(31)-Au(30)-Au(35)	165.2
Au(35)-Au(36)	2.8758	Au(32)-Au(30)-Au(28)	111.6
Au(35)-Au(37)	2.9227	Au(32)-Au(30)-Au(29)	64.8
Au(35)-Au(39)	2.7854	Au(32)-Au(30)-Au(31)	57.8
Au(35)-Au(41)	3.3671	Au(32)-Au(30)-Au(33)	60.5
Au(35)-Au(42)	3.0342	Au(32)-Au(30)-Au(35)	109.9
Au(35)-S(4)	2.3921	Au(32)-Au(30)-Au(37)	68.4
Au(36)-Au(37)	2.8217	Au(32)-Au(30)-Au(39)	64
Au(36)-Au(38)	2.8449	Au(33)-Au(30)-Au(35)	113.8
Au(36)-Au(39)	2.8193	Au(37)-Au(30)-Au(28)	99.5
Au(36)-Au(41)	2.9177	Au(37)-Au(30)-Au(31)	120.1
Au(36)-Au(44)	2.8806	Au(37)-Au(30)-Au(33)	62.8

Au(37)-Au(38)	3.051	Au(37)-Au(30)-Au(35)	54.9
Au(37)-Au(39)	2.7688	Au(39)-Au(30)-Au(28)	54.9
Au(37)-S(3)	2.3568	Au(39)-Au(30)-Au(29)	58.3
Au(38)-Au(40)	3.1405	Au(39)-Au(30)-Au(31)	112.3
Au(38)-Au(44)	2.9625	Au(39)-Au(30)-Au(33)	109.1
Au(38)-S(1)	2.4002	Au(39)-Au(30)-Au(35)	52.9
Au(40)-Au(44)	3.0167	Au(39)-Au(30)-Au(37)	57.9
Au(40)-S(1)	2.3382	S(6)-Au(30)-Au(28)	93
Au(40)-S(25)	2.3192	S(6)-Au(30)-Au(29)	134
Au(41)-S(2)	2.3147	S(6)-Au(30)-Au(31)	110.2
Au(41)-S(4)	2.299	S(6)-Au(30)-Au(32)	155.4
Au(42)-S(7)	2.3154	S(6)-Au(30)-Au(33)	95.7
Au(42)-S(8)	2.2985	S(6)-Au(30)-Au(35)	84.3
Au(43)-S(9)	2.3196	S(6)-Au(30)-Au(37)	108
Au(43)-S(11)	2.2963	S(6)-Au(30)-Au(39)	136.2
Au(44)-S(2)	2.3796	Au(30)-Au(31)-Au(29)	53.3
S(1)-C(1)	1.8045	Au(32)-Au(31)-Au(29)	57.9
S(2)-C(9)	1.8307	Au(32)-Au(31)-Au(30)	54.7
S(3)-C(17)	1.8089	S(5)-Au(31)-Au(29)	140.6
S(4)-C(25)	1.7744	S(5)-Au(31)-Au(30)	90.1
S(5)-C(33)	1.8281	S(5)-Au(31)-Au(32)	90.5
S(6)-C(41)	1.7968	S(5)-Au(31)-S(10)	172.7
S(7)-C(49)	1.8482	S(10)-Au(31)-Au(29)	46
S(8)-C(57)	1.7082	S(10)-Au(31)-Au(30)	97.1
S(9)-C(65)	1.8833	S(10)-Au(31)-Au(32)	92.9
S(10)-C(73)	1.8268	Au(2)-Au(32)-Au(8)	62.9
S(11)-C(81)	1.8295	Au(2)-Au(32)-Au(29)	107.3
S(12)-C(89)	1.7865	Au(2)-Au(32)-Au(30)	108.1
S(13)-C(97)	1.7796	Au(2)-Au(32)-Au(31)	175.3
S(14)-C(105)	1.8624	Au(2)-Au(32)-Au(33)	105.3
S(15)-C(113)	1.811	Au(2)-Au(32)-Au(37)	56.8
S(16)-C(121)	1.7496	Au(2)-Au(32)-Au(39)	59.4
S(17)-C(129)	1.7935	Au(8)-Au(32)-Au(29)	58.8
S(18)-C(137)	1.7862	Au(8)-Au(32)-Au(31)	116.5
S(19)-C(145)	1.8284	Au(8)-Au(32)-Au(33)	166.4
S(20)-C(153)	1.7993	Au(8)-Au(32)-Au(37)	105
S(21)-C(161)	1.8145	Au(8)-Au(32)-Au(39)	59.4
S(22)-C(169)	1.7766	Au(29)-Au(32)-Au(37)	102.1
S(23)-C(177)	1.7834	Au(30)-Au(32)-Au(8)	109.6
S(24)-C(185)	1.8495	Au(30)-Au(32)-Au(29)	60.1
S(25)-C(193)	1.7938	Au(30)-Au(32)-Au(31)	67.5
S(26)-C(201)	1.8188	Au(30)-Au(32)-Au(33)	66.3
C(1)-C(2)	1.39	Au(30)-Au(32)-Au(37)	58.7
C(1)-C(6)	1.39	Au(30)-Au(32)-Au(39)	58.8

C(2)-H(2)	0.95	Au(31)-Au(32)-Au(29)	69.3
C(2)-C(3)	1.39	Au(31)-Au(32)-Au(33)	74.7
C(3)-H(3)	0.95	Au(31)-Au(32)-Au(37)	120.2
C(3)-C(4)	1.39	Au(31)-Au(32)-Au(39)	116.1
C(4)-C(5)	1.39	Au(33)-Au(32)-Au(29)	123.3
C(4)-C(8)	1.6953	Au(33)-Au(32)-Au(37)	61.6
C(5)-H(5)	0.95	Au(39)-Au(32)-Au(29)	55.5
C(5)-C(6)	1.39	Au(39)-Au(32)-Au(33)	109.5
C(6)-C(7)	1.4176	Au(39)-Au(32)-Au(37)	53.7
C(8)-H(8A)	0.98	S(24)-Au(32)-Au(2)	80.8
C(8)-H(8B)	0.98	S(24)-Au(32)-Au(8)	87.9
C(8)-H(8C)	0.98	S(24)-Au(32)-Au(29)	132.8
C(9)-C(10)	1.39	S(24)-Au(32)-Au(30)	162.4
C(9)-C(14)	1.39	S(24)-Au(32)-Au(31)	103.9
C(10)-H(10)	0.95	S(24)-Au(32)-Au(33)	97
C(10)-C(11)	1.39	S(24)-Au(32)-Au(37)	119.4
C(11)-H(11)	0.95	S(24)-Au(32)-Au(39)	136.3
C(11)-C(12)	1.39	Au(30)-Au(33)-Au(37)	55.5
C(12)-C(13)	1.39	Au(32)-Au(33)-Au(30)	53.2
C(12)-C(16)	1.5212	Au(32)-Au(33)-Au(37)	62.5
C(13)-H(13)	0.95	S(3)-Au(33)-Au(30)	98.2
C(13)-C(14)	1.39	S(3)-Au(33)-Au(32)	104.9
C(14)-C(15)	1.5294	S(3)-Au(33)-Au(37)	48
C(17)-C(18)	1.39	S(5)-Au(33)-Au(30)	89.2
C(17)-C(22)	1.39	S(5)-Au(33)-Au(32)	86.9
C(18)-H(18)	0.95	S(5)-Au(33)-Au(37)	142.4
C(18)-C(19)	1.39	S(5)-Au(33)-S(3)	168.2
C(19)-H(19)	0.95	Au(28)-Au(34)-Au(35)	56.1
C(19)-C(20)	1.39	S(6)-Au(34)-Au(28)	97.7
C(20)-C(21)	1.39	S(6)-Au(34)-Au(35)	92.7
C(20)-C(24)	1.6716	S(6)-Au(34)-S(7)	170.1
C(21)-H(21)	0.95	S(7)-Au(34)-Au(28)	92.1
C(21)-C(22)	1.39	S(7)-Au(34)-Au(35)	91.7
C(22)-C(23)	1.4543	Au(4)-Au(35)-Au(30)	108
C(23)-H(23A)	0.98	Au(4)-Au(35)-Au(34)	121.9
C(23)-H(23B)	0.98	Au(4)-Au(35)-Au(41)	82.8
C(23)-H(23C)	0.98	Au(4)-Au(35)-Au(42)	65.1
C(24)-H(24A)	0.98	Au(28)-Au(35)-Au(4)	67.3
C(24)-H(24B)	0.98	Au(28)-Au(35)-Au(30)	59.7
C(24)-H(24C)	0.98	Au(28)-Au(35)-Au(34)	60.5
C(25)-C(26)	1.39	Au(28)-Au(35)-Au(36)	111.4
C(25)-C(30)	1.39	Au(28)-Au(35)-Au(37)	106.8
C(26)-H(26)	0.95	Au(28)-Au(35)-Au(41)	148.5
C(26)-C(27)	1.39	Au(28)-Au(35)-Au(42)	61.8

C(27)-H(27)	0.95	Au(30)-Au(35)-Au(41)	144.6
C(27)-C(28)	1.39	Au(34)-Au(35)-Au(30)	65.4
C(28)-C(29)	1.39	Au(34)-Au(35)-Au(41)	137.5
C(28)-C(32)	1.7037	Au(34)-Au(35)-Au(42)	69.2
C(29)-H(29)	0.95	Au(36)-Au(35)-Au(4)	57.5
C(29)-C(30)	1.39	Au(36)-Au(35)-Au(30)	101.7
C(30)-C(31)	1.527	Au(36)-Au(35)-Au(34)	166.8
C(31)-H(31A)	0.98	Au(36)-Au(35)-Au(37)	58.2
C(31)-H(31B)	0.98	Au(36)-Au(35)-Au(41)	55
C(31)-H(31C)	0.98	Au(36)-Au(35)-Au(42)	117.6
C(32)-H(32A)	0.98	Au(37)-Au(35)-Au(4)	105.2
C(32)-H(32B)	0.98	Au(37)-Au(35)-Au(30)	55
C(32)-H(32C)	0.98	Au(37)-Au(35)-Au(34)	112.4
C(33)-C(34)	1.39	Au(37)-Au(35)-Au(41)	89.8
C(33)-C(38)	1.39	Au(37)-Au(35)-Au(42)	166.8
C(34)-H(34)	0.95	Au(39)-Au(35)-Au(4)	59.1
C(34)-C(35)	1.39	Au(39)-Au(35)-Au(28)	58.4
C(35)-H(35)	0.95	Au(39)-Au(35)-Au(30)	52.9
C(35)-C(36)	1.39	Au(39)-Au(35)-Au(34)	107.9
C(36)-C(37)	1.39	Au(39)-Au(35)-Au(36)	59.7
C(36)-C(40)	1.5025	Au(39)-Au(35)-Au(37)	58
C(37)-H(37)	0.95	Au(39)-Au(35)-Au(41)	114.6
C(37)-C(38)	1.39	Au(39)-Au(35)-Au(42)	108.8
C(38)-C(39)	1.7553	Au(42)-Au(35)-Au(30)	117.8
C(39)-H(39A)	0.98	Au(42)-Au(35)-Au(41)	97.4
C(39)-H(39B)	0.98	S(4)-Au(35)-Au(4)	121.2
C(39)-H(39C)	0.98	S(4)-Au(35)-Au(28)	151.8
C(40)-H(40A)	0.98	S(4)-Au(35)-Au(30)	128.8
C(40)-H(40B)	0.98	S(4)-Au(35)-Au(34)	96.7
C(40)-H(40C)	0.98	S(4)-Au(35)-Au(36)	93.9
C(41)-C(42)	1.39	S(4)-Au(35)-Au(37)	96.9
C(41)-C(46)	1.39	S(4)-Au(35)-Au(39)	149.9
C(42)-H(42)	0.95	S(4)-Au(35)-Au(41)	43
C(42)-C(43)	1.39	S(4)-Au(35)-Au(42)	95.9
C(43)-H(43)	0.95	Au(2)-Au(36)-Au(1)	61.6
C(43)-C(44)	1.39	Au(4)-Au(36)-Au(1)	55.8
C(44)-C(45)	1.39	Au(4)-Au(36)-Au(2)	107.9
C(44)-C(48)	1.5842	Au(4)-Au(36)-Au(5)	63.5
C(45)-H(45)	0.95	Au(4)-Au(36)-Au(35)	62.5
C(45)-C(46)	1.39	Au(4)-Au(36)-Au(37)	112
C(46)-C(47)	1.592	Au(4)-Au(36)-Au(38)	163.2
C(48)-H(48A)	0.98	Au(4)-Au(36)-Au(39)	60.4
C(48)-H(48B)	0.98	Au(4)-Au(36)-Au(41)	94.1
C(48)-H(48C)	0.98	Au(4)-Au(36)-Au(44)	123.8

C(49)-C(50)	1.39	Au(5)-Au(36)-Au(1)	54.5
C(49)-C(54)	1.39	Au(5)-Au(36)-Au(2)	104.9
C(50)-H(50)	0.95	Au(5)-Au(36)-Au(41)	97.8
C(50)-C(51)	1.39	Au(6)-Au(36)-Au(1)	56.6
C(51)-H(51)	0.95	Au(6)-Au(36)-Au(2)	54.6
C(51)-C(52)	1.39	Au(6)-Au(36)-Au(4)	108
C(52)-C(53)	1.39	Au(6)-Au(36)-Au(5)	59.4
C(52)-C(56)	1.6671	Au(6)-Au(36)-Au(35)	156.5
C(53)-H(53)	0.95	Au(6)-Au(36)-Au(37)	107.8
C(53)-C(54)	1.39	Au(6)-Au(36)-Au(38)	60
C(54)-C(55)	1.5586	Au(6)-Au(36)-Au(39)	98
C(55)-H(55A)	0.98	Au(6)-Au(36)-Au(41)	132.4
C(55)-H(55B)	0.98	Au(6)-Au(36)-Au(44)	59.2
C(55)-H(55C)	0.98	Au(35)-Au(36)-Au(1)	104.3
C(56)-H(56A)	0.98	Au(35)-Au(36)-Au(2)	105.9
C(56)-H(56B)	0.98	Au(35)-Au(36)-Au(5)	123.5
C(56)-H(56C)	0.98	Au(35)-Au(36)-Au(41)	71.1
C(57)-C(58)	1.5388	Au(35)-Au(36)-Au(44)	144.3
C(57)-C(62)	1.464	Au(37)-Au(36)-Au(1)	106.4
C(58)-H(58)	0.95	Au(37)-Au(36)-Au(2)	57
C(58)-C(59)	1.258	Au(37)-Au(36)-Au(5)	160.3
C(59)-H(59)	0.95	Au(37)-Au(36)-Au(35)	61.7
C(59)-C(60)	1.4137	Au(37)-Au(36)-Au(38)	65.2
C(60)-C(61)	1.4015	Au(37)-Au(36)-Au(41)	101.7
C(60)-C(64)	1.597	Au(37)-Au(36)-Au(44)	124.2
C(61)-H(61)	0.95	Au(38)-Au(36)-Au(1)	108.1
C(61)-C(62)	1.3498	Au(38)-Au(36)-Au(2)	56.1
C(62)-C(63)	1.655	Au(38)-Au(36)-Au(5)	113.2
C(63)-H(63A)	0.98	Au(38)-Au(36)-Au(35)	123.3
C(63)-H(63B)	0.98	Au(38)-Au(36)-Au(41)	102.7
C(63)-H(63C)	0.98	Au(38)-Au(36)-Au(44)	62.3
C(64)-H(64A)	0.98	Au(39)-Au(36)-Au(1)	55.3
C(64)-H(64B)	0.98	Au(39)-Au(36)-Au(2)	56.3
C(64)-H(64C)	0.98	Au(39)-Au(36)-Au(5)	106
C(65)-C(66)	1.3193	Au(39)-Au(36)-Au(35)	58.6
C(65)-C(70)	1.4319	Au(39)-Au(36)-Au(37)	58.8
C(66)-H(66)	0.95	Au(39)-Au(36)-Au(38)	107.5
C(66)-C(67)	1.4578	Au(39)-Au(36)-Au(41)	129.5
C(67)-H(67)	0.95	Au(39)-Au(36)-Au(44)	157.1
C(67)-C(68)	1.5058	Au(41)-Au(36)-Au(1)	144.8
C(68)-C(69)	1.3584	Au(41)-Au(36)-Au(2)	153.6
C(68)-C(72)	1.5822	Au(44)-Au(36)-Au(1)	106.4
C(69)-H(69)	0.95	Au(44)-Au(36)-Au(2)	104.5
C(69)-C(70)	1.3492	Au(44)-Au(36)-Au(5)	64.4

C(70)-C(71)	1.519	Au(44)-Au(36)-Au(41)	73.4
C(71)-H(71A)	0.98	Au(2)-Au(37)-Au(30)	100
C(71)-H(71B)	0.98	Au(2)-Au(37)-Au(32)	53.3
C(71)-H(71C)	0.98	Au(2)-Au(37)-Au(33)	98
C(72)-H(72A)	0.98	Au(2)-Au(37)-Au(35)	112
C(72)-H(72B)	0.98	Au(2)-Au(37)-Au(38)	56.8
C(72)-H(72C)	0.98	Au(30)-Au(37)-Au(32)	52.9
C(73)-C(78)	1.39	Au(30)-Au(37)-Au(33)	61.6
C(73)-C(74)	1.39	Au(30)-Au(37)-Au(38)	156.7
C(78)-C(77)	1.39	Au(33)-Au(37)-Au(32)	55.9
C(78)-C(79)	1.4818	Au(35)-Au(37)-Au(30)	70.1
C(77)-H(77)	0.95	Au(35)-Au(37)-Au(32)	109.9
C(77)-C(76)	1.39	Au(35)-Au(37)-Au(33)	126.6
C(76)-C(75)	1.39	Au(35)-Au(37)-Au(38)	114.9
C(76)-C(80)	1.5557	Au(36)-Au(37)-Au(2)	66.5
C(75)-H(75)	0.95	Au(36)-Au(37)-Au(30)	114.7
C(75)-C(74)	1.39	Au(36)-Au(37)-Au(32)	108.7
C(74)-H(74)	0.95	Au(36)-Au(37)-Au(33)	163.9
C(79)-H(79A)	0.98	Au(36)-Au(37)-Au(35)	60.1
C(79)-H(79B)	0.98	Au(36)-Au(37)-Au(38)	57.8
C(79)-H(79C)	0.98	Au(38)-Au(37)-Au(32)	106.3
C(80)-H(80A)	0.98	Au(38)-Au(37)-Au(33)	118.5
C(80)-H(80B)	0.98	Au(39)-Au(37)-Au(2)	60
C(80)-H(80C)	0.98	Au(39)-Au(37)-Au(30)	58.4
C(81)-C(82)	1.39	Au(39)-Au(37)-Au(32)	58.4
C(81)-C(86)	1.39	Au(39)-Au(37)-Au(33)	108.5
C(82)-H(82)	0.95	Au(39)-Au(37)-Au(35)	58.5
C(82)-C(83)	1.39	Au(39)-Au(37)-Au(36)	60.6
C(83)-H(83)	0.95	Au(39)-Au(37)-Au(38)	103.4
C(83)-C(84)	1.39	S(3)-Au(37)-Au(2)	113.4
C(84)-C(85)	1.39	S(3)-Au(37)-Au(30)	103.1
C(84)-C(88)	1.5623	S(3)-Au(37)-Au(32)	98.1
C(85)-H(85)	0.95	S(3)-Au(37)-Au(33)	47.2
C(85)-C(86)	1.39	S(3)-Au(37)-Au(35)	134.7
C(86)-C(87)	1.5621	S(3)-Au(37)-Au(36)	141.7
C(87)-H(87A)	0.98	S(3)-Au(37)-Au(38)	89.1
C(87)-H(87B)	0.98	S(3)-Au(37)-Au(39)	155.5
C(87)-H(87C)	0.98	Au(2)-Au(38)-Au(6)	57.8
C(88)-H(88A)	0.98	Au(2)-Au(38)-Au(19)	56.7
C(88)-H(88B)	0.98	Au(2)-Au(38)-Au(21)	106
C(88)-H(88C)	0.98	Au(2)-Au(38)-Au(36)	66.6
C(89)-C(90)	1.39	Au(2)-Au(38)-Au(37)	57.8
C(89)-C(94)	1.39	Au(2)-Au(38)-Au(40)	166.2
C(90)-H(90)	0.95	Au(2)-Au(38)-Au(44)	110.3

C(90)-C(91)	1.39	Au(6)-Au(38)-Au(19)	57.8
C(91)-H(91)	0.95	Au(6)-Au(38)-Au(21)	57.9
C(91)-C(92)	1.39	Au(6)-Au(38)-Au(36)	59
C(92)-C(93)	1.39	Au(6)-Au(38)-Au(37)	101.1
C(92)-C(96)	1.523	Au(6)-Au(38)-Au(40)	108.7
C(93)-H(93)	0.95	Au(6)-Au(38)-Au(44)	57.9
C(93)-C(94)	1.39	Au(19)-Au(38)-Au(37)	111.3
C(94)-C(95)	1.5352	Au(19)-Au(38)-Au(40)	115.2
C(95)-H(95A)	0.98	Au(21)-Au(38)-Au(19)	60.3
C(95)-H(95B)	0.98	Au(21)-Au(38)-Au(37)	158.9
C(95)-H(95C)	0.98	Au(21)-Au(38)-Au(40)	61.2
C(96)-H(96A)	0.98	Au(21)-Au(38)-Au(44)	56.2
C(96)-H(96B)	0.98	Au(36)-Au(38)-Au(19)	110.2
C(96)-H(96C)	0.98	Au(36)-Au(38)-Au(21)	105.8
C(97)-C(98)	1.39	Au(36)-Au(38)-Au(37)	57.1
C(97)-C(102)	1.39	Au(36)-Au(38)-Au(40)	110.2
C(98)-H(98)	0.95	Au(36)-Au(38)-Au(44)	59.4
C(98)-C(99)	1.39	Au(37)-Au(38)-Au(40)	133
C(99)-H(99)	0.95	Au(44)-Au(38)-Au(19)	105.6
C(99)-C(100)	1.39	Au(44)-Au(38)-Au(37)	113.9
C(100)-C(101)	1.39	Au(44)-Au(38)-Au(40)	59.2
C(100)-C(104)	1.54	S(1)-Au(38)-Au(2)	144.3
C(101)-H(101)	0.95	S(1)-Au(38)-Au(6)	152.9
C(101)-C(102)	1.39	S(1)-Au(38)-Au(19)	115.3
C(102)-C(103)	1.5817	S(1)-Au(38)-Au(21)	95.4
C(103)-H(10A)	0.98	S(1)-Au(38)-Au(36)	134.5
C(103)-H(10B)	0.98	S(1)-Au(38)-Au(37)	105.5
C(103)-H(10C)	0.98	S(1)-Au(38)-Au(40)	47.6
C(104)-H(10D)	0.98	S(1)-Au(38)-Au(44)	105.4
C(104)-H(10E)	0.98	Au(1)-Au(39)-Au(2)	70
C(104)-H(10F)	0.98	Au(1)-Au(39)-Au(3)	60.1
C(105)-C(106)	1.39	Au(1)-Au(39)-Au(4)	60
C(105)-C(110)	1.39	Au(1)-Au(39)-Au(8)	60.8
C(106)-H(106)	0.95	Au(1)-Au(39)-Au(32)	112.2
C(106)-C(107)	1.39	Au(1)-Au(39)-Au(36)	68.6
C(107)-H(107)	0.95	Au(2)-Au(39)-Au(4)	116
C(107)-C(108)	1.39	Au(2)-Au(39)-Au(8)	61.6
C(108)-C(109)	1.39	Au(2)-Au(39)-Au(32)	56.7
C(108)-C(112)	1.4844	Au(2)-Au(39)-Au(36)	67
C(109)-H(109)	0.95	Au(3)-Au(39)-Au(2)	121.3
C(109)-C(110)	1.39	Au(3)-Au(39)-Au(4)	62.4
C(113)-C(114)	1.39	Au(3)-Au(39)-Au(8)	68.1
C(113)-C(118)	1.39	Au(3)-Au(39)-Au(32)	117.1
C(114)-H(114)	0.95	Au(3)-Au(39)-Au(36)	115.6

C(114)-C(115)	1.39	Au(4)-Au(39)-Au(8)	115.6
C(115)-H(115)	0.95	Au(4)-Au(39)-Au(32)	171.8
C(115)-C(116)	1.39	Au(8)-Au(39)-Au(32)	58.6
C(116)-C(117)	1.39	Au(28)-Au(39)-Au(1)	117
C(116)-C(120)	1.4086	Au(28)-Au(39)-Au(2)	173
C(117)-H(117)	0.95	Au(28)-Au(39)-Au(3)	64.1
C(117)-C(118)	1.39	Au(28)-Au(39)-Au(4)	70.1
C(118)-C(119)	1.5131	Au(28)-Au(39)-Au(8)	119.9
C(119)-H(11A)	0.98	Au(28)-Au(39)-Au(29)	65.4
C(119)-H(11B)	0.98	Au(28)-Au(39)-Au(30)	68.6
C(119)-H(11C)	0.98	Au(28)-Au(39)-Au(32)	117.5
C(120)-H(12A)	0.98	Au(28)-Au(39)-Au(35)	61.3
C(120)-H(12B)	0.98	Au(28)-Au(39)-Au(36)	115.7
C(120)-H(12C)	0.98	Au(28)-Au(39)-Au(37)	113.8
C(121)-C(122)	1.39	Au(29)-Au(39)-Au(1)	109
C(121)-C(126)	1.39	Au(29)-Au(39)-Au(2)	112.2
C(122)-C(123)	1.39	Au(29)-Au(39)-Au(3)	62.7
C(123)-H(123)	0.95	Au(29)-Au(39)-Au(4)	119.8
C(123)-C(124)	1.39	Au(29)-Au(39)-Au(8)	61.5
C(124)-C(125)	1.39	Au(29)-Au(39)-Au(30)	62.7
C(125)-H(125)	0.95	Au(29)-Au(39)-Au(32)	63.9
C(125)-C(126)	1.39	Au(29)-Au(39)-Au(35)	120.3
C(129)-C(130)	1.39	Au(29)-Au(39)-Au(36)	177.6
C(129)-C(134)	1.39	Au(29)-Au(39)-Au(37)	121.2
C(130)-H(130)	0.95	Au(30)-Au(39)-Au(1)	168.2
C(130)-C(131)	1.39	Au(30)-Au(39)-Au(2)	104.4
C(131)-H(131)	0.95	Au(30)-Au(39)-Au(3)	118.2
C(131)-C(132)	1.39	Au(30)-Au(39)-Au(4)	130.9
C(132)-C(133)	1.39	Au(30)-Au(39)-Au(8)	107.4
C(132)-C(136)	1.6852	Au(30)-Au(39)-Au(32)	57.1
C(133)-H(133)	0.95	Au(30)-Au(39)-Au(35)	74.2
C(133)-C(134)	1.39	Au(30)-Au(39)-Au(36)	119.6
C(134)-C(135)	1.6631	Au(35)-Au(39)-Au(1)	117.6
C(135)-H(13A)	0.98	Au(35)-Au(39)-Au(2)	117.3
C(135)-H(13B)	0.98	Au(35)-Au(39)-Au(3)	112
C(135)-H(13C)	0.98	Au(35)-Au(39)-Au(4)	63.3
C(136)-H(13D)	0.98	Au(35)-Au(39)-Au(8)	178.2
C(136)-H(13E)	0.98	Au(35)-Au(39)-Au(32)	122.3
C(136)-H(13F)	0.98	Au(35)-Au(39)-Au(36)	61.7
C(137)-C(138)	1.39	Au(36)-Au(39)-Au(4)	59.4
C(137)-C(142)	1.39	Au(36)-Au(39)-Au(8)	116.5
C(138)-H(138)	0.95	Au(36)-Au(39)-Au(32)	116.5
C(138)-C(139)	1.39	Au(37)-Au(39)-Au(1)	119.2
C(139)-H(139)	0.95	Au(37)-Au(39)-Au(2)	61.2

C(139)-C(140)	1.39	Au(37)-Au(39)-Au(3)	174.9
C(140)-C(141)	1.39	Au(37)-Au(39)-Au(4)	112.7
C(140)-C(144)	1.5212	Au(37)-Au(39)-Au(8)	116.3
C(141)-H(141)	0.95	Au(37)-Au(39)-Au(30)	63.6
C(141)-C(142)	1.39	Au(37)-Au(39)-Au(32)	68
C(142)-C(143)	1.4304	Au(37)-Au(39)-Au(35)	63.5
C(143)-H(14A)	0.98	Au(37)-Au(39)-Au(36)	60.6
C(143)-H(14B)	0.98	Au(21)-Au(40)-Au(38)	55.4
C(143)-H(14C)	0.98	Au(44)-Au(40)-Au(21)	53.8
C(144)-H(14D)	0.98	Au(44)-Au(40)-Au(38)	57.5
C(144)-H(14E)	0.98	S(1)-Au(40)-Au(21)	91.9
C(144)-H(14F)	0.98	S(1)-Au(40)-Au(38)	49.3
C(145)-C(146)	1.39	S(1)-Au(40)-Au(44)	105.4
C(145)-C(150)	1.39	S(25)-Au(40)-Au(21)	93.8
C(146)-H(146)	0.95	S(25)-Au(40)-Au(38)	139.2
C(146)-C(147)	1.39	S(25)-Au(40)-Au(44)	83.3
C(147)-H(147)	0.95	S(25)-Au(40)-S(1)	171.3
C(147)-C(148)	1.39	Au(36)-Au(41)-Au(35)	53.9
C(148)-C(149)	1.39	S(2)-Au(41)-Au(35)	136.5
C(148)-C(152)	1.5402	S(2)-Au(41)-Au(36)	88.4
C(149)-H(149)	0.95	S(4)-Au(41)-Au(35)	45.2
C(149)-C(150)	1.39	S(4)-Au(41)-Au(36)	94.9
C(150)-C(151)	1.472	S(4)-Au(41)-S(2)	175.6
C(151)-H(15A)	0.98	Au(28)-Au(42)-Au(4)	61.6
C(151)-H(15B)	0.98	Au(28)-Au(42)-Au(35)	55.5
C(151)-H(15C)	0.98	Au(35)-Au(42)-Au(4)	56.1
C(152)-H(15D)	0.98	S(7)-Au(42)-Au(4)	145.6
C(152)-H(15E)	0.98	S(7)-Au(42)-Au(28)	90.8
C(152)-H(15F)	0.98	S(7)-Au(42)-Au(35)	92
C(153)-C(158)	1.39	S(8)-Au(42)-Au(4)	46.8
C(153)-C(154)	1.39	S(8)-Au(42)-Au(28)	96.6
C(158)-C(157)	1.39	S(8)-Au(42)-Au(35)	101
C(158)-C(159)	1.4485	S(8)-Au(42)-S(7)	167.1
C(157)-H(157)	0.95	Au(3)-Au(43)-Au(28)	55.2
C(157)-C(156)	1.39	Au(29)-Au(43)-Au(3)	58.7
C(156)-C(155)	1.39	Au(29)-Au(43)-Au(28)	56.1
C(156)-C(160)	1.4684	S(9)-Au(43)-Au(3)	89.4
C(155)-H(155)	0.95	S(9)-Au(43)-Au(28)	46.2
C(155)-C(154)	1.39	S(9)-Au(43)-Au(29)	99.5
C(154)-H(154)	0.95	S(11)-Au(43)-Au(3)	97.4
C(159)-H(15G)	0.98	S(11)-Au(43)-Au(28)	139.9
C(159)-H(15H)	0.98	S(11)-Au(43)-Au(29)	85.3
C(159)-H(15I)	0.98	S(11)-Au(43)-S(9)	173
C(160)-H(16A)	0.98	Au(6)-Au(44)-Au(5)	57

C(160)-H(16B)	0.98	Au(6)-Au(44)-Au(23)	56.4
C(160)-H(16C)	0.98	Au(6)-Au(44)-Au(24)	109.8
C(161)-C(162)	1.39	Au(6)-Au(44)-Au(36)	58.8
C(161)-C(166)	1.39	Au(6)-Au(44)-Au(38)	58.4
C(162)-H(162)	0.95	Au(6)-Au(44)-Au(40)	112.7
C(162)-C(163)	1.39	Au(21)-Au(44)-Au(5)	110.1
C(163)-H(163)	0.95	Au(21)-Au(44)-Au(6)	59.7
C(163)-C(164)	1.39	Au(21)-Au(44)-Au(23)	66.5
C(164)-C(165)	1.39	Au(21)-Au(44)-Au(24)	62.6
C(164)-C(168)	1.4672	Au(21)-Au(44)-Au(36)	108.5
C(165)-H(165)	0.95	Au(21)-Au(44)-Au(38)	60.7
C(165)-C(166)	1.39	Au(21)-Au(44)-Au(40)	64.3
C(166)-C(167)	1.6681	Au(23)-Au(44)-Au(5)	55.9
C(167)-H(16D)	0.98	Au(24)-Au(44)-Au(5)	116.8
C(167)-H(16E)	0.98	Au(24)-Au(44)-Au(23)	66.4
C(167)-H(16F)	0.98	Au(24)-Au(44)-Au(40)	70.9
C(169)-C(170)	1.39	Au(36)-Au(44)-Au(5)	57.9
C(169)-C(174)	1.39	Au(36)-Au(44)-Au(23)	104
C(170)-H(170)	0.95	Au(36)-Au(44)-Au(24)	168.5
C(170)-C(171)	1.39	Au(36)-Au(44)-Au(38)	58.3
C(171)-H(171)	0.95	Au(36)-Au(44)-Au(40)	112.8
C(171)-C(172)	1.39	Au(38)-Au(44)-Au(5)	104.8
C(172)-C(173)	1.39	Au(38)-Au(44)-Au(23)	109.8
C(172)-C(176)	1.6923	Au(38)-Au(44)-Au(24)	117.8
C(173)-H(173)	0.95	Au(38)-Au(44)-Au(40)	63.4
C(173)-C(174)	1.39	Au(40)-Au(44)-Au(5)	168.1
C(174)-C(175)	1.4926	Au(40)-Au(44)-Au(23)	125.3
C(175)-H(17A)	0.98	S(2)-Au(44)-Au(5)	82
C(175)-H(17B)	0.98	S(2)-Au(44)-Au(6)	136.3
C(175)-H(17C)	0.98	S(2)-Au(44)-Au(21)	162.9
C(176)-H(17D)	0.98	S(2)-Au(44)-Au(23)	114.6
C(176)-H(17E)	0.98	S(2)-Au(44)-Au(24)	101.5
C(176)-H(17F)	0.98	S(2)-Au(44)-Au(36)	88.1
C(177)-C(182)	1.39	S(2)-Au(44)-Au(38)	129.5
C(177)-C(178)	1.39	S(2)-Au(44)-Au(40)	105.9
C(182)-C(181)	1.39	Au(40)-S(1)-Au(38)	83
C(182)-C(183)	1.618	C(1)-S(1)-Au(38)	114.9
C(181)-H(181)	0.95	C(1)-S(1)-Au(40)	103.3
C(181)-C(180)	1.39	Au(41)-S(2)-Au(44)	95.1
C(180)-C(179)	1.39	C(9)-S(2)-Au(41)	112.5
C(180)-C(184)	1.4692	C(9)-S(2)-Au(44)	115
C(179)-H(179)	0.95	Au(33)-S(3)-Au(37)	84.8
C(179)-C(178)	1.39	C(17)-S(3)-Au(33)	96.6
C(178)-H(178)	0.95	C(17)-S(3)-Au(37)	114.5

C(183)-H(18A)	0.98	Au(41)-S(4)-Au(35)	91.7
C(183)-H(18B)	0.98	C(25)-S(4)-Au(35)	109.2
C(183)-H(18C)	0.98	C(25)-S(4)-Au(41)	104.5
C(184)-H(18D)	0.98	Au(31)-S(5)-Au(33)	99.5
C(184)-H(18E)	0.98	C(33)-S(5)-Au(31)	108.2
C(184)-H(18F)	0.98	C(33)-S(5)-Au(33)	105.3
C(185)-C(186)	1.39	Au(34)-S(6)-Au(30)	96.4
C(185)-C(190)	1.39	C(41)-S(6)-Au(30)	114.5
C(186)-H(186)	0.95	C(41)-S(6)-Au(34)	104.1
C(186)-C(187)	1.39	Au(42)-S(7)-Au(34)	95.6
C(187)-H(187)	0.95	C(49)-S(7)-Au(34)	111.9
C(187)-C(188)	1.39	C(49)-S(7)-Au(42)	101.4
C(188)-C(189)	1.39	Au(42)-S(8)-Au(4)	87.6
C(188)-C(192)	1.6543	C(57)-S(8)-Au(4)	118.9
C(189)-H(189)	0.95	C(57)-S(8)-Au(42)	103.9
C(189)-C(190)	1.39	Au(43)-S(9)-Au(28)	89.5
C(190)-C(191)	1.4272	C(65)-S(9)-Au(28)	115.4
C(191)-H(19A)	0.98	C(65)-S(9)-Au(43)	101.1
C(191)-H(19B)	0.98	Au(31)-S(10)-Au(29)	90
C(191)-H(19C)	0.98	C(73)-S(10)-Au(29)	115.6
C(192)-H(19D)	0.98	C(73)-S(10)-Au(31)	100.1
C(192)-H(19E)	0.98	Au(43)-S(11)-Au(12)	92.4
C(192)-H(19F)	0.98	C(81)-S(11)-Au(12)	107.7
C(193)-C(194)	1.39	C(81)-S(11)-Au(43)	107.9
C(193)-C(198)	1.39	Au(13)-S(12)-Au(3)	97.5
C(194)-H(194)	0.95	C(89)-S(12)-Au(3)	111.7
C(194)-C(195)	1.39	C(89)-S(12)-Au(13)	111
C(195)-H(195)	0.95	Au(26)-S(13)-Au(5)	86.6
C(195)-C(196)	1.39	C(97)-S(13)-Au(5)	114.8
C(196)-C(197)	1.39	C(97)-S(13)-Au(26)	104.5
C(196)-C(200)	1.7497	Au(25)-S(14)-Au(26)	93.2
C(197)-H(197)	0.95	C(105)-S(14)-Au(25)	103.2
C(197)-C(198)	1.39	C(105)-S(14)-Au(26)	107.4
C(198)-C(199)	1.5258	Au(13)-S(15)-Au(14)	102.7
C(199)-H(19G)	0.98	C(113)-S(15)-Au(13)	105.8
C(199)-H(19H)	0.98	C(113)-S(15)-Au(14)	108.4
C(199)-H(19I)	0.98	Au(9)-S(16)-Au(27)	97.4
C(200)-H(20B)	0.98	C(121)-S(16)-Au(9)	114.4
C(200)-H(20C)	0.98	C(121)-S(16)-Au(27)	107
C(200)-H(20A)	0.98	Au(14)-S(17)-Au(10)	95.6
C(201)-C(206)	1.39	C(129)-S(17)-Au(10)	107
C(201)-C(202)	1.39	C(129)-S(17)-Au(14)	118.9
C(206)-C(205)	1.39	Au(25)-S(18)-Au(22)	88.7
C(206)-C(207)	1.651	C(137)-S(18)-Au(22)	109.2

C(205)-H(205)	0.95	C(137)-S(18)-Au(25)	106.8
C(205)-C(204)	1.39	Au(15)-S(19)-Au(11)	92.3
C(204)-C(203)	1.39	C(145)-S(19)-Au(11)	108.1
C(204)-C(208)	1.4246	C(145)-S(19)-Au(15)	106.6
C(203)-H(203)	0.95	Au(20)-S(20)-Au(18)	92.3
C(203)-C(202)	1.39	C(153)-S(20)-Au(18)	109.7
C(202)-H(202)	0.95	C(153)-S(20)-Au(20)	111.8
C(208)-H(20D)	0.98	Au(15)-S(21)-Au(16)	109.1
C(208)-H(20E)	0.98	C(161)-S(21)-Au(15)	105.8
C(208)-H(20F)	0.98	C(161)-S(21)-Au(16)	104.8
C(112)-H(11D)	0.98	Au(20)-S(22)-Au(21)	98.7
C(112)-H(11E)	0.98	C(169)-S(22)-Au(20)	103.6
C(112)-H(11F)	0.98	C(169)-S(22)-Au(21)	110
C(207)-H(20G)	0.98	Au(16)-S(23)-Au(19)	102.8
C(207)-H(20H)	0.98	C(177)-S(23)-Au(16)	111.9
C(207)-H(20I)	0.98	C(177)-S(23)-Au(19)	113.4
C(168)-H(16G)	0.98	Au(17)-S(24)-Au(32)	103.4
C(168)-H(16H)	0.98	C(185)-S(24)-Au(17)	115.1
C(168)-H(16I)	0.98	C(185)-S(24)-Au(32)	102.7
C(16)-H(16J)	0.98	Au(24)-S(25)-Au(40)	98.1
C(16)-H(16K)	0.98	C(193)-S(25)-Au(24)	106.9
C(16)-H(16L)	0.98	C(193)-S(25)-Au(40)	103.5
		Au(24)-S(26)-Au(23)	91.2
Au(3)-Au(1)-Au(2)	108.7	C(201)-S(26)-Au(23)	110.7
Au(3)-Au(1)-Au(4)	62.6	C(201)-S(26)-Au(24)	107.5
Au(3)-Au(1)-Au(6)	157.5	C(2)-C(1)-S(1)	121.4
Au(3)-Au(1)-Au(7)	126.4	C(2)-C(1)-C(6)	120
Au(3)-Au(1)-Au(8)	68.1	C(6)-C(1)-S(1)	118.5
Au(3)-Au(1)-Au(9)	77	C(1)-C(2)-H(2)	120
Au(3)-Au(1)-Au(27)	141.1	C(3)-C(2)-C(1)	120
Au(3)-Au(1)-Au(36)	105.7	C(3)-C(2)-H(2)	120
Au(4)-Au(1)-Au(2)	104.8	C(2)-C(3)-H(3)	120
Au(4)-Au(1)-Au(6)	106.3	C(2)-C(3)-C(4)	120
Au(4)-Au(1)-Au(7)	159.8	C(4)-C(3)-H(3)	120
Au(4)-Au(1)-Au(8)	116.2	C(3)-C(4)-C(8)	123.7
Au(4)-Au(1)-Au(9)	136.2	C(5)-C(4)-C(3)	120
Au(4)-Au(1)-Au(36)	55.5	C(5)-C(4)-C(8)	116.2
Au(5)-Au(1)-Au(2)	104.8	C(4)-C(5)-H(5)	120
Au(5)-Au(1)-Au(3)	122.8	C(6)-C(5)-C(4)	120
Au(5)-Au(1)-Au(4)	64.7	C(6)-C(5)-H(5)	120
Au(5)-Au(1)-Au(6)	60.1	C(1)-C(6)-C(7)	115.3
Au(5)-Au(1)-Au(7)	110.7	C(5)-C(6)-C(1)	120
Au(5)-Au(1)-Au(8)	161.6	C(5)-C(6)-C(7)	124.1
Au(5)-Au(1)-Au(9)	136.4	C(4)-C(8)-H(8A)	109.5

Au(5)-Au(1)-Au(27)	63.7	C(4)-C(8)-H(8B)	109.5
Au(5)-Au(1)-Au(36)	57.7	C(4)-C(8)-H(8C)	109.5
Au(5)-Au(1)-Au(39)	109.8	H(8A)-C(8)-H(8B)	109.5
Au(6)-Au(1)-Au(2)	53	H(8A)-C(8)-H(8C)	109.5
Au(6)-Au(1)-Au(7)	58.1	H(8B)-C(8)-H(8C)	109.5
Au(6)-Au(1)-Au(8)	103.9	C(10)-C(9)-S(2)	116.1
Au(6)-Au(1)-Au(9)	117.4	C(10)-C(9)-C(14)	120
Au(6)-Au(1)-Au(36)	55.1	C(14)-C(9)-S(2)	123.8
Au(7)-Au(1)-Au(2)	56.2	C(9)-C(10)-H(10)	120
Au(7)-Au(1)-Au(9)	61.5	C(9)-C(10)-C(11)	120
Au(7)-Au(1)-Au(36)	104.8	C(11)-C(10)-H(10)	120
Au(8)-Au(1)-Au(2)	56.7	C(10)-C(11)-H(11)	120
Au(8)-Au(1)-Au(7)	61.5	C(12)-C(11)-C(10)	120
Au(8)-Au(1)-Au(9)	57.1	C(12)-C(11)-H(11)	120
Au(8)-Au(1)-Au(36)	106.5	C(11)-C(12)-C(13)	120
Au(9)-Au(1)-Au(2)	103.5	C(11)-C(12)-C(16)	97.1
Au(9)-Au(1)-Au(36)	161.7	C(13)-C(12)-C(16)	136.3
Au(27)-Au(1)-Au(2)	105.4	C(12)-C(13)-H(13)	120
Au(27)-Au(1)-Au(4)	125	C(14)-C(13)-C(12)	120
Au(27)-Au(1)-Au(6)	61.4	C(14)-C(13)-H(13)	120
Au(27)-Au(1)-Au(7)	61.6	C(9)-C(14)-C(15)	105.4
Au(27)-Au(1)-Au(8)	118.8	C(13)-C(14)-C(9)	120
Au(27)-Au(1)-Au(9)	77.3	C(13)-C(14)-C(15)	132.6
Au(27)-Au(1)-Au(36)	108	C(18)-C(17)-S(3)	117.7
Au(36)-Au(1)-Au(2)	58.3	C(18)-C(17)-C(22)	120
Au(39)-Au(1)-Au(2)	55.2	C(22)-C(17)-S(3)	122.3
Au(39)-Au(1)-Au(3)	60.1	C(17)-C(18)-H(18)	120
Au(39)-Au(1)-Au(4)	60.7	C(19)-C(18)-C(17)	120
Au(39)-Au(1)-Au(6)	97.4	C(19)-C(18)-H(18)	120
Au(39)-Au(1)-Au(7)	106.1	C(18)-C(19)-H(19)	120
Au(39)-Au(1)-Au(8)	60.7	C(20)-C(19)-C(18)	120
Au(39)-Au(1)-Au(9)	113.6	C(20)-C(19)-H(19)	120
Au(39)-Au(1)-Au(27)	158.7	C(19)-C(20)-C(21)	120
Au(39)-Au(1)-Au(36)	56.1	C(19)-C(20)-C(24)	120.6
Au(6)-Au(2)-Au(1)	56.5	C(21)-C(20)-C(24)	119.3
Au(6)-Au(2)-Au(7)	59.3	C(20)-C(21)-H(21)	120
Au(6)-Au(2)-Au(8)	106	C(22)-C(21)-C(20)	120
Au(6)-Au(2)-Au(19)	61.8	C(22)-C(21)-H(21)	120
Au(6)-Au(2)-Au(32)	162.3	C(17)-C(22)-C(23)	123
Au(6)-Au(2)-Au(36)	56.8	C(21)-C(22)-C(17)	120
Au(6)-Au(2)-Au(37)	109.3	C(21)-C(22)-C(23)	116.4
Au(6)-Au(2)-Au(38)	61.3	C(22)-C(23)-H(23A)	109.5
Au(6)-Au(2)-Au(39)	100.1	C(22)-C(23)-H(23B)	109.5
Au(7)-Au(2)-Au(1)	56	C(22)-C(23)-H(23C)	109.5

Au(7)-Au(2)-Au(8)	60.9	H(23A)-C(23)-H(23B)	109.5
Au(7)-Au(2)-Au(36)	106.2	H(23A)-C(23)-H(23C)	109.5
Au(8)-Au(2)-Au(1)	55.5	H(23B)-C(23)-H(23C)	109.5
Au(8)-Au(2)-Au(36)	107	C(20)-C(24)-H(24A)	109.5
Au(19)-Au(2)-Au(1)	109.1	C(20)-C(24)-H(24B)	109.5
Au(19)-Au(2)-Au(7)	64.7	C(20)-C(24)-H(24C)	109.5
Au(19)-Au(2)-Au(8)	120.6	H(24A)-C(24)-H(24B)	109.5
Au(19)-Au(2)-Au(36)	109.4	H(24A)-C(24)-H(24C)	109.5
Au(19)-Au(2)-Au(37)	126.3	H(24B)-C(24)-H(24C)	109.5
Au(19)-Au(2)-Au(38)	65.2	C(26)-C(25)-S(4)	121.5
Au(19)-Au(2)-Au(39)	161.8	C(26)-C(25)-C(30)	120
Au(32)-Au(2)-Au(1)	106.1	C(30)-C(25)-S(4)	118.2
Au(32)-Au(2)-Au(7)	115.7	C(25)-C(26)-H(26)	120
Au(32)-Au(2)-Au(8)	60.4	C(25)-C(26)-C(27)	120
Au(32)-Au(2)-Au(19)	133.7	C(27)-C(26)-H(26)	120
Au(32)-Au(2)-Au(36)	113.9	C(26)-C(27)-H(27)	120
Au(32)-Au(2)-Au(37)	69.9	C(28)-C(27)-C(26)	120
Au(32)-Au(2)-Au(38)	129.1	C(28)-C(27)-H(27)	120
Au(32)-Au(2)-Au(39)	63.9	C(27)-C(28)-C(29)	120
Au(36)-Au(2)-Au(1)	60.1	C(27)-C(28)-C(32)	109.3
Au(37)-Au(2)-Au(1)	104.9	C(29)-C(28)-C(32)	130.4
Au(37)-Au(2)-Au(7)	160.6	C(28)-C(29)-H(29)	120
Au(37)-Au(2)-Au(8)	112.8	C(30)-C(29)-C(28)	120
Au(37)-Au(2)-Au(36)	56.5	C(30)-C(29)-H(29)	120
Au(38)-Au(2)-Au(1)	107.9	C(25)-C(30)-C(31)	120.7
Au(38)-Au(2)-Au(7)	114.6	C(29)-C(30)-C(25)	120
Au(38)-Au(2)-Au(8)	163.1	C(29)-C(30)-C(31)	118.5
Au(38)-Au(2)-Au(36)	57.3	C(30)-C(31)-H(31A)	109.5
Au(38)-Au(2)-Au(37)	65.5	C(30)-C(31)-H(31B)	109.5
Au(39)-Au(2)-Au(1)	54.8	C(30)-C(31)-H(31C)	109.5
Au(39)-Au(2)-Au(7)	105.6	H(31A)-C(31)-H(31B)	109.5
Au(39)-Au(2)-Au(8)	60.1	H(31A)-C(31)-H(31C)	109.5
Au(39)-Au(2)-Au(36)	56.7	H(31B)-C(31)-H(31C)	109.5
Au(39)-Au(2)-Au(37)	58.8	C(28)-C(32)-H(32A)	109.5
Au(39)-Au(2)-Au(38)	109.1	C(28)-C(32)-H(32B)	109.5
Au(1)-Au(3)-Au(4)	58.9	C(28)-C(32)-H(32C)	109.5
Au(1)-Au(3)-Au(8)	56.8	H(32A)-C(32)-H(32B)	109.5
Au(1)-Au(3)-Au(12)	99	H(32A)-C(32)-H(32C)	109.5
Au(1)-Au(3)-Au(28)	110.4	H(32B)-C(32)-H(32C)	109.5
Au(1)-Au(3)-Au(29)	105.3	C(34)-C(33)-S(5)	118.6
Au(1)-Au(3)-Au(39)	59.8	C(34)-C(33)-C(38)	120
Au(1)-Au(3)-Au(43)	164.7	C(38)-C(33)-S(5)	121.3
Au(4)-Au(3)-Au(8)	104.5	C(33)-C(34)-H(34)	120
Au(4)-Au(3)-Au(28)	66.2	C(35)-C(34)-C(33)	120

Au(4)-Au(3)-Au(43)	129.3	C(35)-C(34)-H(34)	120
Au(12)-Au(3)-Au(4)	156.9	C(34)-C(35)-H(35)	120
Au(12)-Au(3)-Au(8)	53.8	C(34)-C(35)-C(36)	120
Au(12)-Au(3)-Au(28)	122.5	C(36)-C(35)-H(35)	120
Au(12)-Au(3)-Au(29)	63.9	C(35)-C(36)-C(40)	125.2
Au(12)-Au(3)-Au(43)	70.7	C(37)-C(36)-C(35)	120
Au(28)-Au(3)-Au(8)	104.8	C(37)-C(36)-C(40)	114.5
Au(28)-Au(3)-Au(43)	68.6	C(36)-C(37)-H(37)	120
Au(29)-Au(3)-Au(4)	112.9	C(38)-C(37)-C(36)	120
Au(29)-Au(3)-Au(8)	56.4	C(38)-C(37)-H(37)	120
Au(29)-Au(3)-Au(28)	61.2	C(33)-C(38)-C(39)	127.8
Au(29)-Au(3)-Au(43)	60.3	C(37)-C(38)-C(33)	120
Au(39)-Au(3)-Au(4)	59.3	C(37)-C(38)-C(39)	111.7
Au(39)-Au(3)-Au(8)	56.8	C(38)-C(39)-H(39A)	109.5
Au(39)-Au(3)-Au(12)	105.6	C(38)-C(39)-H(39B)	109.5
Au(39)-Au(3)-Au(28)	56.8	C(38)-C(39)-H(39C)	109.5
Au(39)-Au(3)-Au(29)	58.1	H(39A)-C(39)-H(39B)	109.5
Au(39)-Au(3)-Au(43)	111	H(39A)-C(39)-H(39C)	109.5
Au(43)-Au(3)-Au(8)	108.1	H(39B)-C(39)-H(39C)	109.5
S(12)-Au(3)-Au(1)	91.8	C(36)-C(40)-H(40A)	109.5
S(12)-Au(3)-Au(4)	95	C(36)-C(40)-H(40B)	109.5
S(12)-Au(3)-Au(8)	121.6	C(36)-C(40)-H(40C)	109.5
S(12)-Au(3)-Au(12)	91.9	H(40A)-C(40)-H(40B)	109.5
S(12)-Au(3)-Au(28)	133.3	H(40A)-C(40)-H(40C)	109.5
S(12)-Au(3)-Au(29)	151.9	H(40B)-C(40)-H(40C)	109.5
S(12)-Au(3)-Au(39)	148.2	C(42)-C(41)-S(6)	121.9
S(12)-Au(3)-Au(43)	99.7	C(42)-C(41)-C(46)	120
Au(1)-Au(4)-Au(3)	58.5	C(46)-C(41)-S(6)	118
Au(1)-Au(4)-Au(5)	57.1	C(41)-C(42)-H(42)	120
Au(1)-Au(4)-Au(28)	103.1	C(43)-C(42)-C(41)	120
Au(1)-Au(4)-Au(35)	112	C(43)-C(42)-H(42)	120
Au(1)-Au(4)-Au(39)	59.3	C(42)-C(43)-H(43)	120
Au(1)-Au(4)-Au(42)	159.1	C(44)-C(43)-C(42)	120
Au(3)-Au(4)-Au(5)	112	C(44)-C(43)-H(43)	120
Au(3)-Au(4)-Au(28)	57.2	C(43)-C(44)-C(45)	120
Au(3)-Au(4)-Au(35)	104.4	C(43)-C(44)-C(48)	121.5
Au(3)-Au(4)-Au(42)	103.7	C(45)-C(44)-C(48)	118.2
Au(5)-Au(4)-Au(28)	156.4	C(44)-C(45)-H(45)	120
Au(5)-Au(4)-Au(42)	143.3	C(46)-C(45)-C(44)	120
Au(28)-Au(4)-Au(42)	56	C(46)-C(45)-H(45)	120
Au(35)-Au(4)-Au(5)	117.5	C(41)-C(46)-C(47)	124.3
Au(35)-Au(4)-Au(28)	54.4	C(45)-C(46)-C(41)	120
Au(35)-Au(4)-Au(42)	58.8	C(45)-C(46)-C(47)	115.7
Au(36)-Au(4)-Au(1)	68.6	C(44)-C(48)-H(48A)	109.5

Au(36)-Au(4)-Au(3)	112.6	C(44)-C(48)-H(48B)	109.5
Au(36)-Au(4)-Au(5)	59.7	C(44)-C(48)-H(48C)	109.5
Au(36)-Au(4)-Au(28)	103.1	H(48A)-C(48)-H(48B)	109.5
Au(36)-Au(4)-Au(35)	60	H(48A)-C(48)-H(48C)	109.5
Au(36)-Au(4)-Au(39)	60.1	H(48B)-C(48)-H(48C)	109.5
Au(36)-Au(4)-Au(42)	114.2	C(50)-C(49)-S(7)	123.2
Au(39)-Au(4)-Au(3)	58.3	C(50)-C(49)-C(54)	120
Au(39)-Au(4)-Au(5)	103	C(54)-C(49)-S(7)	116.5
Au(39)-Au(4)-Au(28)	53.5	C(49)-C(50)-H(50)	120
Au(39)-Au(4)-Au(35)	57.6	C(49)-C(50)-C(51)	120
Au(39)-Au(4)-Au(42)	103	C(51)-C(50)-H(50)	120
S(8)-Au(4)-Au(1)	144.9	C(50)-C(51)-H(51)	120
S(8)-Au(4)-Au(3)	106.9	C(52)-C(51)-C(50)	120
S(8)-Au(4)-Au(5)	112.6	C(52)-C(51)-H(51)	120
S(8)-Au(4)-Au(28)	90.9	C(51)-C(52)-C(53)	120
S(8)-Au(4)-Au(35)	102.4	C(51)-C(52)-C(56)	109.3
S(8)-Au(4)-Au(36)	139.6	C(53)-C(52)-C(56)	130.7
S(8)-Au(4)-Au(39)	144.4	C(52)-C(53)-H(53)	120
S(8)-Au(4)-Au(42)	45.6	C(52)-C(53)-C(54)	120
Au(1)-Au(5)-Au(4)	58.1	C(54)-C(53)-H(53)	120
Au(1)-Au(5)-Au(6)	61	C(49)-C(54)-C(55)	127.9
Au(1)-Au(5)-Au(23)	106	C(53)-C(54)-C(49)	120
Au(1)-Au(5)-Au(26)	110.3	C(53)-C(54)-C(55)	111.6
Au(1)-Au(5)-Au(27)	58.6	C(54)-C(55)-H(55A)	109.5
Au(1)-Au(5)-Au(36)	67.8	C(54)-C(55)-H(55B)	109.5
Au(1)-Au(5)-Au(44)	111.5	C(54)-C(55)-H(55C)	109.5
Au(4)-Au(5)-Au(26)	133.3	H(55A)-C(55)-H(55B)	109.5
Au(4)-Au(5)-Au(44)	111.3	H(55A)-C(55)-H(55C)	109.5
Au(6)-Au(5)-Au(4)	102.3	H(55B)-C(55)-H(55C)	109.5
Au(6)-Au(5)-Au(23)	58.2	C(52)-C(56)-H(56A)	109.5
Au(6)-Au(5)-Au(26)	109.6	C(52)-C(56)-H(56B)	109.5
Au(6)-Au(5)-Au(27)	60	C(52)-C(56)-H(56C)	109.5
Au(6)-Au(5)-Au(36)	58.6	H(56A)-C(56)-H(56B)	109.5
Au(6)-Au(5)-Au(44)	56.6	H(56A)-C(56)-H(56C)	109.5
Au(23)-Au(5)-Au(4)	160.4	H(56B)-C(56)-H(56C)	109.5
Au(23)-Au(5)-Au(26)	60.2	C(58)-C(57)-S(8)	121.6
Au(23)-Au(5)-Au(27)	56.7	C(62)-C(57)-S(8)	123.8
Au(23)-Au(5)-Au(36)	108.2	C(62)-C(57)-C(58)	114.4
Au(23)-Au(5)-Au(44)	61.3	C(57)-C(58)-H(58)	118.7
Au(27)-Au(5)-Au(4)	114.1	C(59)-C(58)-C(57)	122.6
Au(27)-Au(5)-Au(26)	59.7	C(59)-C(58)-H(58)	118.7
Au(27)-Au(5)-Au(44)	106.9	C(58)-C(59)-H(59)	118.7
Au(36)-Au(5)-Au(4)	56.9	C(58)-C(59)-C(60)	122.5
Au(36)-Au(5)-Au(26)	167.8	C(60)-C(59)-H(59)	118.7

Au(36)-Au(5)-Au(27)	111.8	C(59)-C(60)-C(64)	120.2
Au(36)-Au(5)-Au(44)	57.7	C(61)-C(60)-C(59)	117.2
Au(44)-Au(5)-Au(26)	114.5	C(61)-C(60)-C(64)	122.5
S(13)-Au(5)-Au(1)	138.1	C(60)-C(61)-H(61)	117.3
S(13)-Au(5)-Au(4)	109.4	C(62)-C(61)-C(60)	125.4
S(13)-Au(5)-Au(6)	148.3	C(62)-C(61)-H(61)	117.3
S(13)-Au(5)-Au(23)	90.1	C(57)-C(62)-C(63)	122.4
S(13)-Au(5)-Au(26)	45.6	C(61)-C(62)-C(57)	117.8
S(13)-Au(5)-Au(27)	104.7	C(61)-C(62)-C(63)	119.8
S(13)-Au(5)-Au(36)	143.5	C(62)-C(63)-H(63A)	109.5
S(13)-Au(5)-Au(44)	110.2	C(62)-C(63)-H(63B)	109.5
Au(1)-Au(6)-Au(27)	58.7	C(62)-C(63)-H(63C)	109.5
Au(2)-Au(6)-Au(1)	70.5	H(63A)-C(63)-H(63B)	109.5
Au(2)-Au(6)-Au(5)	118.4	H(63A)-C(63)-H(63C)	109.5
Au(2)-Au(6)-Au(7)	63.2	H(63B)-C(63)-H(63C)	109.5
Au(2)-Au(6)-Au(19)	59.9	C(60)-C(64)-H(64A)	109.5
Au(2)-Au(6)-Au(21)	112.2	C(60)-C(64)-H(64B)	109.5
Au(2)-Au(6)-Au(22)	111.8	C(60)-C(64)-H(64C)	109.5
Au(2)-Au(6)-Au(23)	175.7	H(64A)-C(64)-H(64B)	109.5
Au(2)-Au(6)-Au(27)	117.5	H(64A)-C(64)-H(64C)	109.5
Au(2)-Au(6)-Au(36)	68.6	H(64B)-C(64)-H(64C)	109.5
Au(2)-Au(6)-Au(38)	60.9	C(66)-C(65)-S(9)	117.9
Au(2)-Au(6)-Au(44)	118.2	C(66)-C(65)-C(70)	130.3
Au(5)-Au(6)-Au(1)	58.9	C(70)-C(65)-S(9)	110.2
Au(5)-Au(6)-Au(19)	177.8	C(65)-C(66)-H(66)	121.9
Au(5)-Au(6)-Au(27)	62.3	C(65)-C(66)-C(67)	116.2
Au(5)-Au(6)-Au(38)	116.4	C(67)-C(66)-H(66)	121.9
Au(7)-Au(6)-Au(1)	61.5	C(66)-C(67)-H(67)	122.2
Au(7)-Au(6)-Au(5)	112.7	C(66)-C(67)-C(68)	115.5
Au(7)-Au(6)-Au(19)	65.4	C(68)-C(67)-H(67)	122.2
Au(7)-Au(6)-Au(22)	60.7	C(67)-C(68)-C(72)	122.1
Au(7)-Au(6)-Au(27)	61.9	C(69)-C(68)-C(67)	117.6
Au(7)-Au(6)-Au(36)	118.7	C(69)-C(68)-C(72)	120.2
Au(7)-Au(6)-Au(38)	117.7	C(68)-C(69)-H(69)	115.7
Au(7)-Au(6)-Au(44)	178.6	C(70)-C(69)-C(68)	128.6
Au(19)-Au(6)-Au(1)	118.9	C(70)-C(69)-H(69)	115.7
Au(19)-Au(6)-Au(27)	116.9	C(65)-C(70)-C(71)	128.7
Au(19)-Au(6)-Au(38)	64.3	C(69)-C(70)-C(65)	110.3
Au(21)-Au(6)-Au(1)	177	C(69)-C(70)-C(71)	121.1
Au(21)-Au(6)-Au(5)	118.1	C(70)-C(71)-H(71A)	109.5
Au(21)-Au(6)-Au(7)	120.7	C(70)-C(71)-H(71B)	109.5
Au(21)-Au(6)-Au(19)	64.1	C(70)-C(71)-H(71C)	109.5
Au(21)-Au(6)-Au(22)	70.3	H(71A)-C(71)-H(71B)	109.5
Au(21)-Au(6)-Au(27)	120	H(71A)-C(71)-H(71C)	109.5

Au(21)-Au(6)-Au(36)	111	H(71B)-C(71)-H(71C)	109.5
Au(21)-Au(6)-Au(38)	62.5	C(68)-C(72)-H(72A)	109.5
Au(21)-Au(6)-Au(44)	59.4	C(68)-C(72)-H(72B)	109.5
Au(22)-Au(6)-Au(1)	110.3	C(68)-C(72)-H(72C)	109.5
Au(22)-Au(6)-Au(5)	116.7	H(72A)-C(72)-H(72B)	109.5
Au(22)-Au(6)-Au(19)	63.7	H(72A)-C(72)-H(72C)	109.5
Au(22)-Au(6)-Au(27)	61.7	H(72B)-C(72)-H(72C)	109.5
Au(22)-Au(6)-Au(36)	178.4	C(78)-C(73)-S(10)	118.1
Au(22)-Au(6)-Au(38)	120.5	C(78)-C(73)-C(74)	120
Au(22)-Au(6)-Au(44)	118.5	C(74)-C(73)-S(10)	121.8
Au(23)-Au(6)-Au(1)	107.1	C(73)-C(78)-C(77)	120
Au(23)-Au(6)-Au(5)	61.8	C(73)-C(78)-C(79)	121.5
Au(23)-Au(6)-Au(7)	112.6	C(77)-C(78)-C(79)	117.8
Au(23)-Au(6)-Au(19)	119.8	C(78)-C(77)-H(77)	120
Au(23)-Au(6)-Au(21)	70.3	C(76)-C(77)-C(78)	120
Au(23)-Au(6)-Au(22)	65.3	C(76)-C(77)-H(77)	120
Au(23)-Au(6)-Au(27)	58.5	C(77)-C(76)-C(75)	120
Au(23)-Au(6)-Au(36)	114.2	C(77)-C(76)-C(80)	115.6
Au(23)-Au(6)-Au(38)	123.2	C(75)-C(76)-C(80)	124.2
Au(23)-Au(6)-Au(44)	66.1	C(76)-C(75)-H(75)	120
Au(36)-Au(6)-Au(1)	68.3	C(74)-C(75)-C(76)	120
Au(36)-Au(6)-Au(5)	62	C(74)-C(75)-H(75)	120
Au(36)-Au(6)-Au(19)	117.6	C(73)-C(74)-H(74)	120
Au(36)-Au(6)-Au(27)	116.8	C(75)-C(74)-C(73)	120
Au(36)-Au(6)-Au(38)	61	C(75)-C(74)-H(74)	120
Au(36)-Au(6)-Au(44)	62.1	C(78)-C(79)-H(79A)	109.5
Au(38)-Au(6)-Au(1)	118.8	C(78)-C(79)-H(79B)	109.5
Au(38)-Au(6)-Au(27)	177.5	C(78)-C(79)-H(79C)	109.5
Au(44)-Au(6)-Au(1)	118.3	H(79A)-C(79)-H(79B)	109.5
Au(44)-Au(6)-Au(5)	66.4	H(79A)-C(79)-H(79C)	109.5
Au(44)-Au(6)-Au(19)	115.5	H(79B)-C(79)-H(79C)	109.5
Au(44)-Au(6)-Au(27)	116.7	C(76)-C(80)-H(80A)	109.5
Au(44)-Au(6)-Au(38)	63.7	C(76)-C(80)-H(80B)	109.5
Au(1)-Au(7)-Au(2)	67.8	C(76)-C(80)-H(80C)	109.5
Au(1)-Au(7)-Au(8)	59	H(80A)-C(80)-H(80B)	109.5
Au(1)-Au(7)-Au(9)	60.7	H(80A)-C(80)-H(80C)	109.5
Au(1)-Au(7)-Au(19)	111.5	H(80B)-C(80)-H(80C)	109.5
Au(1)-Au(7)-Au(27)	58.1	C(82)-C(81)-S(11)	117.8
Au(2)-Au(7)-Au(8)	59.9	C(82)-C(81)-C(86)	120
Au(2)-Au(7)-Au(9)	111.5	C(86)-C(81)-S(11)	122
Au(2)-Au(7)-Au(19)	55.8	C(81)-C(82)-H(82)	120
Au(2)-Au(7)-Au(27)	111.7	C(81)-C(82)-C(83)	120
Au(6)-Au(7)-Au(1)	60.4	C(83)-C(82)-H(82)	120
Au(6)-Au(7)-Au(2)	57.5	C(82)-C(83)-H(83)	120

Au(6)-Au(7)-Au(8)	103.8	C(84)-C(83)-C(82)	120
Au(6)-Au(7)-Au(9)	118.8	C(84)-C(83)-H(83)	120
Au(6)-Au(7)-Au(19)	58	C(83)-C(84)-C(85)	120
Au(6)-Au(7)-Au(22)	59.8	C(83)-C(84)-C(88)	121.6
Au(6)-Au(7)-Au(27)	61	C(85)-C(84)-C(88)	116.4
Au(8)-Au(7)-Au(9)	56.1	C(84)-C(85)-H(85)	120
Au(8)-Au(7)-Au(19)	111.5	C(86)-C(85)-C(84)	120
Au(9)-Au(7)-Au(19)	167.1	C(86)-C(85)-H(85)	120
Au(10)-Au(7)-Au(1)	128	C(81)-C(86)-C(87)	116.1
Au(10)-Au(7)-Au(2)	133.3	C(85)-C(86)-C(81)	120
Au(10)-Au(7)-Au(6)	166.6	C(85)-C(86)-C(87)	123.8
Au(10)-Au(7)-Au(8)	89.5	C(86)-C(87)-H(87A)	109.5
Au(10)-Au(7)-Au(9)	67.5	C(86)-C(87)-H(87B)	109.5
Au(10)-Au(7)-Au(19)	118.7	C(86)-C(87)-H(87C)	109.5
Au(10)-Au(7)-Au(22)	106.9	H(87A)-C(87)-H(87B)	109.5
Au(10)-Au(7)-Au(27)	112.7	H(87A)-C(87)-H(87C)	109.5
Au(17)-Au(7)-Au(1)	119.8	H(87B)-C(87)-H(87C)	109.5
Au(17)-Au(7)-Au(2)	74.3	C(84)-C(88)-H(88A)	109.5
Au(17)-Au(7)-Au(6)	128	C(84)-C(88)-H(88B)	109.5
Au(17)-Au(7)-Au(8)	61.9	C(84)-C(88)-H(88C)	109.5
Au(17)-Au(7)-Au(9)	94.9	H(88A)-C(88)-H(88B)	109.5
Au(17)-Au(7)-Au(10)	59.7	H(88A)-C(88)-H(88C)	109.5
Au(17)-Au(7)-Au(18)	62.8	H(88B)-C(88)-H(88C)	109.5
Au(17)-Au(7)-Au(19)	80.2	C(90)-C(89)-S(12)	117.7
Au(17)-Au(7)-Au(22)	126.2	C(90)-C(89)-C(94)	120
Au(17)-Au(7)-Au(27)	169.8	C(94)-C(89)-S(12)	121.3
Au(18)-Au(7)-Au(1)	173.5	C(89)-C(90)-H(90)	120
Au(18)-Au(7)-Au(2)	108.6	C(89)-C(90)-C(91)	120
Au(18)-Au(7)-Au(6)	113.2	C(91)-C(90)-H(90)	120
Au(18)-Au(7)-Au(8)	124.5	C(90)-C(91)-H(91)	120
Au(18)-Au(7)-Au(9)	125.7	C(92)-C(91)-C(90)	120
Au(18)-Au(7)-Au(10)	58.4	C(92)-C(91)-H(91)	120
Au(18)-Au(7)-Au(19)	62.5	C(91)-C(92)-C(93)	120
Au(18)-Au(7)-Au(22)	66.6	C(91)-C(92)-C(96)	108.8
Au(18)-Au(7)-Au(27)	120.5	C(93)-C(92)-C(96)	129.7
Au(22)-Au(7)-Au(1)	108.7	C(92)-C(93)-H(93)	120
Au(22)-Au(7)-Au(2)	106.5	C(92)-C(93)-C(94)	120
Au(22)-Au(7)-Au(8)	163.6	C(94)-C(93)-H(93)	120
Au(22)-Au(7)-Au(9)	130.1	C(89)-C(94)-C(95)	122.8
Au(22)-Au(7)-Au(19)	60.8	C(93)-C(94)-C(89)	120
Au(22)-Au(7)-Au(27)	61.1	C(93)-C(94)-C(95)	117.1
Au(27)-Au(7)-Au(8)	113.2	C(94)-C(95)-H(95A)	109.5
Au(27)-Au(7)-Au(9)	75.3	C(94)-C(95)-H(95B)	109.5
Au(27)-Au(7)-Au(19)	109.9	C(94)-C(95)-H(95C)	109.5

Au(1)-Au(8)-Au(2)	67.8	H(95A)-C(95)-H(95B)	109.5
Au(1)-Au(8)-Au(3)	55.1	H(95A)-C(95)-H(95C)	109.5
Au(1)-Au(8)-Au(7)	59.5	H(95B)-C(95)-H(95C)	109.5
Au(1)-Au(8)-Au(17)	114.3	C(92)-C(96)-H(96A)	109.5
Au(1)-Au(8)-Au(29)	104.3	C(92)-C(96)-H(96B)	109.5
Au(2)-Au(8)-Au(3)	107.2	C(92)-C(96)-H(96C)	109.5
Au(2)-Au(8)-Au(7)	59.2	H(96A)-C(96)-H(96B)	109.5
Au(2)-Au(8)-Au(17)	71.3	H(96A)-C(96)-H(96C)	109.5
Au(7)-Au(8)-Au(3)	112.2	H(96B)-C(96)-H(96C)	109.5
Au(9)-Au(8)-Au(1)	63.3	C(98)-C(97)-S(13)	123.6
Au(9)-Au(8)-Au(2)	117.1	C(98)-C(97)-C(102)	120
Au(9)-Au(8)-Au(3)	73.8	C(102)-C(97)-S(13)	116.3
Au(9)-Au(8)-Au(7)	62.9	C(97)-C(98)-H(98)	120
Au(9)-Au(8)-Au(11)	60.1	C(97)-C(98)-C(99)	120
Au(9)-Au(8)-Au(17)	95.3	C(99)-C(98)-H(98)	120
Au(9)-Au(8)-Au(29)	121.7	C(98)-C(99)-H(99)	120
Au(9)-Au(8)-Au(32)	173.6	C(100)-C(99)-C(98)	120
Au(9)-Au(8)-Au(39)	117.2	C(100)-C(99)-H(99)	120
Au(11)-Au(8)-Au(1)	122.9	C(99)-C(100)-C(104)	110.9
Au(11)-Au(8)-Au(2)	135.7	C(101)-C(100)-C(99)	120
Au(11)-Au(8)-Au(3)	112.8	C(101)-C(100)-C(104)	129.1
Au(11)-Au(8)-Au(7)	88	C(100)-C(101)-H(101)	120
Au(11)-Au(8)-Au(17)	65.4	C(100)-C(101)-C(102)	120
Au(11)-Au(8)-Au(29)	110.7	C(102)-C(101)-H(101)	120
Au(11)-Au(8)-Au(32)	122.4	C(97)-C(102)-C(103)	132.3
Au(11)-Au(8)-Au(39)	165.9	C(101)-C(102)-C(97)	120
Au(12)-Au(8)-Au(1)	100.8	C(101)-C(102)-C(103)	107.2
Au(12)-Au(8)-Au(2)	164.9	C(102)-C(103)-H(10A)	109.5
Au(12)-Au(8)-Au(3)	57.7	C(102)-C(103)-H(10B)	109.5
Au(12)-Au(8)-Au(7)	124.5	C(102)-C(103)-H(10C)	109.5
Au(12)-Au(8)-Au(9)	62.1	H(10A)-C(103)-H(10B)	109.5
Au(12)-Au(8)-Au(11)	58.4	H(10A)-C(103)-H(10C)	109.5
Au(12)-Au(8)-Au(17)	123.5	H(10B)-C(103)-H(10C)	109.5
Au(12)-Au(8)-Au(29)	65.8	C(100)-C(104)-H(10D)	109.5
Au(12)-Au(8)-Au(32)	124.3	C(100)-C(104)-H(10E)	109.5
Au(12)-Au(8)-Au(39)	107.7	C(100)-C(104)-H(10F)	109.5
Au(17)-Au(8)-Au(3)	167.2	H(10D)-C(104)-H(10E)	109.5
Au(17)-Au(8)-Au(7)	55.7	H(10D)-C(104)-H(10F)	109.5
Au(29)-Au(8)-Au(2)	106.5	H(10E)-C(104)-H(10F)	109.5
Au(29)-Au(8)-Au(3)	57	C(106)-C(105)-S(14)	120
Au(29)-Au(8)-Au(7)	160.7	C(106)-C(105)-C(110)	120
Au(29)-Au(8)-Au(17)	135.7	C(110)-C(105)-S(14)	120
Au(32)-Au(8)-Au(1)	113.1	C(105)-C(106)-H(106)	120
Au(32)-Au(8)-Au(2)	56.7	C(107)-C(106)-C(105)	120

Au(32)-Au(8)-Au(3)	108.9	C(107)-C(106)-H(106)	120
Au(32)-Au(8)-Au(7)	110.8	C(106)-C(107)-H(107)	120
Au(32)-Au(8)-Au(17)	81.2	C(106)-C(107)-C(108)	120
Au(32)-Au(8)-Au(29)	63.8	C(108)-C(107)-H(107)	120
Au(32)-Au(8)-Au(39)	61.9	C(107)-C(108)-C(109)	120
Au(39)-Au(8)-Au(1)	58.5	C(107)-C(108)-C(112)	128
Au(39)-Au(8)-Au(2)	58.3	C(109)-C(108)-C(112)	110.6
Au(39)-Au(8)-Au(3)	55.1	C(108)-C(109)-H(109)	120
Au(39)-Au(8)-Au(7)	103	C(108)-C(109)-C(110)	120
Au(39)-Au(8)-Au(17)	128.1	C(110)-C(109)-H(109)	120
Au(39)-Au(8)-Au(29)	57.8	C(109)-C(110)-C(105)	120
Au(1)-Au(9)-Au(7)	57.9	C(114)-C(113)-S(15)	122.2
Au(1)-Au(9)-Au(10)	110.9	C(114)-C(113)-C(118)	120
Au(1)-Au(9)-Au(14)	174.1	C(118)-C(113)-S(15)	117.8
Au(7)-Au(9)-Au(10)	53.1	C(113)-C(114)-H(114)	120
Au(8)-Au(9)-Au(1)	59.7	C(115)-C(114)-C(113)	120
Au(8)-Au(9)-Au(7)	61	C(115)-C(114)-H(114)	120
Au(8)-Au(9)-Au(10)	84	C(114)-C(115)-H(115)	120
Au(8)-Au(9)-Au(11)	60	C(114)-C(115)-C(116)	120
Au(8)-Au(9)-Au(12)	58.4	C(116)-C(115)-H(115)	120
Au(8)-Au(9)-Au(13)	113.3	C(115)-C(116)-C(117)	120
Au(8)-Au(9)-Au(14)	125.4	C(115)-C(116)-C(120)	125.2
Au(11)-Au(9)-Au(1)	119.2	C(117)-C(116)-C(120)	114.7
Au(11)-Au(9)-Au(7)	87	C(116)-C(117)-H(117)	120
Au(11)-Au(9)-Au(10)	55.8	C(118)-C(117)-C(116)	120
Au(11)-Au(9)-Au(12)	57.2	C(118)-C(117)-H(117)	120
Au(11)-Au(9)-Au(13)	103.6	C(113)-C(118)-C(119)	119.7
Au(11)-Au(9)-Au(14)	65.5	C(117)-C(118)-C(113)	120
Au(12)-Au(9)-Au(1)	96	C(117)-C(118)-C(119)	119.2
Au(12)-Au(9)-Au(7)	118.9	C(118)-C(119)-H(11A)	109.5
Au(12)-Au(9)-Au(10)	112.7	C(118)-C(119)-H(11B)	109.5
Au(12)-Au(9)-Au(13)	59.9	C(118)-C(119)-H(11C)	109.5
Au(12)-Au(9)-Au(14)	89.6	H(11A)-C(119)-H(11B)	109.5
Au(13)-Au(9)-Au(1)	105.8	H(11A)-C(119)-H(11C)	109.5
Au(13)-Au(9)-Au(7)	163.6	H(11B)-C(119)-H(11C)	109.5
Au(13)-Au(9)-Au(10)	143.3	C(116)-C(120)-H(12A)	109.5
Au(13)-Au(9)-Au(14)	75.5	C(116)-C(120)-H(12B)	109.5
Au(14)-Au(9)-Au(7)	120.7	C(116)-C(120)-H(12C)	109.5
Au(14)-Au(9)-Au(10)	68.3	H(12A)-C(120)-H(12B)	109.5
S(16)-Au(9)-Au(1)	89.1	H(12A)-C(120)-H(12C)	109.5
S(16)-Au(9)-Au(7)	79.1	H(12B)-C(120)-H(12C)	109.5
S(16)-Au(9)-Au(8)	138	C(122)-C(121)-S(16)	126.3
S(16)-Au(9)-Au(10)	82.1	C(122)-C(121)-C(126)	120
S(16)-Au(9)-Au(11)	134.7	C(126)-C(121)-S(16)	113.7

S(16)-Au(9)-Au(12)	161.1	C(123)-C(122)-C(121)	120
S(16)-Au(9)-Au(13)	101.2	C(122)-C(123)-H(123)	120
S(16)-Au(9)-Au(14)	85.1	C(122)-C(123)-C(124)	120
Au(7)-Au(10)-Au(9)	59.4	C(124)-C(123)-H(123)	120
Au(7)-Au(10)-Au(11)	90.4	C(123)-C(124)-C(125)	120
Au(7)-Au(10)-Au(15)	117.2	C(124)-C(125)-H(125)	120
Au(11)-Au(10)-Au(9)	54.6	C(126)-C(125)-C(124)	120
Au(11)-Au(10)-Au(15)	69	C(126)-C(125)-H(125)	120
Au(15)-Au(10)-Au(9)	122.9	C(125)-C(126)-C(121)	120
Au(17)-Au(10)-Au(7)	59.4	C(130)-C(129)-S(17)	118.4
Au(17)-Au(10)-Au(9)	89.9	C(130)-C(129)-C(134)	120
Au(17)-Au(10)-Au(11)	67.2	C(134)-C(129)-S(17)	121.6
Au(17)-Au(10)-Au(15)	57.9	C(129)-C(130)-H(130)	120
Au(18)-Au(10)-Au(7)	60.4	C(131)-C(130)-C(129)	120
Au(18)-Au(10)-Au(9)	119.6	C(131)-C(130)-H(130)	120
Au(18)-Au(10)-Au(11)	130.4	C(130)-C(131)-H(131)	120
Au(18)-Au(10)-Au(15)	88.7	C(132)-C(131)-C(130)	120
Au(18)-Au(10)-Au(17)	63.5	C(132)-C(131)-H(131)	120
S(17)-Au(10)-Au(7)	132.4	C(131)-C(132)-C(133)	120
S(17)-Au(10)-Au(9)	87.4	C(131)-C(132)-C(136)	119
S(17)-Au(10)-Au(11)	96.8	C(133)-C(132)-C(136)	113.1
S(17)-Au(10)-Au(15)	109.2	C(132)-C(133)-H(133)	120
S(17)-Au(10)-Au(17)	161.8	C(134)-C(133)-C(132)	120
S(17)-Au(10)-Au(18)	132.7	C(134)-C(133)-H(133)	120
Au(8)-Au(11)-Au(9)	59.9	C(129)-C(134)-C(135)	122.8
Au(8)-Au(11)-Au(10)	91.5	C(133)-C(134)-C(129)	120
Au(8)-Au(11)-Au(14)	120	C(133)-C(134)-C(135)	115.7
Au(8)-Au(11)-Au(17)	59.4	C(134)-C(135)-H(13A)	109.5
Au(9)-Au(11)-Au(10)	69.6	C(134)-C(135)-H(13B)	109.5
Au(9)-Au(11)-Au(14)	60.2	C(134)-C(135)-H(13C)	109.5
Au(9)-Au(11)-Au(17)	91.6	H(13A)-C(135)-H(13B)	109.5
Au(10)-Au(11)-Au(14)	71.3	H(13A)-C(135)-H(13C)	109.5
Au(10)-Au(11)-Au(17)	55.1	H(13B)-C(135)-H(13C)	109.5
Au(12)-Au(11)-Au(8)	60.1	C(132)-C(136)-H(13D)	109.5
Au(12)-Au(11)-Au(9)	62.7	C(132)-C(136)-H(13E)	109.5
Au(12)-Au(11)-Au(10)	131.9	C(132)-C(136)-H(13F)	109.5
Au(12)-Au(11)-Au(14)	89.5	H(13D)-C(136)-H(13E)	109.5
Au(12)-Au(11)-Au(17)	119.2	H(13D)-C(136)-H(13F)	109.5
Au(17)-Au(11)-Au(14)	125.8	H(13E)-C(136)-H(13F)	109.5
S(19)-Au(11)-Au(8)	151.1	C(138)-C(137)-S(18)	119.7
S(19)-Au(11)-Au(9)	141.6	C(138)-C(137)-C(142)	120
S(19)-Au(11)-Au(10)	84	C(142)-C(137)-S(18)	120.2
S(19)-Au(11)-Au(12)	139.5	C(137)-C(138)-H(138)	120
S(19)-Au(11)-Au(14)	85.5	C(137)-C(138)-C(139)	120

S(19)-Au(11)-Au(17)	95.6	C(139)-C(138)-H(138)	120
Au(3)-Au(12)-Au(13)	76.3	C(138)-C(139)-H(139)	120
Au(3)-Au(12)-Au(29)	58.3	C(140)-C(139)-C(138)	120
Au(8)-Au(12)-Au(3)	68.5	C(140)-C(139)-H(139)	120
Au(8)-Au(12)-Au(9)	59.5	C(139)-C(140)-C(141)	120
Au(8)-Au(12)-Au(13)	115.6	C(139)-C(140)-C(144)	118.3
Au(8)-Au(12)-Au(29)	59.2	C(141)-C(140)-C(144)	121.6
Au(9)-Au(12)-Au(3)	77.5	C(140)-C(141)-H(141)	120
Au(9)-Au(12)-Au(13)	61.4	C(142)-C(141)-C(140)	120
Au(9)-Au(12)-Au(29)	113.4	C(142)-C(141)-H(141)	120
Au(11)-Au(12)-Au(3)	125.7	C(137)-C(142)-C(143)	117.3
Au(11)-Au(12)-Au(8)	61.5	C(141)-C(142)-C(137)	120
Au(11)-Au(12)-Au(9)	60.2	C(141)-C(142)-C(143)	122.7
Au(11)-Au(12)-Au(13)	107	C(142)-C(143)-H(14A)	109.5
Au(11)-Au(12)-Au(29)	107.8	C(142)-C(143)-H(14B)	109.5
Au(13)-Au(12)-Au(29)	133.4	C(142)-C(143)-H(14C)	109.5
S(11)-Au(12)-Au(3)	97.7	H(14A)-C(143)-H(14B)	109.5
S(11)-Au(12)-Au(8)	139.9	H(14A)-C(143)-H(14C)	109.5
S(11)-Au(12)-Au(9)	157.1	H(14B)-C(143)-H(14C)	109.5
S(11)-Au(12)-Au(11)	134.3	C(140)-C(144)-H(14D)	109.5
S(11)-Au(12)-Au(13)	95.7	C(140)-C(144)-H(14E)	109.5
S(11)-Au(12)-Au(29)	81.3	C(140)-C(144)-H(14F)	109.5
Au(12)-Au(13)-Au(9)	58.7	H(14D)-C(144)-H(14E)	109.5
S(12)-Au(13)-Au(9)	89.4	H(14D)-C(144)-H(14F)	109.5
S(12)-Au(13)-Au(12)	94.1	H(14E)-C(144)-H(14F)	109.5
S(15)-Au(13)-Au(9)	89.3	C(146)-C(145)-S(19)	117.9
S(15)-Au(13)-Au(12)	84.2	C(146)-C(145)-C(150)	120
S(15)-Au(13)-S(12)	178.2	C(150)-C(145)-S(19)	122
Au(9)-Au(14)-Au(11)	54.3	C(145)-C(146)-H(146)	120
S(15)-Au(14)-Au(9)	87.8	C(145)-C(146)-C(147)	120
S(15)-Au(14)-Au(11)	95.3	C(147)-C(146)-H(146)	120
S(15)-Au(14)-S(17)	174.5	C(146)-C(147)-H(147)	120
S(17)-Au(14)-Au(9)	93.2	C(148)-C(147)-C(146)	120
S(17)-Au(14)-Au(11)	89.6	C(148)-C(147)-H(147)	120
Au(17)-Au(15)-Au(10)	54.1	C(147)-C(148)-C(149)	120
S(19)-Au(15)-Au(10)	77.9	C(147)-C(148)-C(152)	126.7
S(19)-Au(15)-Au(17)	102.5	C(149)-C(148)-C(152)	113.2
S(21)-Au(15)-Au(10)	111.1	C(148)-C(149)-H(149)	120
S(21)-Au(15)-Au(17)	86.8	C(148)-C(149)-C(150)	120
S(21)-Au(15)-S(19)	169.9	C(150)-C(149)-H(149)	120
Au(18)-Au(16)-Au(17)	57.1	C(145)-C(150)-C(151)	120.5
S(21)-Au(16)-Au(17)	83.3	C(149)-C(150)-C(145)	120
S(21)-Au(16)-Au(18)	96.2	C(149)-C(150)-C(151)	119.5
S(23)-Au(16)-Au(17)	104.2	C(150)-C(151)-H(15A)	109.5

S(23)-Au(16)-Au(18)	82.5	C(150)-C(151)-H(15B)	109.5
S(23)-Au(16)-S(21)	169.8	C(150)-C(151)-H(15C)	109.5
Au(7)-Au(17)-Au(8)	62.4	H(15A)-C(151)-H(15B)	109.5
Au(7)-Au(17)-Au(10)	60.9	H(15A)-C(151)-H(15C)	109.5
Au(7)-Au(17)-Au(11)	86	H(15B)-C(151)-H(15C)	109.5
Au(7)-Au(17)-Au(15)	128.8	C(148)-C(152)-H(15D)	109.5
Au(7)-Au(17)-Au(16)	111.6	C(148)-C(152)-H(15E)	109.5
Au(7)-Au(17)-Au(18)	58.9	C(148)-C(152)-H(15F)	109.5
Au(8)-Au(17)-Au(11)	55.2	H(15D)-C(152)-H(15E)	109.5
Au(8)-Au(17)-Au(16)	155	H(15D)-C(152)-H(15F)	109.5
Au(10)-Au(17)-Au(8)	90.4	H(15E)-C(152)-H(15F)	109.5
Au(10)-Au(17)-Au(11)	57.7	C(158)-C(153)-S(20)	119.6
Au(10)-Au(17)-Au(15)	68	C(158)-C(153)-C(154)	120
Au(10)-Au(17)-Au(16)	108	C(154)-C(153)-S(20)	120.3
Au(10)-Au(17)-Au(18)	57.5	C(153)-C(158)-C(157)	120
Au(15)-Au(17)-Au(8)	123.2	C(153)-C(158)-C(159)	123.6
Au(15)-Au(17)-Au(11)	69.4	C(157)-C(158)-C(159)	115.9
Au(15)-Au(17)-Au(16)	80.3	C(158)-C(157)-H(157)	120
Au(16)-Au(17)-Au(11)	149.5	C(156)-C(157)-C(158)	120
Au(18)-Au(17)-Au(8)	121.1	C(156)-C(157)-H(157)	120
Au(18)-Au(17)-Au(11)	115.1	C(157)-C(156)-C(155)	120
Au(18)-Au(17)-Au(15)	91.2	C(157)-C(156)-C(160)	115
Au(18)-Au(17)-Au(16)	60.8	C(155)-C(156)-C(160)	124.2
S(24)-Au(17)-Au(7)	122.6	C(156)-C(155)-H(155)	120
S(24)-Au(17)-Au(8)	86.2	C(154)-C(155)-C(156)	120
S(24)-Au(17)-Au(10)	172.8	C(154)-C(155)-H(155)	120
S(24)-Au(17)-Au(11)	115.3	C(153)-C(154)-H(154)	120
S(24)-Au(17)-Au(15)	108.6	C(155)-C(154)-C(153)	120
S(24)-Au(17)-Au(16)	77.1	C(155)-C(154)-H(154)	120
S(24)-Au(17)-Au(18)	129.6	C(158)-C(159)-H(15G)	109.5
Au(7)-Au(18)-Au(16)	112.1	C(158)-C(159)-H(15H)	109.5
Au(7)-Au(18)-Au(17)	58.2	C(158)-C(159)-H(15I)	109.5
Au(7)-Au(18)-Au(19)	63.1	H(15G)-C(159)-H(15H)	109.5
Au(7)-Au(18)-Au(20)	105.5	H(15G)-C(159)-H(15I)	109.5
Au(7)-Au(18)-Au(22)	57.5	H(15H)-C(159)-H(15I)	109.5
Au(10)-Au(18)-Au(7)	61.1	C(156)-C(160)-H(16A)	109.5
Au(10)-Au(18)-Au(16)	110.4	C(156)-C(160)-H(16B)	109.5
Au(10)-Au(18)-Au(17)	59	C(156)-C(160)-H(16C)	109.5
Au(10)-Au(18)-Au(19)	121.8	H(16A)-C(160)-H(16B)	109.5
Au(10)-Au(18)-Au(20)	154.1	H(16A)-C(160)-H(16C)	109.5
Au(10)-Au(18)-Au(22)	102.2	H(16B)-C(160)-H(16C)	109.5
Au(16)-Au(18)-Au(19)	76.4	C(162)-C(161)-S(21)	115.8
Au(16)-Au(18)-Au(20)	95.1	C(162)-C(161)-C(166)	120
Au(16)-Au(18)-Au(22)	133.6	C(166)-C(161)-S(21)	123.1

Au(17)-Au(18)-Au(16)	62.1	C(161)-C(162)-H(162)	120
Au(17)-Au(18)-Au(19)	78.5	C(163)-C(162)-C(161)	120
Au(17)-Au(18)-Au(20)	135.6	C(163)-C(162)-H(162)	120
Au(17)-Au(18)-Au(22)	113.3	C(162)-C(163)-H(163)	120
Au(19)-Au(18)-Au(20)	58.5	C(162)-C(163)-C(164)	120
Au(19)-Au(18)-Au(22)	58.3	C(164)-C(163)-H(163)	120
Au(22)-Au(18)-Au(20)	54.2	C(163)-C(164)-C(165)	120
S(20)-Au(18)-Au(7)	141.8	C(163)-C(164)-C(168)	121.9
S(20)-Au(18)-Au(10)	134.8	C(165)-C(164)-C(168)	116.5
S(20)-Au(18)-Au(16)	94.7	C(164)-C(165)-H(165)	120
S(20)-Au(18)-Au(17)	156.7	C(166)-C(165)-C(164)	120
S(20)-Au(18)-Au(19)	99.9	C(166)-C(165)-H(165)	120
S(20)-Au(18)-Au(20)	43	C(161)-C(166)-C(167)	116.3
S(20)-Au(18)-Au(22)	84.2	C(165)-C(166)-C(161)	120
Au(2)-Au(19)-Au(6)	58.3	C(165)-C(166)-C(167)	123.7
Au(2)-Au(19)-Au(7)	59.5	C(166)-C(167)-H(16D)	109.5
Au(2)-Au(19)-Au(18)	104.8	C(166)-C(167)-H(16E)	109.5
Au(2)-Au(19)-Au(20)	163.2	C(166)-C(167)-H(16F)	109.5
Au(2)-Au(19)-Au(21)	105.3	H(16D)-C(167)-H(16E)	109.5
Au(2)-Au(19)-Au(22)	105.7	H(16D)-C(167)-H(16F)	109.5
Au(2)-Au(19)-Au(38)	58.1	H(16E)-C(167)-H(16F)	109.5
Au(6)-Au(19)-Au(7)	56.6	C(170)-C(169)-S(22)	120.6
Au(6)-Au(19)-Au(18)	104.7	C(170)-C(169)-C(174)	120
Au(6)-Au(19)-Au(20)	108.6	C(174)-C(169)-S(22)	119.1
Au(6)-Au(19)-Au(21)	57.1	C(169)-C(170)-H(170)	120
Au(6)-Au(19)-Au(22)	57.6	C(169)-C(170)-C(171)	120
Au(6)-Au(19)-Au(38)	57.9	C(171)-C(170)-H(170)	120
Au(7)-Au(19)-Au(20)	105.1	C(170)-C(171)-H(171)	120
Au(18)-Au(19)-Au(7)	54.3	C(172)-C(171)-C(170)	120
Au(18)-Au(19)-Au(20)	66.6	C(172)-C(171)-H(171)	120
Au(21)-Au(19)-Au(7)	107.1	C(171)-C(172)-C(176)	116.8
Au(21)-Au(19)-Au(18)	124.1	C(173)-C(172)-C(171)	120
Au(21)-Au(19)-Au(20)	71.2	C(173)-C(172)-C(176)	123.2
Au(21)-Au(19)-Au(38)	58.1	C(172)-C(173)-H(173)	120
Au(22)-Au(19)-Au(7)	56	C(172)-C(173)-C(174)	120
Au(22)-Au(19)-Au(18)	61.6	C(174)-C(173)-H(173)	120
Au(22)-Au(19)-Au(20)	57.6	C(169)-C(174)-C(175)	114.8
Au(22)-Au(19)-Au(21)	65.4	C(173)-C(174)-C(169)	120
Au(22)-Au(19)-Au(38)	109.6	C(173)-C(174)-C(175)	124.8
Au(38)-Au(19)-Au(7)	105.3	C(174)-C(175)-H(17A)	109.5
Au(38)-Au(19)-Au(18)	159.6	C(174)-C(175)-H(17B)	109.5
Au(38)-Au(19)-Au(20)	126.4	C(174)-C(175)-H(17C)	109.5
S(23)-Au(19)-Au(2)	119	H(17A)-C(175)-H(17B)	109.5
S(23)-Au(19)-Au(6)	174.9	H(17A)-C(175)-H(17C)	109.5

S(23)-Au(19)-Au(7)	126.8	H(17B)-C(175)-H(17C)	109.5
S(23)-Au(19)-Au(18)	80	C(172)-C(176)-H(17D)	109.5
S(23)-Au(19)-Au(20)	74.8	C(172)-C(176)-H(17E)	109.5
S(23)-Au(19)-Au(21)	121.8	C(172)-C(176)-H(17F)	109.5
S(23)-Au(19)-Au(22)	127.1	H(17D)-C(176)-H(17E)	109.5
S(23)-Au(19)-Au(38)	117.1	H(17D)-C(176)-H(17F)	109.5
Au(19)-Au(20)-Au(18)	54.9	H(17E)-C(176)-H(17F)	109.5
Au(22)-Au(20)-Au(18)	57.4	C(182)-C(177)-S(23)	115.2
Au(22)-Au(20)-Au(19)	58.1	C(182)-C(177)-C(178)	120
S(20)-Au(20)-Au(18)	44.7	C(178)-C(177)-S(23)	124.8
S(20)-Au(20)-Au(19)	98	C(177)-C(182)-C(183)	126.8
S(20)-Au(20)-Au(22)	88.2	C(181)-C(182)-C(177)	120
S(20)-Au(20)-S(22)	172.8	C(181)-C(182)-C(183)	111.5
S(22)-Au(20)-Au(18)	140.5	C(182)-C(181)-H(181)	120
S(22)-Au(20)-Au(19)	88.4	C(182)-C(181)-C(180)	120
S(22)-Au(20)-Au(22)	92.5	C(180)-C(181)-H(181)	120
Au(6)-Au(21)-Au(19)	58.7	C(181)-C(180)-C(179)	120
Au(6)-Au(21)-Au(22)	55.1	C(181)-C(180)-C(184)	122.4
Au(6)-Au(21)-Au(23)	54.8	C(179)-C(180)-C(184)	116.6
Au(6)-Au(21)-Au(24)	111	C(180)-C(179)-H(179)	120
Au(6)-Au(21)-Au(38)	59.6	C(180)-C(179)-C(178)	120
Au(6)-Au(21)-Au(40)	111.7	C(178)-C(179)-H(179)	120
Au(19)-Au(21)-Au(22)	57.1	C(177)-C(178)-H(178)	120
Au(19)-Au(21)-Au(23)	103.4	C(179)-C(178)-C(177)	120
Au(19)-Au(21)-Au(24)	168	C(179)-C(178)-H(178)	120
Au(19)-Au(21)-Au(40)	118.1	C(182)-C(183)-H(18A)	109.5
Au(23)-Au(21)-Au(22)	56	C(182)-C(183)-H(18B)	109.5
Au(24)-Au(21)-Au(22)	112.7	C(182)-C(183)-H(18C)	109.5
Au(24)-Au(21)-Au(23)	64.6	H(18A)-C(183)-H(18B)	109.5
Au(24)-Au(21)-Au(40)	70.2	H(18A)-C(183)-H(18C)	109.5
Au(38)-Au(21)-Au(19)	61.6	H(18B)-C(183)-H(18C)	109.5
Au(38)-Au(21)-Au(22)	105.8	C(180)-C(184)-H(18D)	109.5
Au(38)-Au(21)-Au(23)	107.6	C(180)-C(184)-H(18E)	109.5
Au(38)-Au(21)-Au(24)	120.3	C(180)-C(184)-H(18F)	109.5
Au(38)-Au(21)-Au(40)	63.3	H(18D)-C(184)-H(18E)	109.5
Au(40)-Au(21)-Au(22)	166.8	H(18D)-C(184)-H(18F)	109.5
Au(40)-Au(21)-Au(23)	118.2	H(18E)-C(184)-H(18F)	109.5
Au(44)-Au(21)-Au(6)	60.9	C(186)-C(185)-S(24)	120.6
Au(44)-Au(21)-Au(19)	112.1	C(186)-C(185)-C(190)	120
Au(44)-Au(21)-Au(22)	107.2	C(190)-C(185)-S(24)	119.2
Au(44)-Au(21)-Au(23)	60.9	C(185)-C(186)-H(186)	120
Au(44)-Au(21)-Au(24)	62.9	C(185)-C(186)-C(187)	120
Au(44)-Au(21)-Au(38)	63.2	C(187)-C(186)-H(186)	120
Au(44)-Au(21)-Au(40)	61.9	C(186)-C(187)-H(187)	120

S(22)-Au(21)-Au(6)	138.3	C(186)-C(187)-C(188)	120
S(22)-Au(21)-Au(19)	91.3	C(188)-C(187)-H(187)	120
S(22)-Au(21)-Au(22)	85.1	C(187)-C(188)-C(189)	120
S(22)-Au(21)-Au(23)	115.2	C(187)-C(188)-C(192)	111.5
S(22)-Au(21)-Au(24)	94.1	C(189)-C(188)-C(192)	127.9
S(22)-Au(21)-Au(38)	133.7	C(188)-C(189)-H(189)	120
S(22)-Au(21)-Au(40)	107.8	C(188)-C(189)-C(190)	120
S(22)-Au(21)-Au(44)	156.6	C(190)-C(189)-H(189)	120
Au(6)-Au(22)-Au(7)	59.5	C(185)-C(190)-C(191)	122.8
Au(6)-Au(22)-Au(18)	104.3	C(189)-C(190)-C(185)	120
Au(6)-Au(22)-Au(19)	58.7	C(189)-C(190)-C(191)	116.8
Au(6)-Au(22)-Au(20)	115.2	C(190)-C(191)-H(19A)	109.5
Au(6)-Au(22)-Au(21)	54.6	C(190)-C(191)-H(19B)	109.5
Au(6)-Au(22)-Au(23)	57	C(190)-C(191)-H(19C)	109.5
Au(6)-Au(22)-Au(25)	108	H(19A)-C(191)-H(19B)	109.5
Au(6)-Au(22)-Au(27)	60.9	H(19A)-C(191)-H(19C)	109.5
Au(7)-Au(22)-Au(18)	55.8	H(19B)-C(191)-H(19C)	109.5
Au(7)-Au(22)-Au(19)	63.2	C(188)-C(192)-H(19D)	109.5
Au(7)-Au(22)-Au(20)	116.5	C(188)-C(192)-H(19E)	109.5
Au(7)-Au(22)-Au(21)	106.5	C(188)-C(192)-H(19F)	109.5
Au(7)-Au(22)-Au(23)	105	H(19D)-C(192)-H(19E)	109.5
Au(7)-Au(22)-Au(25)	111.5	H(19D)-C(192)-H(19F)	109.5
Au(7)-Au(22)-Au(27)	61.2	H(19E)-C(192)-H(19F)	109.5
Au(18)-Au(22)-Au(21)	115.1	C(194)-C(193)-S(25)	120.4
Au(18)-Au(22)-Au(25)	128.6	C(194)-C(193)-C(198)	120
Au(19)-Au(22)-Au(18)	60	C(198)-C(193)-S(25)	118.9
Au(19)-Au(22)-Au(21)	57.5	C(193)-C(194)-H(194)	120
Au(19)-Au(22)-Au(23)	108.5	C(193)-C(194)-C(195)	120
Au(19)-Au(22)-Au(25)	166.7	C(195)-C(194)-H(194)	120
Au(20)-Au(22)-Au(18)	68.4	C(194)-C(195)-H(195)	120
Au(20)-Au(22)-Au(19)	64.2	C(194)-C(195)-C(196)	120
Au(20)-Au(22)-Au(21)	70.6	C(196)-C(195)-H(195)	120
Au(20)-Au(22)-Au(23)	123.5	C(195)-C(196)-C(200)	127.4
Au(20)-Au(22)-Au(25)	126.7	C(197)-C(196)-C(195)	120
Au(21)-Au(22)-Au(25)	116.2	C(197)-C(196)-C(200)	112.4
Au(23)-Au(22)-Au(18)	160.1	C(196)-C(197)-H(197)	120
Au(23)-Au(22)-Au(21)	61.8	C(198)-C(197)-C(196)	120
Au(23)-Au(22)-Au(25)	60	C(198)-C(197)-H(197)	120
Au(27)-Au(22)-Au(18)	111.1	C(193)-C(198)-C(199)	105.7
Au(27)-Au(22)-Au(19)	112	C(197)-C(198)-C(193)	120
Au(27)-Au(22)-Au(20)	176	C(197)-C(198)-C(199)	133.7
Au(27)-Au(22)-Au(21)	106.6	C(198)-C(199)-H(19G)	109.5
Au(27)-Au(22)-Au(23)	55.8	C(198)-C(199)-H(19H)	109.5
Au(27)-Au(22)-Au(25)	56.9	C(198)-C(199)-H(19I)	109.5

S(18)-Au(22)-Au(6)	144.5	H(19G)-C(199)-H(19H)	109.5
S(18)-Au(22)-Au(7)	142.2	H(19G)-C(199)-H(19I)	109.5
S(18)-Au(22)-Au(18)	111	H(19H)-C(199)-H(19I)	109.5
S(18)-Au(22)-Au(19)	146.5	C(196)-C(200)-H(20B)	109.5
S(18)-Au(22)-Au(20)	82.4	C(196)-C(200)-H(20C)	109.5
S(18)-Au(22)-Au(21)	110.8	C(196)-C(200)-H(20A)	109.5
S(18)-Au(22)-Au(23)	87.5	H(20B)-C(200)-H(20C)	109.5
S(18)-Au(22)-Au(25)	44.8	H(20B)-C(200)-H(20A)	109.5
S(18)-Au(22)-Au(27)	101.4	H(20C)-C(200)-H(20A)	109.5
Au(5)-Au(23)-Au(21)	104.5	C(206)-C(201)-S(26)	121.4
Au(5)-Au(23)-Au(22)	108.8	C(206)-C(201)-C(202)	120
Au(5)-Au(23)-Au(24)	114.1	C(202)-C(201)-S(26)	118.6
Au(5)-Au(23)-Au(25)	115.9	C(201)-C(206)-C(205)	120
Au(5)-Au(23)-Au(26)	65.3	C(201)-C(206)-C(207)	114
Au(5)-Au(23)-Au(44)	62.8	C(205)-C(206)-C(207)	125.3
Au(6)-Au(23)-Au(5)	60	C(206)-C(205)-H(205)	120
Au(6)-Au(23)-Au(21)	54.9	C(204)-C(205)-C(206)	120
Au(6)-Au(23)-Au(22)	57.7	C(204)-C(205)-H(205)	120
Au(6)-Au(23)-Au(24)	102.8	C(205)-C(204)-C(203)	120
Au(6)-Au(23)-Au(25)	112.5	C(205)-C(204)-C(208)	109.4
Au(6)-Au(23)-Au(26)	115.4	C(203)-C(204)-C(208)	129.6
Au(6)-Au(23)-Au(44)	57.6	C(204)-C(203)-H(203)	120
Au(21)-Au(23)-Au(24)	55.1	C(202)-C(203)-C(204)	120
Au(22)-Au(23)-Au(21)	62.2	C(202)-C(203)-H(203)	120
Au(22)-Au(23)-Au(24)	109.9	C(201)-C(202)-H(202)	120
Au(22)-Au(23)-Au(25)	64.7	C(203)-C(202)-C(201)	120
Au(22)-Au(23)-Au(26)	117.5	C(203)-C(202)-H(202)	120
Au(22)-Au(23)-Au(44)	105.6	C(204)-C(208)-H(20D)	109.5
Au(25)-Au(23)-Au(21)	120.8	C(204)-C(208)-H(20E)	109.5
Au(25)-Au(23)-Au(24)	128.4	C(204)-C(208)-H(20F)	109.5
Au(26)-Au(23)-Au(21)	169.6	H(20D)-C(208)-H(20E)	109.5
Au(26)-Au(23)-Au(24)	129.8	H(20D)-C(208)-H(20F)	109.5
Au(26)-Au(23)-Au(25)	64.9	H(20E)-C(208)-H(20F)	109.5
Au(27)-Au(23)-Au(5)	63.2	C(108)-C(112)-H(11D)	109.5
Au(27)-Au(23)-Au(6)	63	C(108)-C(112)-H(11E)	109.5
Au(27)-Au(23)-Au(21)	110.7	C(108)-C(112)-H(11F)	109.5
Au(27)-Au(23)-Au(22)	60.5	H(11D)-C(112)-H(11E)	109.5
Au(27)-Au(23)-Au(24)	165.4	H(11D)-C(112)-H(11F)	109.5
Au(27)-Au(23)-Au(25)	59.8	H(11E)-C(112)-H(11F)	109.5
Au(27)-Au(23)-Au(26)	63.4	C(206)-C(207)-H(20G)	109.5
Au(27)-Au(23)-Au(44)	113.3	C(206)-C(207)-H(20H)	109.5
Au(44)-Au(23)-Au(21)	52.6	C(206)-C(207)-H(20I)	109.5
Au(44)-Au(23)-Au(24)	56.6	H(20G)-C(207)-H(20H)	109.5
Au(44)-Au(23)-Au(25)	169.7	H(20G)-C(207)-H(20I)	109.5

Au(44)-Au(23)-Au(26)	120.3	H(20H)-C(207)-H(20I)	109.5
S(26)-Au(23)-Au(5)	145.4	C(164)-C(168)-H(16G)	109.5
S(26)-Au(23)-Au(6)	138.6	C(164)-C(168)-H(16H)	109.5
S(26)-Au(23)-Au(21)	83.7	C(164)-C(168)-H(16I)	109.5
S(26)-Au(23)-Au(22)	104.8	H(16G)-C(168)-H(16H)	109.5
S(26)-Au(23)-Au(24)	43.9	H(16G)-C(168)-H(16I)	109.5
S(26)-Au(23)-Au(25)	86	H(16H)-C(168)-H(16I)	109.5
S(26)-Au(23)-Au(26)	106	C(12)-C(16)-H(16J)	109.5
S(26)-Au(23)-Au(27)	145.7	C(12)-C(16)-H(16K)	109.5
S(26)-Au(23)-Au(44)	100.2	C(12)-C(16)-H(16L)	109.5
Au(21)-Au(24)-Au(23)	60.2	H(16J)-C(16)-H(16K)	109.5
Au(21)-Au(24)-Au(44)	54.5	H(16J)-C(16)-H(16L)	109.5
Au(44)-Au(24)-Au(23)	57	H(16K)-C(16)-H(16L)	109.5
S(25)-Au(24)-Au(21)	95.8		

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Au}_{44}(\text{2,4-DMBT})_{26}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	42(1)	40(1)	44(1)	-5(1)	5(1)	-9(1)
Au(2)	45(1)	39(1)	46(1)	-6(1)	3(1)	-14(1)
Au(3)	42(1)	39(1)	47(1)	-4(1)	6(1)	-12(1)
Au(4)	44(1)	41(1)	51(1)	-2(1)	2(1)	-10(1)
Au(5)	47(1)	45(1)	49(1)	-4(1)	3(1)	-7(1)
Au(6)	40(1)	40(1)	44(1)	-8(1)	2(1)	-9(1)
Au(7)	40(1)	39(1)	47(1)	-8(1)	3(1)	-6(1)
Au(8)	40(1)	38(1)	44(1)	-4(1)	4(1)	-11(1)
Au(9)	42(1)	47(1)	46(1)	-3(1)	7(1)	-14(1)
Au(10)	42(1)	49(1)	59(1)	-11(1)	3(1)	-8(1)
Au(11)	41(1)	42(1)	55(1)	-6(1)	0(1)	-7(1)
Au(12)	44(1)	40(1)	49(1)	-6(1)	6(1)	-14(1)
Au(13)	45(1)	48(1)	54(1)	-1(1)	8(1)	-14(1)
Au(14)	41(1)	55(1)	63(1)	-5(1)	5(1)	-11(1)
Au(15)	56(1)	43(1)	74(1)	-1(1)	-7(1)	-8(1)
Au(16)	64(1)	42(1)	65(1)	-2(1)	-2(1)	-12(1)
Au(17)	51(1)	38(1)	51(1)	-4(1)	2(1)	-8(1)
Au(18)	50(1)	42(1)	58(1)	-11(1)	3(1)	-6(1)

Au(19)	48(1)	38(1)	55(1)	-7(1)	1(1)	-10(1)
Au(20)	63(1)	47(1)	64(1)	-16(1)	-1(1)	-6(1)
Au(21)	54(1)	43(1)	56(1)	-11(1)	0(1)	-11(1)
Au(22)	50(1)	46(1)	49(1)	-12(1)	5(1)	-8(1)
Au(23)	50(1)	60(1)	47(1)	-11(1)	1(1)	-10(1)
Au(24)	66(1)	51(1)	56(1)	-8(1)	-7(1)	-13(1)
Au(25)	60(1)	71(1)	50(1)	-3(1)	11(1)	-7(1)
Au(26)	84(1)	74(1)	53(1)	2(1)	9(1)	6(1)
Au(27)	44(1)	51(1)	46(1)	-6(1)	7(1)	-10(1)
Au(28)	43(1)	40(1)	53(1)	-9(1)	9(1)	-13(1)
Au(29)	47(1)	40(1)	43(1)	-6(1)	6(1)	-15(1)
Au(30)	49(1)	46(1)	51(1)	-10(1)	12(1)	-16(1)
Au(31)	63(1)	49(1)	46(1)	-5(1)	4(1)	-21(1)
Au(32)	48(1)	39(1)	43(1)	-3(1)	5(1)	-13(1)
Au(33)	64(1)	55(1)	55(1)	-3(1)	9(1)	-27(1)
Au(34)	46(1)	52(1)	60(1)	-10(1)	10(1)	-13(1)
Au(35)	40(1)	45(1)	55(1)	-11(1)	8(1)	-12(1)
Au(36)	42(1)	41(1)	48(1)	-9(1)	5(1)	-10(1)
Au(37)	49(1)	49(1)	50(1)	-7(1)	11(1)	-21(1)
Au(38)	46(1)	45(1)	52(1)	-8(1)	4(1)	-17(1)
Au(39)	38(1)	36(1)	45(1)	-4(1)	6(1)	-11(1)
Au(40)	56(1)	58(1)	67(1)	-14(1)	2(1)	-21(1)
Au(41)	44(1)	50(1)	75(1)	-11(1)	3(1)	-7(1)
Au(42)	61(1)	48(1)	65(1)	-7(1)	-5(1)	-9(1)
Au(43)	49(1)	43(1)	51(1)	-8(1)	8(1)	-16(1)
Au(44)	43(1)	45(1)	51(1)	-9(1)	0(1)	-9(1)
S(1)	61(6)	52(5)	72(6)	-15(4)	5(5)	-24(4)
S(2)	57(6)	52(5)	63(5)	0(4)	-6(4)	-4(4)
S(3)	60(6)	61(5)	52(5)	-8(4)	17(4)	-30(5)
S(4)	43(5)	56(5)	80(6)	-10(5)	5(4)	-15(4)
S(5)	65(6)	69(6)	48(5)	4(4)	-5(4)	-18(5)
S(6)	35(4)	65(5)	52(5)	-9(4)	8(3)	-18(4)
S(7)	48(5)	56(5)	72(6)	-6(5)	-2(4)	-5(4)
S(8)	60(6)	48(5)	70(6)	2(4)	-23(5)	-7(4)
S(9)	42(5)	42(4)	54(4)	-3(3)	4(3)	-11(3)
S(10)	52(5)	59(5)	37(4)	-11(3)	-2(3)	-20(4)
S(11)	55(5)	42(4)	47(4)	-9(3)	2(3)	-17(4)
S(12)	47(5)	48(4)	52(4)	4(4)	8(4)	-9(4)

S(13)	66(7)	58(6)	75(7)	-10(5)	8(5)	-3(5)
S(14)	97(10)	71(7)	65(7)	10(5)	22(6)	3(7)
S(15)	44(5)	57(5)	62(5)	-11(4)	10(4)	-15(4)
S(16)	68(7)	92(8)	52(5)	-13(5)	18(5)	-23(6)
S(17)	53(6)	61(5)	56(5)	-10(4)	3(4)	-10(4)
S(18)	49(5)	55(5)	47(4)	-12(4)	6(3)	-4(4)
S(19)	40(5)	44(4)	76(6)	-6(4)	-4(4)	-8(4)
S(20)	61(6)	53(5)	63(6)	-21(4)	-11(4)	-4(4)
S(21)	74(8)	56(6)	77(7)	6(5)	-13(5)	-16(5)
S(22)	60(6)	36(4)	75(6)	-16(4)	-6(4)	-7(4)
S(23)	62(6)	41(4)	76(6)	10(4)	0(5)	-20(4)
S(24)	82(7)	42(4)	45(4)	-1(3)	10(4)	-23(4)
S(25)	67(7)	71(7)	69(6)	-8(5)	-6(5)	-28(5)
S(26)	74(7)	66(6)	54(5)	-19(5)	-4(5)	-4(5)
C(1)	70(5)	69(5)	70(5)	-2(3)	0(3)	-24(3)
C(2)	69(5)	69(5)	69(5)	-2(3)	0(3)	-23(3)
C(3)	69(5)	69(5)	70(5)	-2(3)	-1(3)	-23(3)
C(4)	70(5)	70(5)	72(5)	-1(3)	0(3)	-23(3)
C(5)	71(5)	71(5)	72(5)	-1(3)	0(3)	-23(3)
C(6)	72(5)	70(5)	72(5)	-1(3)	0(3)	-23(3)
C(7)	80(9)	77(9)	79(9)	-2(7)	-1(7)	-23(7)
C(8)	76(9)	79(9)	80(9)	-1(7)	-1(7)	-25(7)
C(9)	158(13)	158(13)	158(13)	-4(3)	0(3)	-50(5)
C(10)	158(13)	158(13)	159(13)	-4(3)	-1(3)	-51(5)
C(11)	159(13)	159(13)	159(13)	-4(3)	-1(3)	-51(5)
C(12)	159(13)	159(13)	159(13)	-3(3)	0(3)	-51(5)
C(13)	159(13)	159(13)	159(13)	-4(3)	0(3)	-51(5)
C(14)	158(13)	158(13)	158(13)	-3(3)	0(3)	-50(5)
C(15)	158(15)	158(15)	158(15)	-1(7)	0(7)	-51(8)
C(17)	87(6)	87(6)	87(6)	-2(3)	0(3)	-28(4)
C(18)	87(7)	87(7)	87(6)	-3(3)	0(3)	-27(4)
C(19)	86(6)	87(6)	87(6)	-3(3)	0(3)	-27(4)
C(20)	87(6)	88(6)	87(6)	-3(3)	0(3)	-27(4)
C(21)	88(6)	88(6)	88(6)	-3(3)	0(3)	-28(4)
C(22)	88(6)	87(6)	88(6)	-2(3)	0(3)	-28(4)
C(23)	94(10)	89(10)	90(10)	-3(7)	-2(7)	-29(7)
C(24)	92(10)	91(10)	93(10)	-1(7)	0(7)	-25(7)
C(25)	50(9)	49(9)	53(9)	-1(5)	0(5)	-15(5)

C(26)	58(10)	58(10)	57(10)	1(5)	1(5)	-17(5)
C(27)	53(9)	51(9)	51(9)	-2(5)	0(5)	-17(5)
C(28)	78(14)	76(14)	78(14)	-2(5)	-3(5)	-24(6)
C(29)	93(17)	93(17)	92(17)	-2(5)	0(5)	-29(7)
C(30)	49(9)	51(9)	53(9)	0(5)	0(5)	-17(5)
C(31)	120(30)	130(30)	120(30)	-2(10)	3(10)	-39(12)
C(32)	100(20)	100(20)	90(20)	-2(10)	-3(10)	-26(11)
C(33)	86(15)	83(15)	85(15)	-2(5)	0(5)	-28(7)
C(34)	69(12)	69(12)	70(12)	-2(5)	1(5)	-22(6)
C(35)	73(13)	74(13)	73(13)	-2(5)	0(5)	-23(6)
C(36)	76(13)	74(13)	75(13)	1(5)	3(5)	-26(6)
C(37)	72(12)	69(12)	70(12)	-3(5)	0(5)	-24(6)
C(38)	77(14)	77(13)	76(13)	0(5)	0(5)	-25(6)
C(39)	160(40)	160(40)	160(40)	-5(10)	1(10)	-52(15)
C(40)	97(19)	92(18)	87(18)	-5(10)	-1(10)	-26(10)
C(41)	43(8)	41(8)	42(8)	-2(5)	-1(5)	-14(5)
C(42)	54(10)	57(10)	54(10)	-3(5)	-3(5)	-17(5)
C(43)	80(14)	79(14)	79(14)	-3(5)	1(5)	-25(6)
C(44)	79(14)	80(14)	80(14)	-3(5)	-1(5)	-26(6)
C(45)	76(13)	76(13)	75(13)	-1(5)	2(5)	-25(6)
C(46)	67(12)	67(12)	68(12)	-3(5)	1(5)	-24(6)
C(47)	87(17)	88(17)	86(17)	-6(10)	0(10)	-27(10)
C(48)	84(17)	88(17)	87(17)	-4(10)	-7(10)	-23(10)
C(49)	58(10)	60(10)	57(10)	-2(5)	-2(5)	-19(5)
C(50)	65(11)	66(11)	65(11)	-4(5)	0(5)	-20(6)
C(51)	57(10)	55(10)	57(10)	-3(5)	1(5)	-17(5)
C(52)	97(18)	95(18)	95(18)	-3(5)	1(5)	-30(7)
C(53)	75(13)	74(13)	75(13)	-3(5)	-2(5)	-23(6)
C(54)	38(8)	38(8)	38(7)	-3(5)	0(5)	-11(5)
C(55)	110(20)	110(20)	110(20)	-2(10)	7(10)	-37(11)
C(56)	94(19)	91(18)	92(18)	-8(10)	0(10)	-27(10)
C(57)	65(5)	64(5)	64(5)	0(3)	0(3)	-21(3)
C(58)	64(5)	64(5)	63(5)	0(3)	0(3)	-21(3)
C(59)	63(5)	64(5)	63(5)	0(3)	1(3)	-21(3)
C(60)	64(5)	65(5)	64(5)	0(3)	1(3)	-21(3)
C(61)	66(5)	66(5)	65(5)	0(3)	1(3)	-21(3)
C(62)	67(5)	66(5)	66(5)	0(3)	0(3)	-21(3)
C(63)	74(9)	76(9)	75(9)	-2(7)	-3(7)	-21(7)

C(64)	67(9)	72(9)	65(8)	-1(7)	0(7)	-19(7)
C(65)	55(10)	56(10)	55(10)	-1(5)	1(5)	-17(5)
C(66)	63(11)	64(11)	62(11)	-1(5)	2(5)	-20(6)
C(67)	67(12)	65(12)	67(12)	-2(5)	1(5)	-20(6)
C(68)	67(12)	67(12)	67(12)	-3(5)	1(5)	-22(6)
C(69)	45(9)	45(8)	48(8)	-2(5)	0(5)	-17(5)
C(70)	53(9)	45(9)	50(9)	-1(5)	1(5)	-20(5)
C(71)	50(12)	53(11)	55(11)	0(9)	1(9)	-18(9)
C(72)	73(15)	73(14)	68(14)	-5(9)	-3(9)	-20(9)
C(73)	50(9)	49(9)	50(9)	1(5)	0(5)	-17(5)
C(78)	43(8)	42(8)	43(8)	-4(5)	-1(5)	-14(5)
C(77)	80(14)	80(14)	77(14)	-3(5)	0(5)	-26(6)
C(76)	68(12)	70(12)	69(12)	-1(5)	-2(5)	-22(6)
C(75)	70(12)	71(12)	70(12)	-3(5)	-2(5)	-21(6)
C(74)	77(14)	78(14)	77(14)	-3(5)	-1(5)	-24(6)
C(79)	52(11)	44(10)	44(10)	6(8)	11(8)	-17(8)
C(80)	52(11)	38(10)	54(11)	-9(8)	8(8)	-22(8)
C(81)	55(5)	54(5)	55(5)	-2(3)	0(3)	-19(3)
C(82)	55(5)	56(5)	56(5)	-1(3)	-1(3)	-19(3)
C(83)	57(5)	58(5)	58(5)	0(3)	-1(3)	-18(3)
C(84)	59(5)	60(5)	60(5)	0(3)	0(3)	-19(3)
C(85)	57(5)	57(5)	57(5)	0(3)	1(3)	-18(3)
C(86)	56(5)	55(5)	55(5)	-1(3)	1(3)	-19(3)
C(87)	57(8)	58(8)	54(8)	-3(7)	-1(7)	-19(7)
C(88)	68(8)	69(8)	72(8)	3(7)	-3(7)	-19(7)
C(89)	92(7)	91(7)	92(7)	-2(3)	0(3)	-29(4)
C(90)	91(7)	91(7)	92(7)	-2(3)	0(3)	-30(4)
C(91)	92(7)	92(7)	93(7)	-2(3)	-1(3)	-29(4)
C(92)	93(7)	93(7)	94(7)	-2(3)	-1(3)	-30(4)
C(93)	93(7)	92(7)	94(7)	-1(3)	-1(3)	-30(4)
C(94)	92(7)	92(7)	93(7)	-1(3)	0(3)	-30(4)
C(95)	92(10)	93(10)	96(10)	4(7)	2(7)	-31(7)
C(96)	98(10)	95(10)	100(10)	1(7)	1(7)	-31(7)
C(97)	71(13)	70(12)	71(12)	0(5)	1(5)	-22(6)
C(98)	68(12)	69(12)	69(12)	0(5)	-1(5)	-21(6)
C(99)	100(19)	99(19)	100(19)	-2(5)	1(5)	-32(7)
C(100)	96(18)	96(18)	97(18)	-2(5)	0(5)	-31(7)
C(101)	100(20)	100(20)	100(20)	-2(5)	-1(5)	-32(8)

C(102)	126(19)	125(19)	126(19)	-3(5)	-1(5)	-40(7)
C(103)	130(20)	130(20)	130(20)	-3(8)	-1(8)	-39(9)
C(104)	140(30)	140(30)	140(30)	-2(10)	-1(10)	-47(14)
C(105)	117(10)	117(10)	116(10)	-3(3)	0(3)	-37(4)
C(106)	117(10)	117(10)	116(10)	-2(3)	0(3)	-37(4)
C(107)	117(10)	117(10)	116(10)	-2(3)	0(3)	-37(4)
C(108)	117(10)	116(10)	116(10)	-2(3)	-1(3)	-37(4)
C(109)	118(10)	117(10)	117(10)	-3(3)	-1(3)	-37(4)
C(110)	117(10)	117(10)	117(10)	-3(3)	0(3)	-37(4)
C(113)	48(9)	52(9)	49(9)	0(5)	3(5)	-13(5)
C(114)	69(12)	69(12)	70(12)	-1(5)	1(5)	-23(6)
C(115)	90(17)	91(17)	90(16)	-2(5)	0(5)	-29(7)
C(116)	64(11)	65(11)	67(11)	-2(5)	-1(5)	-20(6)
C(117)	63(11)	63(11)	64(11)	0(5)	1(5)	-22(6)
C(118)	73(13)	73(13)	73(13)	-1(5)	1(5)	-21(6)
C(119)	73(15)	72(15)	75(15)	9(9)	-3(9)	-21(10)
C(120)	110(20)	110(20)	110(20)	-1(10)	-1(10)	-37(11)
C(121)	150(13)	150(13)	150(13)	-3(3)	-1(3)	-48(5)
C(122)	150(13)	150(13)	150(13)	-3(3)	0(3)	-48(5)
C(123)	150(13)	150(13)	150(13)	-3(3)	-1(3)	-48(5)
C(124)	151(13)	151(13)	151(13)	-3(3)	-1(3)	-48(5)
C(125)	151(13)	151(13)	151(13)	-3(3)	0(3)	-48(5)
C(126)	151(13)	151(13)	151(13)	-3(3)	0(3)	-48(5)
C(129)	103(9)	103(9)	104(8)	-3(3)	0(3)	-33(4)
C(130)	104(9)	105(9)	105(8)	-4(3)	-1(3)	-33(4)
C(131)	105(9)	105(9)	106(8)	-3(3)	-1(3)	-33(4)
C(132)	105(9)	104(9)	106(8)	-3(3)	-1(3)	-33(4)
C(133)	103(9)	103(9)	105(8)	-3(3)	0(3)	-34(4)
C(134)	104(9)	104(9)	105(8)	-3(3)	0(3)	-33(4)
C(135)	110(20)	110(20)	110(20)	-1(10)	0(10)	-36(11)
C(136)	100(20)	100(20)	110(20)	-9(10)	-4(10)	-33(11)
C(137)	78(6)	78(6)	78(6)	-3(3)	0(3)	-25(3)
C(138)	79(6)	80(6)	80(6)	-3(3)	0(3)	-25(4)
C(139)	80(6)	82(6)	81(6)	-3(3)	0(3)	-25(4)
C(140)	81(6)	81(6)	81(6)	-2(3)	0(3)	-25(3)
C(141)	79(6)	79(6)	79(6)	-2(3)	0(3)	-24(3)
C(142)	78(6)	77(6)	77(6)	-3(3)	1(3)	-24(3)
C(143)	74(9)	69(9)	69(9)	-5(7)	6(7)	-23(7)

C(144)	80(9)	80(9)	84(9)	-2(7)	-2(7)	-26(7)
C(145)	66(12)	66(11)	66(11)	0(5)	-1(5)	-23(6)
C(146)	81(14)	80(14)	80(14)	-2(5)	0(5)	-25(6)
C(147)	54(10)	54(10)	54(10)	-1(5)	1(5)	-17(5)
C(148)	120(20)	120(20)	120(20)	-3(5)	0(5)	-38(9)
C(149)	85(16)	86(15)	87(15)	-2(5)	1(5)	-29(7)
C(150)	61(11)	61(11)	62(11)	2(5)	0(5)	-21(6)
C(151)	79(17)	85(17)	87(17)	-3(10)	-5(10)	-29(10)
C(152)	150(40)	150(40)	150(40)	-5(10)	0(10)	-48(15)
C(153)	88(6)	86(6)	87(6)	-2(3)	-1(3)	-28(4)
C(158)	88(6)	87(6)	88(6)	-2(3)	-1(3)	-29(4)
C(157)	89(6)	88(6)	89(6)	-2(3)	-2(3)	-28(4)
C(156)	89(6)	89(6)	89(6)	-1(3)	-1(3)	-28(4)
C(155)	89(6)	88(6)	89(6)	-1(3)	-1(3)	-28(4)
C(154)	88(6)	87(6)	88(6)	-2(3)	0(3)	-28(4)
C(159)	86(10)	87(9)	90(9)	-2(7)	-2(7)	-32(7)
C(160)	90(10)	91(10)	90(10)	2(7)	-3(7)	-27(7)
C(161)	94(7)	93(7)	94(7)	-2(3)	-1(3)	-30(4)
C(162)	93(7)	92(7)	92(7)	-2(3)	-1(3)	-30(4)
C(163)	93(7)	93(7)	93(7)	-2(3)	-1(3)	-30(4)
C(164)	96(7)	94(7)	95(7)	-1(3)	-1(3)	-30(4)
C(165)	96(7)	95(7)	95(7)	-1(3)	-2(3)	-30(4)
C(166)	96(7)	95(7)	95(7)	-1(3)	-2(3)	-30(4)
C(167)	100(10)	95(10)	100(10)	0(7)	-3(7)	-32(7)
C(169)	111(8)	110(8)	111(8)	-3(3)	0(3)	-35(4)
C(170)	111(8)	110(8)	111(8)	-3(3)	0(3)	-35(4)
C(171)	111(8)	111(8)	112(8)	-2(3)	0(3)	-35(4)
C(172)	112(8)	111(8)	112(8)	-2(3)	0(3)	-36(4)
C(173)	112(8)	111(8)	112(8)	-3(3)	0(3)	-35(4)
C(174)	112(8)	111(8)	111(8)	-3(3)	0(3)	-35(4)
C(175)	113(11)	108(11)	112(11)	-3(7)	-1(7)	-37(7)
C(176)	113(11)	114(11)	115(11)	-3(7)	-2(7)	-35(7)
C(177)	83(6)	81(6)	83(6)	-1(3)	0(3)	-26(4)
C(182)	83(6)	82(6)	84(6)	-1(3)	1(3)	-26(3)
C(181)	83(6)	82(6)	84(6)	-1(3)	1(3)	-27(4)
C(180)	84(6)	83(6)	84(6)	-1(3)	0(3)	-27(3)
C(179)	84(6)	83(6)	84(6)	-2(3)	0(3)	-27(4)
C(178)	83(6)	82(6)	84(6)	-2(3)	0(3)	-27(4)

C(183)	81(9)	80(9)	83(9)	0(7)	-1(7)	-23(7)
C(184)	86(9)	84(9)	88(9)	1(7)	0(7)	-26(7)
C(185)	69(12)	69(12)	69(12)	-2(5)	1(5)	-21(6)
C(186)	44(8)	46(8)	46(8)	1(5)	0(5)	-16(5)
C(187)	86(15)	85(15)	84(15)	-2(5)	-1(5)	-27(7)
C(188)	76(13)	75(13)	76(13)	-3(5)	-2(5)	-24(6)
C(189)	74(13)	74(13)	75(13)	-3(5)	0(5)	-24(6)
C(190)	55(10)	57(10)	55(10)	2(5)	2(5)	-18(5)
C(191)	58(12)	53(11)	45(11)	16(8)	5(8)	-21(9)
C(192)	110(20)	110(20)	110(20)	-9(10)	-6(10)	-37(11)
C(193)	122(9)	122(9)	122(9)	-3(3)	0(3)	-39(4)
C(194)	122(9)	122(9)	123(9)	-4(3)	-1(3)	-39(4)
C(195)	123(9)	122(9)	123(9)	-4(3)	-1(3)	-39(4)
C(196)	123(9)	122(9)	123(9)	-3(3)	-1(3)	-39(4)
C(197)	122(9)	122(9)	123(9)	-4(3)	-1(3)	-39(4)
C(198)	122(9)	122(9)	123(9)	-3(3)	0(3)	-39(4)
C(199)	124(12)	123(12)	124(12)	-1(7)	0(7)	-37(7)
C(200)	123(12)	123(12)	122(12)	-2(7)	-3(7)	-39(7)
C(201)	98(7)	97(7)	97(7)	-3(3)	-1(3)	-31(4)
C(206)	100(7)	99(7)	99(7)	-2(3)	-1(3)	-31(4)
C(205)	100(7)	100(7)	99(7)	-2(3)	-1(3)	-31(4)
C(204)	100(7)	100(7)	99(7)	-2(3)	-1(3)	-31(4)
C(203)	98(7)	98(7)	98(7)	-3(3)	-1(3)	-31(4)
C(202)	97(7)	97(7)	97(7)	-3(3)	-1(3)	-31(4)
C(208)	102(10)	103(10)	102(10)	-2(7)	-1(7)	-34(7)
C(112)	150(40)	150(40)	150(40)	-6(10)	-1(10)	-49(14)
C(207)	103(10)	100(10)	101(10)	-5(7)	0(7)	-31(7)
C(168)	98(10)	96(10)	96(10)	3(7)	0(7)	-33(7)
C(16)	162(15)	160(15)	162(15)	-3(7)	-3(7)	-51(8)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Au}_{44}(2,4\text{-DMBT})_{26}$.

	x	y	z	U(eq)
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H(2)	9070	7594	7516	82
H(3)	10112	7120	7087	83
H(5)	10251	8700	6669	85
H(8A)	11281	7170	6601	117
H(8B)	11331	7810	6487	117
H(8C)	10825	7547	6188	117
H(10)	10151	6921	8443	190
H(11)	11152	7135	8757	191
H(13)	10346	6999	10003	190
H(18)	8839	7041	6385	104
H(19)	9859	6598	5929	104
H(21)	9814	8201	5446	106
H(23A)	8110	8933	5815	137
H(23B)	8821	8979	5547	137
H(23C)	8760	9073	6078	137
H(24A)	11127	7011	5509	139
H(24B)	10675	7300	5066	139
H(24C)	10684	6662	5239	139
H(26)	9590	5280	7925	70
H(27)	10290	4283	7935	62
H(29)	11193	4504	6735	111
H(31A)	9922	5812	6450	186
H(31B)	10696	5356	6301	186
H(31C)	10679	5911	6593	186
H(32A)	11699	3456	7486	148
H(32B)	11119	3364	7135	148
H(32C)	10914	3428	7657	148
H(34)	7916	7756	5293	84
H(35)	8781	7313	4741	88
H(37)	7133	7153	3960	84
H(39A)	5590	7530	4592	241
H(39B)	5874	7488	4083	241
H(39C)	5635	8107	4328	241
H(40A)	8752	7117	3769	139
H(40B)	8256	6693	3734	139
H(40C)	8938	6531	4075	139
H(42)	6750	6399	5354	67
H(43)	6515	6089	4649	95

H(45)	8716	5440	4411	91
H(48A)	7082	5374	3970	131
H(48B)	7920	5310	3845	131
H(48C)	7289	5931	3781	131
H(50)	8370	3869	7090	78
H(51)	8141	3024	6847	68
H(53)	8997	3222	5627	90
H(55A)	9663	3895	5508	163
H(55B)	9463	4478	5797	163
H(55C)	8856	4369	5475	163
H(56A)	8620	2116	6308	140
H(56B)	8345	2354	5813	140
H(56C)	7785	2525	6228	140
H(58)	8535	5656	8558	76
H(59)	9386	5431	9071	76
H(61)	9634	3703	8983	79
H(63A)	8211	3634	8401	114
H(63B)	9059	3247	8465	114
H(63C)	8794	3615	8008	114
H(64A)	9915	4642	9764	103
H(64B)	10594	4511	9420	103
H(64C)	10299	3989	9590	103
H(66)	7530	5188	5871	76
H(67)	7626	4917	5072	80
H(69)	6869	3563	5465	55
H(71A)	6621	3817	6592	78
H(71B)	6615	3358	6213	78
H(71C)	5915	3934	6274	78
H(72A)	7362	4178	4489	108
H(72B)	7016	3687	4663	108
H(72C)	7885	3575	4708	108
H(77)	4656	6385	4358	95
H(75)	5947	5055	5139	85
H(74)	5804	5699	5734	93
H(79A)	3833	7255	5135	70
H(79B)	4093	7291	4626	70
H(79C)	4487	7518	5021	70
H(80A)	4965	5413	4085	70

H(80B)	5519	4867	4354	70
H(80C)	5832	5325	4088	70
H(82)	4800	4842	7100	67
H(83)	4220	4266	7506	70
H(85)	2229	5298	7043	69
H(87A)	2718	6439	6612	84
H(87B)	2157	6098	6477	84
H(87C)	2900	6009	6194	84
H(88A)	3090	4145	7833	106
H(88B)	2377	4335	7516	106
H(88C)	2488	4781	7879	106
H(90)	6525	4776	7485	110
H(91)	7066	3755	7465	111
H(93)	5501	3554	8324	112
H(95A)	4815	4925	8684	140
H(95B)	4633	4321	8647	140
H(95C)	4281	4850	8296	140
H(96A)	6716	2923	7414	146
H(96B)	6377	2691	7845	146
H(96C)	7179	2766	7870	146
H(98)	6534	5531	8735	82
H(99)	6523	4563	8681	120
H(101)	7964	4069	9717	124
H(10A)	8390	5260	9937	193
H(10B)	8502	4581	10044	193
H(10C)	7801	5077	10241	193
H(10D)	6867	3518	9347	213
H(10E)	7629	3327	9074	213
H(10F)	6871	3655	8819	213
H(106)	6040	6244	10646	140
H(107)	6254	6284	11414	140
H(109)	4840	7950	11431	141
H(114)	3212	5773	8579	83
H(115)	2550	5308	9034	109
H(117)	873	5762	8134	76
H(11A)	1124	6834	7673	111
H(11B)	971	6285	7448	111
H(11C)	1712	6434	7331	111

H(12A)	1489	4908	9055	161
H(12B)	866	5124	8676	161
H(12C)	881	5544	9082	161
H(123)	5085	5272	9308	180
H(125)	3108	6331	9753	182
H(130)	2098	9505	8178	126
H(131)	1011	10275	8021	126
H(133)	-116	9107	7952	125
H(13A)	1433	7809	7897	165
H(13B)	576	8078	7770	165
H(13C)	816	7891	8279	165
H(13D)	-400	10384	8439	158
H(13E)	-849	10077	8133	158
H(13F)	-582	10598	7928	158
H(138)	3598	8637	9178	96
H(139)	2330	9128	9102	98
H(141)	2576	10541	9718	95
H(14A)	4128	9983	10164	106
H(14B)	3806	10553	9846	106
H(14C)	4495	10018	9683	106
H(14D)	1408	10194	9002	122
H(14E)	1391	10604	9420	122
H(14F)	1223	9996	9494	122
H(146)	3029	7514	6360	96
H(147)	2824	7336	5612	65
H(149)	1216	8916	5521	103
H(15A)	1179	9206	6663	125
H(15B)	758	9414	6197	125
H(15C)	1481	9585	6308	125
H(15D)	2206	7750	4860	232
H(15E)	1811	8447	4842	232
H(15F)	1342	8019	4968	232
H(157)	2087	11607	7732	107
H(155)	4112	11813	7734	107
H(154)	4566	10956	8175	105
H(15G)	2642	10206	8152	130
H(15H)	1993	10719	7914	130
H(15I)	2112	10723	8445	130

H(16A)	2252	12352	7316	136
H(16B)	3029	12470	7272	136
H(16C)	2533	12665	7712	136
H(162)	2822	9566	6216	111
H(163)	2573	9852	5463	111
H(165)	2990	11373	5694	114
H(16D)	3010	11290	6887	147
H(16E)	3283	11636	6493	147
H(16F)	3849	11057	6718	147
H(170)	7061	9662	8066	133
H(171)	7581	10293	7677	133
H(173)	6972	11458	8682	134
H(17A)	5716	10930	9143	166
H(17B)	6291	11227	9332	166
H(17C)	6414	10544	9429	166
H(17D)	8143	11406	8033	172
H(17E)	7390	11730	7772	172
H(17F)	7964	11147	7575	172
H(181)	6587	11128	6807	99
H(179)	7179	9464	6352	101
H(178)	6364	9243	6863	99
H(18A)	5244	11298	7473	123
H(18B)	6025	11412	7448	123
H(18C)	5904	10933	7796	123
H(18D)	7378	10619	5988	129
H(18E)	7913	10007	6184	129
H(18F)	7838	10603	6437	129
H(186)	3937	8341	6200	54
H(187)	3390	8431	5492	102
H(189)	4534	9510	5078	88
H(19A)	4915	9896	6017	77
H(19B)	5265	9772	5525	77
H(19C)	5650	9354	5940	77
H(19D)	3829	8527	4603	161
H(19E)	3573	9224	4523	161
H(19F)	3033	8925	4772	161
H(194)	7861	9509	9293	147
H(195)	7944	10449	9395	147

H(197)	10177	9768	9426	147
H(19G)	10330	8316	9506	187
H(19H)	10678	8623	9121	187
H(19I)	10022	8370	9004	187
H(20B)	9440	10897	9752	184
H(20C)	8806	11189	9392	184
H(20A)	9635	10870	9228	184
H(205)	7187	7554	11393	120
H(203)	8071	6280	10492	118
H(202)	7664	6968	9904	116
H(20D)	8475	6562	11441	153
H(20E)	7984	6137	11388	153
H(20F)	7665	6734	11657	153
H(11D)	5388	6851	12125	228
H(11E)	5085	7549	12054	228
H(11F)	5952	7221	12111	228
H(20G)	6510	8756	10527	152
H(20H)	6607	8694	11060	152
H(20I)	5966	8511	10825	152
H(16G)	2955	10415	4860	144
H(16H)	3118	11009	4976	144
H(16I)	2284	11010	4925	144
H(16J)	11917	6636	9227	242
H(16K)	11849	6848	9735	242
H(16L)	11797	7311	9332	242

Table S6. Torsion angles [°] for Au₄₄(2,4-DMBT)₂₆.

Au(3)-S(12)-C(89)-C(90)	24.2
Au(3)-S(12)-C(89)-C(94)	-167.3
Au(4)-S(8)-C(57)-C(58)	-0.1
Au(4)-S(8)-C(57)-C(62)	174.6
Au(5)-S(13)-C(97)-C(98)	-19.1
Au(5)-S(13)-C(97)-C(102)	158.3
Au(9)-S(16)-C(121)-C(122)	58.2
Au(9)-S(16)-C(121)-C(126)	-121.5
Au(10)-S(17)-C(129)-C(130)	-39.3
Au(10)-S(17)-C(129)-C(134)	142.1
Au(11)-S(19)-C(145)-C(146)	20.1
Au(11)-S(19)-C(145)-C(150)	-164.0
Au(12)-S(11)-C(81)-C(82)	-87.6
Au(12)-S(11)-C(81)-C(86)	87.4
Au(13)-S(12)-C(89)-C(90)	131.9
Au(13)-S(12)-C(89)-C(94)	-59.7
Au(13)-S(15)-C(113)-C(114)	25.6
Au(13)-S(15)-C(113)-C(118)	-154.4
Au(14)-S(15)-C(113)-C(114)	-84.0
Au(14)-S(15)-C(113)-C(118)	96.0
Au(14)-S(17)-C(129)-C(130)	-145.9
Au(14)-S(17)-C(129)-C(134)	35.6
Au(15)-S(19)-C(145)-C(146)	118.3
Au(15)-S(19)-C(145)-C(150)	-65.8
Au(15)-S(21)-C(161)-C(162)	5.5
Au(15)-S(21)-C(161)-C(166)	173.1
Au(16)-S(21)-C(161)-C(162)	120.7
Au(16)-S(21)-C(161)-C(166)	-71.7
Au(16)-S(23)-C(177)-C(182)	103.1
Au(16)-S(23)-C(177)-C(178)	-77.8
Au(17)-S(24)-C(185)-C(186)	-39.5
Au(17)-S(24)-C(185)-C(190)	145.7
Au(18)-S(20)-C(153)-C(158)	77.3
Au(18)-S(20)-C(153)-C(154)	-100.9
Au(19)-S(23)-C(177)-C(182)	-141.1
Au(19)-S(23)-C(177)-C(178)	38.0

Au(20)-S(20)-C(153)-C(158)	178.2
Au(20)-S(20)-C(153)-C(154)	0.0
Au(20)-S(22)-C(169)-C(170)	-89.8
Au(20)-S(22)-C(169)-C(174)	96.0
Au(21)-S(22)-C(169)-C(170)	14.9
Au(21)-S(22)-C(169)-C(174)	-159.4
Au(22)-S(18)-C(137)-C(138)	52.0
Au(22)-S(18)-C(137)-C(142)	-124.3
Au(23)-S(26)-C(201)-C(206)	-145.1
Au(23)-S(26)-C(201)-C(202)	32.9
Au(24)-S(25)-C(193)-C(194)	-38.8
Au(24)-S(25)-C(193)-C(198)	151.0
Au(24)-S(26)-C(201)-C(206)	116.6
Au(24)-S(26)-C(201)-C(202)	-65.3
Au(25)-S(14)-C(105)-C(106)	-144.6
Au(25)-S(14)-C(105)-C(110)	37.5
Au(25)-S(18)-C(137)-C(138)	-42.6
Au(25)-S(18)-C(137)-C(142)	141.1
Au(26)-S(13)-C(97)-C(98)	73.9
Au(26)-S(13)-C(97)-C(102)	-108.7
Au(26)-S(14)-C(105)-C(106)	-47.0
Au(26)-S(14)-C(105)-C(110)	135.2
Au(27)-S(16)-C(121)-C(122)	-48.5
Au(27)-S(16)-C(121)-C(126)	131.8
Au(28)-S(9)-C(65)-C(66)	11.5
Au(28)-S(9)-C(65)-C(70)	178.4
Au(29)-S(10)-C(73)-C(78)	-171.3
Au(29)-S(10)-C(73)-C(74)	11.9
Au(30)-S(6)-C(41)-C(42)	2.8
Au(30)-S(6)-C(41)-C(46)	179.2
Au(31)-S(5)-C(33)-C(34)	-120.4
Au(31)-S(5)-C(33)-C(38)	63.4
Au(31)-S(10)-C(73)-C(78)	-76.4
Au(31)-S(10)-C(73)-C(74)	106.7
Au(32)-S(24)-C(185)-C(186)	72.2
Au(32)-S(24)-C(185)-C(190)	-102.7
Au(33)-S(3)-C(17)-C(18)	-86.4
Au(33)-S(3)-C(17)-C(22)	90.9

Au(33)-S(5)-C(33)-C(34)	-14.8
Au(33)-S(5)-C(33)-C(38)	169.0
Au(34)-S(6)-C(41)-C(42)	106.8
Au(34)-S(6)-C(41)-C(46)	-76.8
Au(34)-S(7)-C(49)-C(50)	-119.9
Au(34)-S(7)-C(49)-C(54)	66.3
Au(35)-S(4)-C(25)-C(26)	-68.3
Au(35)-S(4)-C(25)-C(30)	105.5
Au(37)-S(3)-C(17)-C(18)	0.9
Au(37)-S(3)-C(17)-C(22)	178.2
Au(38)-S(1)-C(1)-C(2)	-23.9
Au(38)-S(1)-C(1)-C(6)	152.4
Au(40)-S(1)-C(1)-C(2)	64.5
Au(40)-S(1)-C(1)-C(6)	-119.2
Au(40)-S(25)-C(193)-C(194)	64.2
Au(40)-S(25)-C(193)-C(198)	-106.1
Au(41)-S(2)-C(9)-C(10)	17.0
Au(41)-S(2)-C(9)-C(14)	-167.3
Au(41)-S(4)-C(25)-C(26)	28.8
Au(41)-S(4)-C(25)-C(30)	-157.5
Au(42)-S(7)-C(49)-C(50)	-19.1
Au(42)-S(7)-C(49)-C(54)	167.1
Au(42)-S(8)-C(57)-C(58)	95.0
Au(42)-S(8)-C(57)-C(62)	-90.4
Au(43)-S(9)-C(65)-C(66)	106.3
Au(43)-S(9)-C(65)-C(70)	-86.7
Au(43)-S(11)-C(81)-C(82)	11.0
Au(43)-S(11)-C(81)-C(86)	-174.0
Au(44)-S(2)-C(9)-C(10)	-90.5
Au(44)-S(2)-C(9)-C(14)	85.2
S(1)-C(1)-C(2)-C(3)	176.3
S(1)-C(1)-C(6)-C(5)	-176.4
S(1)-C(1)-C(6)-C(7)	-5.0
S(2)-C(9)-C(10)-C(11)	175.9
S(2)-C(9)-C(14)-C(13)	-175.5
S(2)-C(9)-C(14)-C(15)	18.6
S(3)-C(17)-C(18)-C(19)	177.3
S(3)-C(17)-C(22)-C(21)	-177.2

S(3)-C(17)-C(22)-C(23)	-6.6
S(4)-C(25)-C(26)-C(27)	173.6
S(4)-C(25)-C(30)-C(29)	-173.8
S(4)-C(25)-C(30)-C(31)	-3.7
S(5)-C(33)-C(34)-C(35)	-176.3
S(5)-C(33)-C(38)-C(37)	176.2
S(5)-C(33)-C(38)-C(39)	5.0
S(6)-C(41)-C(42)-C(43)	176.3
S(6)-C(41)-C(46)-C(45)	-176.5
S(6)-C(41)-C(46)-C(47)	1.4
S(7)-C(49)-C(50)-C(51)	-173.6
S(7)-C(49)-C(54)-C(53)	174.0
S(7)-C(49)-C(54)-C(55)	-14.8
S(8)-C(57)-C(58)-C(59)	176.3
S(8)-C(57)-C(62)-C(61)	-174.6
S(8)-C(57)-C(62)-C(63)	4.8
S(9)-C(65)-C(66)-C(67)	179.2
S(9)-C(65)-C(70)-C(69)	-173.3
S(9)-C(65)-C(70)-C(71)	5.4
S(10)-C(73)-C(78)-C(77)	-176.9
S(10)-C(73)-C(78)-C(79)	-6.3
S(10)-C(73)-C(74)-C(75)	176.8
S(11)-C(81)-C(82)-C(83)	175.1
S(11)-C(81)-C(86)-C(85)	-174.9
S(11)-C(81)-C(86)-C(87)	8.2
S(12)-C(89)-C(90)-C(91)	168.6
S(12)-C(89)-C(94)-C(93)	-168.2
S(12)-C(89)-C(94)-C(95)	9.1
S(13)-C(97)-C(98)-C(99)	177.3
S(13)-C(97)-C(102)-C(101)	-177.5
S(13)-C(97)-C(102)-C(103)	11.6
S(14)-C(105)-C(106)-C(107)	-177.8
S(14)-C(105)-C(110)-C(109)	177.8
S(15)-C(113)-C(114)-C(115)	-180.0
S(15)-C(113)-C(118)-C(117)	180.0
S(15)-C(113)-C(118)-C(119)	-11.9
S(16)-C(121)-C(122)-C(123)	-179.6
S(16)-C(121)-C(126)-C(125)	179.7

S(17)-C(129)-C(130)-C(131)	-178.6
S(17)-C(129)-C(134)-C(133)	178.5
S(17)-C(129)-C(134)-C(135)	-16.0
S(18)-C(137)-C(138)-C(139)	-176.3
S(18)-C(137)-C(142)-C(141)	176.3
S(18)-C(137)-C(142)-C(143)	-2.4
S(19)-C(145)-C(146)-C(147)	176.0
S(19)-C(145)-C(150)-C(149)	-175.8
S(19)-C(145)-C(150)-C(151)	1.8
S(20)-C(153)-C(158)-C(157)	-178.1
S(20)-C(153)-C(158)-C(159)	-6.6
S(20)-C(153)-C(154)-C(155)	178.1
S(21)-C(161)-C(162)-C(163)	168.0
S(21)-C(161)-C(166)-C(165)	-167.1
S(21)-C(161)-C(166)-C(167)	12.2
S(22)-C(169)-C(170)-C(171)	-174.2
S(22)-C(169)-C(174)-C(173)	174.3
S(22)-C(169)-C(174)-C(175)	-12.1
S(23)-C(177)-C(182)-C(181)	179.1
S(23)-C(177)-C(182)-C(183)	15.0
S(23)-C(177)-C(178)-C(179)	-179.0
S(24)-C(185)-C(186)-C(187)	-174.8
S(24)-C(185)-C(190)-C(189)	174.9
S(24)-C(185)-C(190)-C(191)	-13.0
S(25)-C(193)-C(194)-C(195)	-170.1
S(25)-C(193)-C(198)-C(197)	170.3
S(25)-C(193)-C(198)-C(199)	-1.7
S(26)-C(201)-C(206)-C(205)	178.0
S(26)-C(201)-C(206)-C(207)	7.0
S(26)-C(201)-C(202)-C(203)	-178.1
C(1)-C(2)-C(3)-C(4)	0.0
C(2)-C(1)-C(6)-C(5)	0.0
C(2)-C(1)-C(6)-C(7)	171.4
C(2)-C(3)-C(4)-C(5)	0.0
C(2)-C(3)-C(4)-C(8)	-176.3
C(3)-C(4)-C(5)-C(6)	0.0
C(4)-C(5)-C(6)-C(1)	0.0
C(4)-C(5)-C(6)-C(7)	-170.6

C(6)-C(1)-C(2)-C(3)	0.0
C(8)-C(4)-C(5)-C(6)	176.6
C(9)-C(10)-C(11)-C(12)	0.0
C(10)-C(9)-C(14)-C(13)	0.0
C(10)-C(9)-C(14)-C(15)	-165.9
C(10)-C(11)-C(12)-C(13)	0.0
C(10)-C(11)-C(12)-C(16)	155.9
C(11)-C(12)-C(13)-C(14)	0.0
C(12)-C(13)-C(14)-C(9)	0.0
C(12)-C(13)-C(14)-C(15)	161.4
C(14)-C(9)-C(10)-C(11)	0.0
C(17)-C(18)-C(19)-C(20)	0.0
C(18)-C(17)-C(22)-C(21)	0.0
C(18)-C(17)-C(22)-C(23)	170.5
C(18)-C(19)-C(20)-C(21)	0.0
C(18)-C(19)-C(20)-C(24)	177.4
C(19)-C(20)-C(21)-C(22)	0.0
C(20)-C(21)-C(22)-C(17)	0.0
C(20)-C(21)-C(22)-C(23)	-171.1
C(22)-C(17)-C(18)-C(19)	0.0
C(24)-C(20)-C(21)-C(22)	-177.5
C(25)-C(26)-C(27)-C(28)	0.0
C(26)-C(25)-C(30)-C(29)	0.0
C(26)-C(25)-C(30)-C(31)	170.1
C(26)-C(27)-C(28)-C(29)	0.0
C(26)-C(27)-C(28)-C(32)	-174.4
C(27)-C(28)-C(29)-C(30)	0.0
C(28)-C(29)-C(30)-C(25)	0.0
C(28)-C(29)-C(30)-C(31)	-170.3
C(30)-C(25)-C(26)-C(27)	0.0
C(32)-C(28)-C(29)-C(30)	173.1
C(33)-C(34)-C(35)-C(36)	0.0
C(34)-C(33)-C(38)-C(37)	0.0
C(34)-C(33)-C(38)-C(39)	-171.1
C(34)-C(35)-C(36)-C(37)	0.0
C(34)-C(35)-C(36)-C(40)	-174.1
C(35)-C(36)-C(37)-C(38)	0.0
C(36)-C(37)-C(38)-C(33)	0.0

C(36)-C(37)-C(38)-C(39)	172.4
C(38)-C(33)-C(34)-C(35)	0.0
C(40)-C(36)-C(37)-C(38)	174.7
C(41)-C(42)-C(43)-C(44)	0.0
C(42)-C(41)-C(46)-C(45)	0.0
C(42)-C(41)-C(46)-C(47)	177.8
C(42)-C(43)-C(44)-C(45)	0.0
C(42)-C(43)-C(44)-C(48)	-174.2
C(43)-C(44)-C(45)-C(46)	0.0
C(44)-C(45)-C(46)-C(41)	0.0
C(44)-C(45)-C(46)-C(47)	-178.0
C(46)-C(41)-C(42)-C(43)	0.0
C(48)-C(44)-C(45)-C(46)	174.4
C(49)-C(50)-C(51)-C(52)	0.0
C(50)-C(49)-C(54)-C(53)	0.0
C(50)-C(49)-C(54)-C(55)	171.2
C(50)-C(51)-C(52)-C(53)	0.0
C(50)-C(51)-C(52)-C(56)	-178.3
C(51)-C(52)-C(53)-C(54)	0.0
C(52)-C(53)-C(54)-C(49)	0.0
C(52)-C(53)-C(54)-C(55)	-172.5
C(54)-C(49)-C(50)-C(51)	0.0
C(56)-C(52)-C(53)-C(54)	177.9
C(57)-C(58)-C(59)-C(60)	-2.8
C(58)-C(57)-C(62)-C(61)	0.4
C(58)-C(57)-C(62)-C(63)	179.8
C(58)-C(59)-C(60)-C(61)	2.8
C(58)-C(59)-C(60)-C(64)	-175.1
C(59)-C(60)-C(61)-C(62)	-1.3
C(60)-C(61)-C(62)-C(57)	-0.2
C(60)-C(61)-C(62)-C(63)	-179.7
C(62)-C(57)-C(58)-C(59)	1.1
C(64)-C(60)-C(61)-C(62)	176.7
C(65)-C(66)-C(67)-C(68)	-12.4
C(66)-C(65)-C(70)-C(69)	-8.5
C(66)-C(65)-C(70)-C(71)	170.2
C(66)-C(67)-C(68)-C(69)	5.1
C(66)-C(67)-C(68)-C(72)	-176.5

C(67)-C(68)-C(69)-C(70)	1.7
C(68)-C(69)-C(70)-C(65)	-1.0
C(68)-C(69)-C(70)-C(71)	-179.8
C(70)-C(65)-C(66)-C(67)	15.4
C(72)-C(68)-C(69)-C(70)	-176.7
C(73)-C(78)-C(77)-C(76)	0.0
C(78)-C(73)-C(74)-C(75)	0.0
C(78)-C(77)-C(76)-C(75)	0.0
C(78)-C(77)-C(76)-C(80)	-175.8
C(77)-C(76)-C(75)-C(74)	0.0
C(76)-C(75)-C(74)-C(73)	0.0
C(74)-C(73)-C(78)-C(77)	0.0
C(74)-C(73)-C(78)-C(79)	170.6
C(79)-C(78)-C(77)-C(76)	-171.0
C(80)-C(76)-C(75)-C(74)	175.5
C(81)-C(82)-C(83)-C(84)	0.0
C(82)-C(81)-C(86)-C(85)	0.0
C(82)-C(81)-C(86)-C(87)	-177.0
C(82)-C(83)-C(84)-C(85)	0.0
C(82)-C(83)-C(84)-C(88)	-163.3
C(83)-C(84)-C(85)-C(86)	0.0
C(84)-C(85)-C(86)-C(81)	0.0
C(84)-C(85)-C(86)-C(87)	176.7
C(86)-C(81)-C(82)-C(83)	0.0
C(88)-C(84)-C(85)-C(86)	164.2
C(89)-C(90)-C(91)-C(92)	0.0
C(90)-C(89)-C(94)-C(93)	0.0
C(90)-C(89)-C(94)-C(95)	177.3
C(90)-C(91)-C(92)-C(93)	0.0
C(90)-C(91)-C(92)-C(96)	167.7
C(91)-C(92)-C(93)-C(94)	0.0
C(92)-C(93)-C(94)-C(89)	0.0
C(92)-C(93)-C(94)-C(95)	-177.4
C(94)-C(89)-C(90)-C(91)	0.0
C(96)-C(92)-C(93)-C(94)	-164.8
C(97)-C(98)-C(99)-C(100)	0.0
C(98)-C(97)-C(102)-C(101)	0.0
C(98)-C(97)-C(102)-C(103)	-170.9

C(98)-C(99)-C(100)-C(101)	0.0
C(98)-C(99)-C(100)-C(104)	179.4
C(99)-C(100)-C(101)-C(102)	0.0
C(100)-C(101)-C(102)-C(97)	0.0
C(100)-C(101)-C(102)-C(103)	173.0
C(102)-C(97)-C(98)-C(99)	0.0
C(104)-C(100)-C(101)-C(102)	-179.3
C(105)-C(106)-C(107)-C(108)	0.0
C(106)-C(105)-C(110)-C(109)	0.0
C(106)-C(107)-C(108)-C(109)	0.0
C(106)-C(107)-C(108)-C(112)	164.8
C(107)-C(108)-C(109)-C(110)	0.0
C(108)-C(109)-C(110)-C(105)	0.0
C(110)-C(105)-C(106)-C(107)	0.0
C(113)-C(114)-C(115)-C(116)	0.0
C(114)-C(113)-C(118)-C(117)	0.0
C(114)-C(113)-C(118)-C(119)	168.1
C(114)-C(115)-C(116)-C(117)	0.0
C(114)-C(115)-C(116)-C(120)	-177.3
C(115)-C(116)-C(117)-C(118)	0.0
C(116)-C(117)-C(118)-C(113)	0.0
C(116)-C(117)-C(118)-C(119)	-168.1
C(118)-C(113)-C(114)-C(115)	0.0
C(120)-C(116)-C(117)-C(118)	177.6
C(121)-C(122)-C(123)-C(124)	0.0
C(122)-C(121)-C(126)-C(125)	0.0
C(122)-C(123)-C(124)-C(125)	0.0
C(123)-C(124)-C(125)-C(126)	0.0
C(124)-C(125)-C(126)-C(121)	0.0
C(126)-C(121)-C(122)-C(123)	0.0
C(129)-C(130)-C(131)-C(132)	0.0
C(130)-C(129)-C(134)-C(133)	0.0
C(130)-C(129)-C(134)-C(135)	165.5
C(130)-C(131)-C(132)-C(133)	0.0
C(130)-C(131)-C(132)-C(136)	146.9
C(131)-C(132)-C(133)-C(134)	0.0
C(132)-C(133)-C(134)-C(129)	0.0
C(132)-C(133)-C(134)-C(135)	-166.5

C(134)-C(129)-C(130)-C(131)	0.0
C(136)-C(132)-C(133)-C(134)	-148.8
C(137)-C(138)-C(139)-C(140)	0.0
C(138)-C(137)-C(142)-C(141)	0.0
C(138)-C(137)-C(142)-C(143)	-178.7
C(138)-C(139)-C(140)-C(141)	0.0
C(138)-C(139)-C(140)-C(144)	176.5
C(139)-C(140)-C(141)-C(142)	0.0
C(140)-C(141)-C(142)-C(137)	0.0
C(140)-C(141)-C(142)-C(143)	178.6
C(142)-C(137)-C(138)-C(139)	0.0
C(144)-C(140)-C(141)-C(142)	-176.3
C(145)-C(146)-C(147)-C(148)	0.0
C(146)-C(145)-C(150)-C(149)	0.0
C(146)-C(145)-C(150)-C(151)	177.7
C(146)-C(147)-C(148)-C(149)	0.0
C(146)-C(147)-C(148)-C(152)	176.4
C(147)-C(148)-C(149)-C(150)	0.0
C(148)-C(149)-C(150)-C(145)	0.0
C(148)-C(149)-C(150)-C(151)	-177.7
C(150)-C(145)-C(146)-C(147)	0.0
C(152)-C(148)-C(149)-C(150)	-176.9
C(153)-C(158)-C(157)-C(156)	0.0
C(158)-C(153)-C(154)-C(155)	0.0
C(158)-C(157)-C(156)-C(155)	0.0
C(158)-C(157)-C(156)-C(160)	-170.3
C(157)-C(156)-C(155)-C(154)	0.0
C(156)-C(155)-C(154)-C(153)	0.0
C(154)-C(153)-C(158)-C(157)	0.0
C(154)-C(153)-C(158)-C(159)	171.5
C(159)-C(158)-C(157)-C(156)	-172.2
C(160)-C(156)-C(155)-C(154)	169.4
C(161)-C(162)-C(163)-C(164)	0.0
C(162)-C(161)-C(166)-C(165)	0.0
C(162)-C(161)-C(166)-C(167)	179.3
C(162)-C(163)-C(164)-C(165)	0.0
C(162)-C(163)-C(164)-C(168)	165.4
C(163)-C(164)-C(165)-C(166)	0.0

C(164)-C(165)-C(166)-C(161)	0.0
C(164)-C(165)-C(166)-C(167)	-179.3
C(166)-C(161)-C(162)-C(163)	0.0
C(169)-C(170)-C(171)-C(172)	0.0
C(170)-C(169)-C(174)-C(173)	0.0
C(170)-C(169)-C(174)-C(175)	173.7
C(170)-C(171)-C(172)-C(173)	0.0
C(170)-C(171)-C(172)-C(176)	177.2
C(171)-C(172)-C(173)-C(174)	0.0
C(172)-C(173)-C(174)-C(169)	0.0
C(172)-C(173)-C(174)-C(175)	-173.0
C(174)-C(169)-C(170)-C(171)	0.0
C(176)-C(172)-C(173)-C(174)	-177.0
C(177)-C(182)-C(181)-C(180)	0.0
C(182)-C(177)-C(178)-C(179)	0.0
C(182)-C(181)-C(180)-C(179)	0.0
C(182)-C(181)-C(180)-C(184)	-168.6
C(181)-C(180)-C(179)-C(178)	0.0
C(180)-C(179)-C(178)-C(177)	0.0
C(178)-C(177)-C(182)-C(181)	0.0
C(178)-C(177)-C(182)-C(183)	-164.1
C(183)-C(182)-C(181)-C(180)	166.4
C(184)-C(180)-C(179)-C(178)	169.3
C(185)-C(186)-C(187)-C(188)	0.0
C(186)-C(185)-C(190)-C(189)	0.0
C(186)-C(185)-C(190)-C(191)	172.1
C(186)-C(187)-C(188)-C(189)	0.0
C(186)-C(187)-C(188)-C(192)	172.3
C(187)-C(188)-C(189)-C(190)	0.0
C(188)-C(189)-C(190)-C(185)	0.0
C(188)-C(189)-C(190)-C(191)	-172.5
C(190)-C(185)-C(186)-C(187)	0.0
C(192)-C(188)-C(189)-C(190)	-170.9
C(193)-C(194)-C(195)-C(196)	0.0
C(194)-C(193)-C(198)-C(197)	0.0
C(194)-C(193)-C(198)-C(199)	-172.0
C(194)-C(195)-C(196)-C(197)	0.0
C(194)-C(195)-C(196)-C(200)	174.4

C(195)-C(196)-C(197)-C(198)	0.0
C(196)-C(197)-C(198)-C(193)	0.0
C(196)-C(197)-C(198)-C(199)	169.3
C(198)-C(193)-C(194)-C(195)	0.0
C(200)-C(196)-C(197)-C(198)	-175.2
C(201)-C(206)-C(205)-C(204)	0.0
C(206)-C(201)-C(202)-C(203)	0.0
C(206)-C(205)-C(204)-C(203)	0.0
C(206)-C(205)-C(204)-C(208)	169.3
C(205)-C(204)-C(203)-C(202)	0.0
C(204)-C(203)-C(202)-C(201)	0.0
C(202)-C(201)-C(206)-C(205)	0.0
C(202)-C(201)-C(206)-C(207)	-171.0
C(208)-C(204)-C(203)-C(202)	-166.9
C(112)-C(108)-C(109)-C(110)	-167.3
C(207)-C(206)-C(205)-C(204)	169.9
C(168)-C(164)-C(165)-C(166)	-166.2
C(16)-C(12)-C(13)-C(14)	-144.1
