Supporting Information

Heavily doped $Au_{25-x}Ag_x(SC_6H_{11})_{18}^-$ nanoclusters: silver goes from core to surface

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Experimental

Synthesis of $Au_{23}(SC_6H_{11})_{16}^-$

$Au_{23}(SC_6H_{11})_{16}^-$ cluster was synthesized by a previously reported method. $HAuCl_4 \cdot 3H_2O$ (0.3 mmol, 118 mg) and tetraoctylammonium bromide (TOAB, 0.348 mmol, 190 mg) were dissolved in methanol (15 mL) in a round-bottom flask. After vigorously stirring for 15 min, the solution color changed from yellow to dark reddish orange. Then, excess 1-cyclohexanethiol (1.6 mmol, 196 μL) was added to the mixture at room temperature. The reddish orange solution turned yellowish immediately, indicating the conversion of Au(III) to Au(I) complexes. After ~15 min, $NaBH_4$ (3 mmol, 114 mg dissolved freshly in 6 mL of cold Nanopure water) was rapidly added to the solution under vigorous stirring. The solution turned black immediately, indicating formation of Au clusters. The clusters spontaneously precipitated out of the methanol solution. The reaction mixture was stirred overnight and finally gave rise to pure $[Au_{23}(c\text{-}C_6)_{16}]^-$ nanoclusters. After washing with ethanol for at least 5 times, 20 mg $[Au_{23}(c\text{-}C_6)_{16}]^-$ nanoclusters were dissolved in dichloromethane.

Synthesis of Ag(1)-cyclohexanethiolate

1 mL solution of $AgNO_3$ (1g dissolved in 5 mL methanol) was mixed with another methanol solution (7 mL) containing cyclohexane (0.7 mL) under vigorous stirring for 30 mins. After centrifugation at ~6500 rpm, the solution was then removed and the precipitate was washed several times with ethanol/water to remove the redundant cyclohexanethiol. The Ag-cyclohexanethiol (solid) was obtained.

Reaction of Ag(1)-cyclohexanethiol with $Au_{23}(SC_6H_{11})_{16}^-$

20 mg $[Au_{23}(c\text{-}C_6H_{11})_{16}]^-$ was dissolved in 3 ml dichloromethane, and Ag(1)-cyclohexanethiol (powder) was added to the solution. The reaction was allowed to proceed for 4 hr at room temperature. The mixture was taken to a centrifuge tube and centrifuged at ~10000 rpm to remove excess Ag(I)-cyclohexanethiol and byproducts. The alloy clusters were then crystallized in a dichloromethane-acetonitrile (3:2) mixed solvent.

Characterization

UV-vis spectra of the Au clusters (dissolved in CH_2Cl_2) were acquired on Hewlett-Packard (HP) Agilent 8453 diode array spectrophotometer and Varian Cary 5000 at room temperature. Energy dispersive X-ray spectroscopy (EDX) was conducted on a JOEL JSM-7500F Field Emission Scanning Electron Microscope equipped with an EDX Detector (Bruker AXS: XFlash Detector 5010).

X-ray crystallography

The total exposure time was 41.46 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 53704 reflections to a maximum θ angle of 62.50° (0.87 Å resolution), of which 53704 were independent (average redundancy 1.000, completeness = 94.7%, R_{int} = 13.19%, R_{sig} = 12.61% indicating poor quality data) and 34471 (64.19%) were greater than $2\sigma(F^2)$. The final cell constants of $\underline{a}$ = 17.0545(11) Å, $\underline{b}$ = 29.3289(19) Å, $\underline{c}$ = 35.668(2) Å, α = 85.911(4)°, β = 89.317(4)°, γ = 86.562(4)°, volume = 17763.(2) $Å^3$, are based upon the refinement of the XYZ-centroids of 9966 reflections above 20 σ(I) with 5.625° < 2θ < 133.3°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.268.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 4 for the formula unit, $C_{140}H_{266}Ag_{19.40}Au_{5.60}NS_{18}$. The final anisotropic full-matrix least-squares refinement on F^2 with 1850 variables converged at R1 = 11.59%, for the observed data and wR2 = 33.20% for all data. The goodness-of-fit was 1.092. The largest peak in the final difference electron density synthesis was 11.401 $e^-/Å^3$ and the largest hole was -4.571 $e^-/Å^3$ with an RMS deviation of 0.558 $e^-/Å^3$. On the basis of the final model, the calculated density was 2.145 g/cm^3 and F(000), 11021 e^-.

There are three crystallographically independent $[(Au,Ag)_{25}(SC_6H_{11})_{18}]^-$ anions. One is located on a general position, the other two are located over inversion centers with the central gold atoms Au26 and Au39 on (0.0, 0.5, 1.0) and (0.0, 0.5, 0.5), respectively. All heavy metal atoms, S, N, and C -atoms were obtained by direct methods and subsequent difference Fourier techniques. During initial refinements almost 300 restraints and constraints were used (EXYZ, EADP, SIMU, SADI), during successive refinements more than 80% could be released. H-atoms were geometrically determined and included in the final refinements as riding atoms with the exception of disordered H-atoms. Au, Ag, S and N atoms were refined with anisotropic displacement parameters. All C-atoms were refined with isotropic displacement parameters, one cyclohexyl-ring is disordered over 2 positions with equal occupancies.

The occupancies of the Au and Ag atoms were refined revealing compositional disorder for most of the heavy metal positions, with the exception that in all three clusters, the central atoms are 100% Au atoms and each staple has one metal atom with a 100% Ag occupancy. However, crystallographically, occupancies of 0.97(2) Ag and 0.03(2) Au could not be distinguished from 100% Ag, therefore the occupancies were fixed to an approximate value.

One of the $[N(C_8H_{17})_4]^+$ cations was located by subsequent difference Fourier techniques on a general position and refined. However, the other cations and potential solvent molecules could not be identified from the X-ray structure data. Although several aliphatic C-chain fragments were identified, no chemically reasonable model could be established. These cations are disordered over the inversion center. PLATON[s1] was used to calculate the total accessible void volume and estimate the total electron count per void as well as producing a 'solvent-free' dataset. Based on this calculation, the two accessible void volume were found around (0, 0, 0) and (0, 0, 0.5) estimated to be 1,000 $Å^3$ and 1,300 $Å^3$ with an electron count of 527 and 538 electrons, respectively (electron counts for the $[N(C_8H_{17})_4]^+$ cation is 266). This electron count of the cation (but not the potential solvent molecules) has been included in F(000), density and the molecular weight. Final refinements were done with the solvent-free dataset produced by the SQUEEZE procedure in PLATON.

s1. Spek, A.L., Acta Cryst. D65, 148-155, 2009

Supporting Figures and Tables

Table S1. The occupancies of metal sites 1-25 in one of the three crystallographically independent $Au_{25-x}Ag_x(SR)_{18}^-$ nanoclusters.

sites	1	2	3	4	5	6	7	8	9	10	11	12	13
Au%	100	18	18	15	0	10	18	7	7	18	10	15	7
Ag%	0	82	82	85	100	90	82	93	93	82	90	85	93

sites	14	15	16	17	18	19	20	21	22	23	24	25
Au%	0	55	0	55	0	50	55	0	50	0	0	55
Ag%	100	45	100	45	100	50	45	100	50	100	100	45

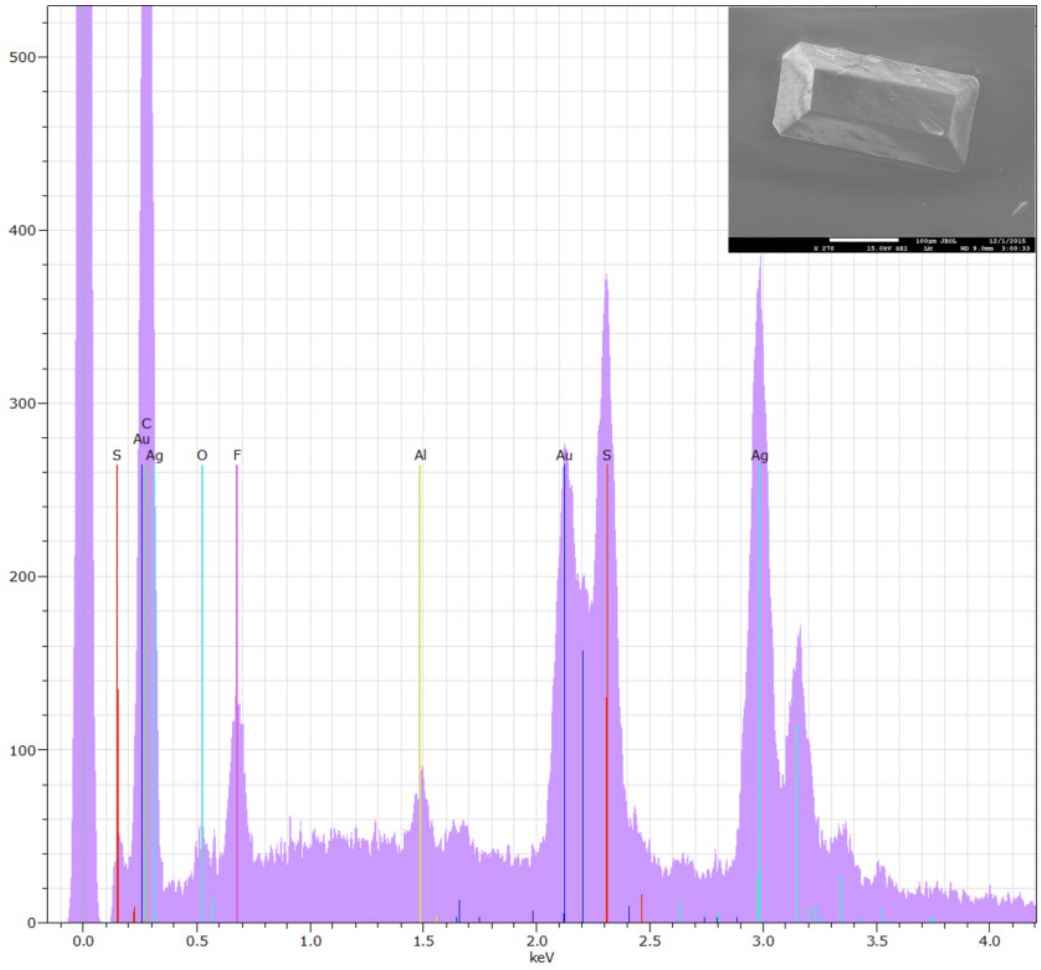

Figure S1. Energy dispersive X-ray spectroscopy by scanning electron microscopy. Inset: SEM image of the single crystal. The crystal was mounted on an Al sample holder and was still covered with a little fluorinated oil used to mount this crystal for single crystal X-ray analysis.

Table S2. The composition of the final $(AuAg)_{25}$ cluster obtained by EDX measurement.

	Gold	Silver	Sulfur
Atomic percent	13.03	43.67	43.29
Normalized to 1	1	3.4	3.3
Normalized to Au+Ag=25	5.68	19.32	18.75

Table S3. Sample and crystal data

Chemical formula	$C_{140}H_{266}Ag_{19.40}Au_{5.60}NS_{18}$	
Formula weight	5736.29 g/mol	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 17.0545(11) Å	α = 85.911(4)°
	b = 29.3289(19) Å	β = 89.317(4)°
	c = 35.668(2) Å	γ = 86.562(4)°
Volume	17763.(2) $Å^3$	
Z	4	
Density (calculated)	2.145 g/cm^3	
Absorption coefficient	27.431 mm^{-1}	
F(000)	11021	

Table S4. Data collection and structure refinement

Theta range for data collection	2.82 to 62.50°
Index ranges	-19<=h<=19, -31<=k<=33, -37<=l<=41
Reflections collected	53704
Independent reflections	53704 [R(int) = 0.1319]
Coverage of independent reflections	94.7%
Absorption correction	Multi-Scan
Structure solution technique	direct methods
Structure solution program	XT, VERSION 2014/4
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	53704 / 54 / 1850
Goodness-of-fit on F^2	1.092
Δ/σ_{max}	0.001
Final R indices	34471 data; I>2σ(I) R1 = 0.1159, wR2 = 0.2973
	all data R1 = 0.1674, wR2 = 0.3320
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1946P)^2+296.9710P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	11.401 and -4.571 eÅ^{-3}
R.M.S. deviation from mean	0.558 eÅ^{-3}

Table S5. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Au1	0.48628(6)	0.01284(3)	0.76334(3)	0.0212(2)
Au2	0.48245(10)	0.97925(6)	0.83810(5)	0.0274(4)
Au3	0.48894(11)	0.04622(6)	0.68829(5)	0.0343(4)
Au4	0.45496(10)	0.07693(5)	0.81627(5)	0.0240(4)
Au6	0.42396(11)	0.92886(6)	0.77814(5)	0.0285(4)
Au7	0.59378(10)	0.94004(6)	0.78543(5)	0.0283(4)
Au8	0.61020(11)	0.03331(6)	0.80700(5)	0.0272(4)
Au9	0.54912(11)	0.09740(6)	0.74850(5)	0.0283(4)
Au10	0.37882(10)	0.08477(6)	0.74235(5)	0.0291(4)
Au11	0.36087(11)	0.99278(7)	0.72022(5)	0.0324(4)
Au12	0.51820(11)	0.94828(6)	0.71098(5)	0.0306(4)
Au13	0.63261(11)	0.01314(6)	0.72973(5)	0.0307(4)
Au15	0.59421(8)	0.13932(5)	0.82326(4)	0.0295(3)
Au17	0.37995(10)	0.88970(5)	0.70070(4)	0.0377(4)
Au19	0.20989(9)	0.05238(5)	0.73915(4)	0.0284(3)
Au20	0.33484(8)	0.93084(4)	0.85534(4)	0.0258(3)
Au22	0.76052(9)	0.96682(5)	0.78980(4)	0.0311(3)
Au25	0.64102(9)	0.09273(5)	0.66979(4)	0.0371(4)
Au26	0.0	0.5	0.0	0.0232(4)
Au27	0.92553(12)	0.43399(6)	0.96333(5)	0.0330(5)
Au28	0.99343(11)	0.58806(6)	0.96653(5)	0.0298(4)
Au29	0.00957(11)	0.50725(6)	0.92191(5)	0.0298(4)
Au30	0.09947(11)	0.43718(6)	0.96661(5)	0.0296(4)
Au31	0.13614(11)	0.47170(6)	0.03911(5)	0.0300(4)
Au32	0.14053(11)	0.53121(6)	0.97068(5)	0.0301(4)
Au34	0.85965(12)	0.48262(7)	0.88521(5)	0.0482(5)
Au37	0.27488(9)	0.45420(5)	0.98430(4)	0.0329(4)
Au38	0.13986(9)	0.64076(5)	0.97873(4)	0.0329(4)
Au39	0.0	0.5	0.5	0.0232(3)
Au40	0.85828(11)	0.48062(6)	0.53354(5)	0.0307(4)
Au41	0.11170(11)	0.42691(6)	0.49673(5)	0.0300(4)
Au42	0.97376(11)	0.53433(6)	0.57034(5)	0.0286(4)
Au43	0.00669(11)	0.43579(6)	0.56189(5)	0.0292(4)
Au44	0.05599(11)	0.58489(7)	0.51002(5)	0.0331(4)
Au45	0.12800(11)	0.50172(7)	0.54634(5)	0.0294(4)
Au46	0.85948(9)	0.38071(5)	0.56763(4)	0.0326(4)
Au48	0.10546(9)	0.59257(5)	0.59277(4)	0.0325(3)
Au50	0.27785(9)	0.45441(5)	0.51095(4)	0.0355(4)
Ag2	0.48245(10)	0.97925(6)	0.83810(5)	0.0274(4)
Ag3	0.48894(11)	0.04622(6)	0.68829(5)	0.0343(4)
Ag4	0.45496(10)	0.07693(5)	0.81627(5)	0.0240(4)
Ag5	0.33898(10)	0.01223(6)	0.79735(5)	0.0220(4)

	x/a	y/b	z/c	U(eq)
Ag6	0.42396(11)	0.92886(6)	0.77814(5)	0.0285(4)
Ag7	0.59378(10)	0.94004(6)	0.78543(5)	0.0283(4)
Ag8	0.61020(11)	0.03331(6)	0.80700(5)	0.0272(4)
Ag9	0.54912(11)	0.09740(6)	0.74850(5)	0.0283(4)
Ag10	0.37882(10)	0.08477(6)	0.74235(5)	0.0291(4)
Ag11	0.36087(11)	0.99278(7)	0.72022(5)	0.0324(4)
Ag12	0.51820(11)	0.94828(6)	0.71098(5)	0.0306(4)
Ag13	0.63261(11)	0.01314(6)	0.72973(5)	0.0307(4)
Ag14	0.57260(14)	0.03988(7)	0.88727(6)	0.0393(5)
Ag15	0.59421(8)	0.13932(5)	0.82326(4)	0.0295(3)
Ag16	0.3864(2)	0.99031(9)	0.63978(7)	0.0595(8)
Ag17	0.37995(10)	0.88970(5)	0.70070(4)	0.0377(4)
Ag18	0.27412(12)	0.09857(7)	0.82342(6)	0.0315(5)
Ag19	0.20989(9)	0.05238(5)	0.73915(4)	0.0284(3)
Ag20	0.33484(8)	0.93084(4)	0.85534(4)	0.0258(3)
Ag21	0.51141(12)	0.86717(7)	0.83207(6)	0.0331(5)
Ag22	0.76052(9)	0.96682(5)	0.78980(4)	0.0311(3)
Ag23	0.69480(14)	0.92490(9)	0.70712(8)	0.0485(6)
Ag24	0.46425(13)	0.15599(7)	0.69061(6)	0.0410(6)
Ag25	0.64102(9)	0.09273(5)	0.66979(4)	0.0371(4)
Ag27	0.92553(12)	0.43399(6)	0.96333(5)	0.0330(5)
Ag28	0.99343(11)	0.58806(6)	0.96653(5)	0.0298(4)
Ag29	0.00957(11)	0.50725(6)	0.92191(5)	0.0298(4)
Ag30	0.09947(11)	0.43718(6)	0.96661(5)	0.0296(4)
Ag31	0.13614(11)	0.47170(6)	0.03911(5)	0.0300(4)
Ag32	0.14053(11)	0.53121(6)	0.97068(5)	0.0301(4)
Ag33	0.88384(16)	0.59455(8)	0.89486(7)	0.0506(7)
Ag34	0.85965(12)	0.48262(7)	0.88521(5)	0.0482(5)
Ag35	0.02473(14)	0.34732(7)	0.95987(7)	0.0442(6)
Ag36	0.17635(13)	0.49132(7)	0.89822(6)	0.0360(5)
Ag37	0.27488(9)	0.45420(5)	0.98430(4)	0.0329(4)
Ag38	0.13986(9)	0.64076(5)	0.97873(4)	0.0329(4)
Ag40	0.85828(11)	0.48062(6)	0.53354(5)	0.0307(4)
Ag41	0.11170(11)	0.42691(6)	0.49673(5)	0.0300(4)
Ag42	0.97376(11)	0.53433(6)	0.57034(5)	0.0286(4)
Ag43	0.00669(11)	0.43579(6)	0.56189(5)	0.0292(4)
Ag44	0.05599(11)	0.58489(7)	0.51002(5)	0.0331(4)
Ag45	0.12800(11)	0.50172(7)	0.54634(5)	0.0294(4)
Ag46	0.85948(9)	0.38071(5)	0.56763(4)	0.0326(4)
Ag47	0.03481(14)	0.33637(8)	0.52731(7)	0.0439(6)
Ag48	0.10546(9)	0.59257(5)	0.59277(4)	0.0325(3)
Ag49	0.09939(14)	0.47180(8)	0.62552(6)	0.0407(6)
Ag50	0.27785(9)	0.45441(5)	0.51095(4)	0.0355(4)

	x/a	y/b	z/c	U(eq)
Ag51	0.19966(13)	0.44915(9)	0.41861(6)	0.0411(5)
S1	0.5122(4)	0.9687(3)	0.90532(19)	0.0368(18)
S2	0.6245(4)	0.1145(2)	0.88503(18)	0.0284(14)
S3	0.5636(4)	0.1770(2)	0.7652(2)	0.0303(15)
S4	0.4520(6)	0.0596(3)	0.6219(2)	0.047(2)
S5	0.3404(5)	0.9149(3)	0.6397(2)	0.0438(19)
S6	0.4121(5)	0.8509(2)	0.75866(19)	0.0335(16)
S7	0.3789(4)	0.1264(2)	0.8575(2)	0.0288(14)
S8	0.1559(4)	0.0919(2)	0.78915(19)	0.0270(14)
S9	0.2402(4)	0.0155(2)	0.68314(18)	0.0332(16)
S10	0.2632(4)	0.0012(2)	0.85773(19)	0.0276(15)
S11	0.3852(4)	0.8554(2)	0.86140(18)	0.0258(14)
S12	0.6506(4)	0.8709(2)	0.82279(19)	0.0315(16)
S13	0.7243(4)	0.0054(2)	0.84471(18)	0.0302(15)
S14	0.8164(5)	0.9287(3)	0.7400(2)	0.0387(17)
S15	0.5938(5)	0.8945(4)	0.6714(2)	0.054(2)
S16	0.3278(4)	0.1552(2)	0.7067(2)	0.0344(16)
S17	0.5886(5)	0.1678(3)	0.6612(3)	0.047(2)
S18	0.7097(4)	0.0213(3)	0.66976(19)	0.0358(17)
S19	0.8802(6)	0.4041(3)	0.9058(2)	0.058(3)
S20	0.8139(5)	0.5505(3)	0.8556(2)	0.049(2)
S21	0.9510(5)	0.6521(2)	0.9221(2)	0.047(2)
S22	0.0645(5)	0.4986(2)	0.85718(18)	0.0388(18)
S23	0.3070(5)	0.4788(2)	0.9222(2)	0.0372(17)
S24	0.2608(4)	0.4236(2)	0.04637(19)	0.0331(16)
S25	0.1483(5)	0.3704(2)	0.93414(19)	0.0342(16)
S26	0.2193(4)	0.5930(2)	0.9426(2)	0.0357(17)
S27	0.0784(4)	0.6975(2)	0.0136(2)	0.0372(17)
S28	0.7857(4)	0.4446(3)	0.58741(19)	0.0340(17)
S29	0.9205(5)	0.3092(3)	0.5581(2)	0.0421(19)
S30	0.1617(5)	0.3463(2)	0.4994(2)	0.0424(19)
S31	0.0455(4)	0.3978(2)	0.62244(19)	0.0347(17)
S32	0.1465(4)	0.5431(2)	0.64337(19)	0.0346(17)
S33	0.0689(4)	0.6517(3)	0.54737(19)	0.0335(16)
S34	0.2471(5)	0.4611(3)	0.5748(2)	0.0395(18)
S35	0.3237(4)	0.4449(3)	0.4502(2)	0.0415(19)
S36	0.0981(4)	0.4410(3)	0.37341(19)	0.0334(16)
N1	0.4037(19)	0.5830(10)	0.7569(8)	0.054(8)
C1A	0.334(2)	0.5557(14)	0.7604(11)	0.060(10)
C2A	0.325(3)	0.5190(14)	0.7317(13)	0.070(11)
C3A	0.288(2)	0.4780(13)	0.7478(11)	0.057(9)
C4A	0.279(2)	0.4440(11)	0.7176(9)	0.044(8)
C5A	0.239(2)	0.3999(13)	0.7308(11)	0.057(9)

	x/a	y/b	z/c	U(eq)
C6A	0.233(2)	0.3672(13)	0.7002(11)	0.061(10)
C7A	0.191(2)	0.3232(13)	0.7157(11)	0.057(9)
C8A	0.192(4)	0.289(2)	0.681(2)	0.15(3)
C1B	0.406(2)	0.6122(13)	0.7177(11)	0.056(9)
C2B	0.347(2)	0.6491(13)	0.7112(11)	0.059(10)
C3B	0.354(2)	0.6692(13)	0.6693(11)	0.057(9)
C4B	0.302(2)	0.7144(14)	0.6619(12)	0.062(10)
C5B	0.212(2)	0.7098(13)	0.6680(11)	0.055(9)
C6B	0.165(2)	0.7513(13)	0.6573(12)	0.060(10)
C7B	0.081(3)	0.7481(18)	0.6639(16)	0.090(15)
C8B	0.037(3)	0.791(2)	0.6551(18)	0.109(19)
C1C	0.480(3)	0.5509(15)	0.7561(12)	0.075(12)
C2C	0.479(3)	0.5161(15)	0.7916(12)	0.081(12)
C3C	0.558(3)	0.486(2)	0.7888(17)	0.120(18)
C4C	0.573(4)	0.4561(19)	0.7545(18)	0.131(19)
C5C	0.523(3)	0.4130(18)	0.7554(17)	0.117(17)
C6C	0.547(3)	0.3813(18)	0.7229(17)	0.112(17)
C7C	0.486(3)	0.3436(19)	0.7289(17)	0.121(19)
C8C	0.490(4)	0.314(2)	0.6942(17)	0.13(2)
C1D	0.396(2)	0.6161(15)	0.7888(13)	0.070(11)
C2D	0.459(2)	0.6512(15)	0.7888(13)	0.068(11)
C3D	0.441(3)	0.680(2)	0.8191(18)	0.107(18)
C4D	0.495(4)	0.719(2)	0.822(2)	0.13(2)
C5D	0.568(3)	0.697(2)	0.8450(18)	0.108(19)
C6D	0.636(3)	0.723(2)	0.8501(18)	0.105(18)
C7D	0.703(3)	0.7092(19)	0.8659(17)	0.097(16)
C8D	0.781(3)	0.7405(18)	0.8654(16)	0.099(17)
C11	0.4276(19)	0.9861(11)	0.9304(10)	0.044(8)
C12	0.401(3)	0.0351(19)	0.9321(17)	0.104(18)
C13	0.333(4)	0.051(2)	0.959(2)	0.13(2)
C14	0.333(3)	0.0242(17)	0.9959(15)	0.088(14)
C15	0.341(5)	0.973(3)	0.989(3)	0.19(4)
C16	0.425(4)	0.958(2)	0.9706(18)	0.12(2)
C21	0.5560(19)	0.1499(11)	0.9129(9)	0.041(7)
C22	0.5754(16)	0.2025(9)	0.9067(8)	0.032(6)
C23	0.522(2)	0.2310(12)	0.9283(10)	0.050(8)
C24	0.525(2)	0.2168(12)	0.9710(10)	0.048(8)
C25	0.504(2)	0.1658(13)	0.9753(12)	0.062(10)
C26	0.558(2)	0.1357(12)	0.9539(9)	0.046(8)
C31	0.6483(19)	0.2051(11)	0.7468(10)	0.045(8)
C32	0.664(3)	0.2473(15)	0.7689(13)	0.074(12)
C33	0.733(2)	0.2721(14)	0.7500(12)	0.066(11)
C34	0.805(3)	0.2404(15)	0.7468(13)	0.073(12)

	x/a	y/b	z/c	U(eq)
C35	0.789(2)	0.1970(12)	0.7285(10)	0.050(8)
C36	0.7254(18)	0.1732(11)	0.7465(9)	0.042(7)
C41	0.532(2)	0.0373(11)	0.5926(9)	0.053(9)
C42	0.520(3)	0.049(2)	0.5510(12)	0.105(18)
C43	0.599(5)	0.037(4)	0.533(3)	0.23(5)
C44	0.631(5)	0.986(3)	0.5378(17)	0.15(3)
C45	0.631(3)	0.976(2)	0.5799(14)	0.112(19)
C46	0.559(2)	0.9880(10)	0.6029(10)	0.053(9)
C51	0.408(2)	0.8823(14)	0.6102(12)	0.065(11)
C52	0.402(3)	0.8993(16)	0.5702(13)	0.072(12)
C53	0.455(2)	0.8711(14)	0.5464(13)	0.069(11)
C54	0.428(3)	0.8191(17)	0.5505(15)	0.090(15)
C55	0.438(3)	0.8008(16)	0.5930(13)	0.078(13)
C56	0.382(2)	0.8307(14)	0.6139(13)	0.067(11)
C61	0.3268(19)	0.8227(11)	0.7734(10)	0.044(8)
C62	0.310(2)	0.7857(14)	0.7493(12)	0.064(10)
C63	0.234(3)	0.7611(16)	0.7620(14)	0.079(13)
C64	0.165(3)	0.7945(16)	0.7620(14)	0.080(13)
C65	0.183(3)	0.8340(17)	0.7874(15)	0.083(14)
C66	0.257(2)	0.8563(13)	0.7763(12)	0.059(10)
C71	0.3874(16)	0.1861(9)	0.8378(8)	0.029(6)
C72	0.3716(16)	0.1930(9)	0.7966(7)	0.027(6)
C73	0.3762(18)	0.2432(10)	0.7837(9)	0.038(7)
C74	0.3212(16)	0.2744(9)	0.8057(8)	0.029(6)
C75	0.340(2)	0.2676(12)	0.8467(10)	0.050(8)
C76	0.3265(19)	0.2159(11)	0.8626(9)	0.042(7)
C81	0.1322(15)	0.1509(9)	0.7687(7)	0.026(6)
C82	0.0548(15)	0.1507(9)	0.7451(8)	0.028(6)
C83	0.036(2)	0.1999(12)	0.7280(11)	0.053(9)
C84	0.026(2)	0.2331(12)	0.7580(10)	0.050(8)
C85	0.101(2)	0.2317(13)	0.7832(12)	0.061(10)
C86	0.1220(18)	0.1837(10)	0.7983(8)	0.035(7)
C91	0.1768(18)	0.9660(11)	0.6814(8)	0.036(7)
C92	0.133(3)	0.9685(18)	0.6449(15)	0.091(15)
C93	0.080(3)	0.9245(19)	0.6428(17)	0.100(17)
C94	0.025(2)	0.9246(14)	0.6747(11)	0.062(10)
C95	0.065(3)	0.9176(19)	0.7093(16)	0.094(16)
C96	0.125(3)	0.958(2)	0.7121(17)	0.101(17)
C100	0.1610(14)	0.9868(8)	0.8542(7)	0.019(5)
C101	0.1433(17)	0.9653(10)	0.8172(8)	0.036(7)
C103	0.053(2)	0.9550(13)	0.8197(11)	0.055(9)
C104	0.038(2)	0.9232(13)	0.8501(11)	0.058(10)
C105	0.0554(18)	0.9399(11)	0.8897(9)	0.043(8)

	x/a	y/b	z/c	U(eq)
C106	0.1425(15)	0.9526(9)	0.8884(7)	0.026(6)
C111	0.4088(16)	0.8441(9)	0.9108(8)	0.028(6)
C112	0.333(2)	0.8531(13)	0.9360(11)	0.054(9)
C113	0.2718(19)	0.8194(11)	0.9300(10)	0.044(8)
C114	0.305(2)	0.7708(14)	0.9349(12)	0.065(11)
C115	0.377(2)	0.7617(13)	0.9100(11)	0.053(9)
C116	0.4370(18)	0.7925(10)	0.9179(9)	0.040(7)
C121	0.6774(16)	0.8864(10)	0.8702(8)	0.032(6)
C122	0.7656(16)	0.8839(10)	0.8730(8)	0.033(6)
C123	0.787(2)	0.9010(12)	0.9131(10)	0.048(8)
C124	0.751(2)	0.8706(14)	0.9440(11)	0.059(10)
C125	0.6616(17)	0.8726(11)	0.9402(8)	0.036(7)
C126	0.6408(16)	0.8590(9)	0.9014(7)	0.028(6)
C131	0.7967(18)	0.0501(11)	0.8487(9)	0.038(7)
C132	0.8701(17)	0.0284(11)	0.8633(9)	0.039(7)
C133	0.9312(18)	0.0653(11)	0.8665(9)	0.040(7)
C134	0.946(2)	0.0919(13)	0.8298(11)	0.054(9)
C135	0.872(2)	0.1094(12)	0.8139(11)	0.052(9)
C136	0.8094(17)	0.0753(10)	0.8101(8)	0.033(6)
C141	0.8319(17)	0.8656(10)	0.7598(8)	0.034(7)
C142	0.8487(19)	0.8374(11)	0.7288(9)	0.042(7)
C143	0.8649(18)	0.7879(11)	0.7429(9)	0.041(7)
C144	0.930(2)	0.7827(13)	0.7713(11)	0.059(10)
C145	0.9202(19)	0.8156(11)	0.8022(9)	0.043(8)
C146	0.9061(18)	0.8646(11)	0.7842(9)	0.039(7)
C151	0.588(2)	0.8336(12)	0.6926(10)	0.051(9)
C152	0.630(4)	0.805(2)	0.6634(18)	0.11(2)
C153	0.620(4)	0.756(2)	0.6788(19)	0.12(2)
C154	0.646(3)	0.7464(17)	0.7202(14)	0.080(13)
C155	0.602(4)	0.781(2)	0.740(2)	0.14(3)
C156	0.610(3)	0.8289(15)	0.7280(12)	0.069(11)
C161	0.2871(17)	0.1383(10)	0.6618(8)	0.035(7)
C162	0.2004(19)	0.1444(12)	0.6662(10)	0.047(8)
C163	0.161(2)	0.1315(12)	0.6296(10)	0.048(8)
C164	0.190(3)	0.1628(17)	0.5955(14)	0.081(13)
C165	0.281(2)	0.1536(13)	0.5913(10)	0.051(9)
C166	0.3164(17)	0.1646(10)	0.6291(8)	0.034(6)
C171	0.567(2)	0.1757(13)	0.6120(11)	0.055(9)
C172	0.535(3)	0.2252(15)	0.6047(12)	0.068(11)
C173	0.524(4)	0.238(2)	0.563(2)	0.13(2)
C174	0.604(6)	0.234(3)	0.546(3)	0.20(4)
C175	0.633(4)	0.186(3)	0.550(2)	0.14(3)
C176	0.651(3)	0.1718(19)	0.5899(15)	0.091(15)

	x/a	y/b	z/c	U(eq)
C181	0.8149(15)	0.0314(9)	0.6733(7)	0.027(6)
C182	0.8401(16)	0.0606(10)	0.6396(8)	0.031(6)
C183	0.928(3)	0.0664(18)	0.6431(14)	0.084(14)
C184	0.954(3)	0.0836(16)	0.6792(13)	0.078(13)
C185	0.9223(18)	0.0585(11)	0.7127(9)	0.042(7)
C186	0.8317(16)	0.0532(10)	0.7104(8)	0.035(7)
C191	0.777(2)	0.3864(15)	0.9018(13)	0.068(11)
C192	0.777(3)	0.3388(18)	0.9109(17)	0.097(16)
C193	0.691(3)	0.3221(17)	0.9098(13)	0.077(12)
C194	0.670(3)	0.3270(16)	0.8675(13)	0.076(12)
C195	0.675(3)	0.3758(17)	0.8504(16)	0.091(15)
C196	0.757(2)	0.3956(15)	0.8606(12)	0.065(11)
C201	0.866(2)	0.5556(13)	0.8105(11)	0.055(9)
C202	0.826(2)	0.5288(15)	0.7824(13)	0.069(11)
C203	0.739(4)	0.544(3)	0.771(2)	0.14(3)
C204	0.738(5)	0.586(3)	0.757(2)	0.16(3)
C205	0.778(3)	0.625(2)	0.7822(17)	0.104(18)
C206	0.862(3)	0.6087(16)	0.7937(15)	0.081(13)
C211	0.0336(17)	0.6626(10)	0.8916(8)	0.034(7)
C212	0.070(2)	0.6220(12)	0.8721(10)	0.050(8)
C213	0.146(2)	0.6354(14)	0.8469(12)	0.062(10)
C214	0.116(3)	0.6751(16)	0.8184(14)	0.082(14)
C215	0.079(2)	0.7147(12)	0.8383(10)	0.051(9)
C216	0.009(2)	0.7035(12)	0.8597(10)	0.048(8)
C221	0.0569(19)	0.4364(12)	0.8476(10)	0.047(8)
C222	0.1339(16)	0.4171(9)	0.8330(8)	0.029(6)
C223	0.1238(19)	0.3659(11)	0.8245(9)	0.044(8)
C224	0.056(2)	0.3625(14)	0.7997(11)	0.058(10)
C225	0.9812(18)	0.3824(11)	0.8131(9)	0.043(7)
C226	0.9861(17)	0.4328(10)	0.8214(8)	0.035(7)
C231	0.3383(17)	0.4252(10)	0.8985(8)	0.035(7)
C232	0.4129(17)	0.4046(10)	0.9198(8)	0.034(6)
C233	0.4439(17)	0.3615(10)	0.8996(8)	0.035(7)
C234	0.4515(18)	0.3717(11)	0.8570(9)	0.041(7)
C235	0.3763(17)	0.3934(10)	0.8391(9)	0.038(7)
C236	0.3521(16)	0.4360(9)	0.8602(8)	0.029(6)
C241	0.333(2)	0.4491(15)	0.0762(12)	0.066(11)
C242	0.412(3)	0.4114(18)	0.0729(17)	0.035(13)
C243	0.466(4)	0.4289(19)	0.1010(18)	0.039(14)
C42B	0.374(4)	0.418(2)	0.1048(19)	0.045(16)
C43B	0.434(3)	0.438(2)	0.1272(17)	0.036(13)
C244	0.482(3)	0.4709(16)	0.1002(13)	0.071(12)
C245	0.397(4)	0.507(2)	0.104(2)	0.047(16)

	x/a	y/b	z/c	U(eq)
C246	0.339(3)	0.4882(17)	0.0737(15)	0.027(12)
C45B	0.468(5)	0.490(3)	0.073(2)	0.06(2)
C46B	0.399(4)	0.472(3)	0.047(2)	0.051(17)
C251	0.2216(16)	0.3392(9)	0.9653(7)	0.027(6)
C252	0.2540(19)	0.2961(11)	0.9461(10)	0.044(8)
C253	0.319(3)	0.2697(17)	0.9683(14)	0.079(13)
C254	0.2883(19)	0.2578(11)	0.0069(9)	0.042(7)
C255	0.256(2)	0.3001(12)	0.0279(11)	0.053(9)
C256	0.192(2)	0.3261(12)	0.0044(10)	0.051(9)
C261	0.3192(16)	0.5974(10)	0.9615(8)	0.030(6)
C262	0.324(2)	0.5889(15)	0.0021(12)	0.068(11)
C263	0.407(2)	0.5934(14)	0.0150(12)	0.066(11)
C264	0.437(2)	0.6410(13)	0.0027(11)	0.058(10)
C265	0.433(2)	0.6460(16)	0.9592(13)	0.072(12)
C266	0.349(2)	0.6449(13)	0.9498(12)	0.060(10)
C271	0.0284(18)	0.7362(11)	0.9811(9)	0.049(8)
C272	0.971(2)	0.7696(12)	0.0019(10)	0.060(10)
C273	0.929(3)	0.8052(15)	0.9735(13)	0.092(15)
C274	0.988(3)	0.8313(16)	0.9480(13)	0.086(14)
C275	0.042(4)	0.7975(18)	0.9258(15)	0.14(3)
C276	0.086(2)	0.7625(13)	0.9545(10)	0.059(10)
C281	0.6813(16)	0.4322(10)	0.5797(8)	0.030(6)
C282	0.6587(18)	0.3912(11)	0.6048(9)	0.042(7)
C283	0.575(2)	0.3806(15)	0.6002(12)	0.064(10)
C284	0.553(3)	0.3804(18)	0.5586(15)	0.091(15)
C285	0.574(2)	0.4221(12)	0.5351(10)	0.049(8)
C286	0.6575(17)	0.4306(11)	0.5400(8)	0.037(7)
C291	0.950(2)	0.2905(12)	0.6056(10)	0.048(8)
C292	0.994(2)	0.2432(12)	0.6066(11)	0.054(9)
C293	0.945(2)	0.2030(12)	0.5961(10)	0.051(9)
C294	0.871(2)	0.2003(14)	0.6220(12)	0.063(10)
C295	0.823(2)	0.2461(12)	0.6215(11)	0.053(9)
C296	0.877(2)	0.2832(13)	0.6315(10)	0.052(9)
C301	0.238(3)	0.3376(18)	0.5311(15)	0.086(14)
C302	0.213(3)	0.342(2)	0.5687(17)	0.109(19)
C303	0.286(3)	0.3374(18)	0.5977(16)	0.091(15)
C304	0.313(2)	0.2917(14)	0.6022(12)	0.066(11)
C305	0.343(4)	0.279(2)	0.5620(19)	0.13(2)
C306	0.270(3)	0.2883(16)	0.5308(14)	0.077(13)
C311	0.9616(17)	0.3973(10)	0.6529(8)	0.034(7)
C312	0.9284(17)	0.4428(10)	0.6615(9)	0.037(7)
C313	0.856(2)	0.4423(12)	0.6895(10)	0.047(8)
C314	0.877(2)	0.4119(13)	0.7225(11)	0.056(9)

	x/a	y/b	z/c	U(eq)
C315	0.905(2)	0.3634(13)	0.7179(11)	0.057(9)
C316	0.9789(18)	0.3675(11)	0.6913(9)	0.040(7)
C321	0.0871(14)	0.5591(8)	0.6819(7)	0.020(5)
C322	0.0988(19)	0.6069(11)	0.6930(9)	0.042(7)
C323	0.054(2)	0.6213(13)	0.7272(10)	0.053(9)
C324	0.0641(19)	0.5841(11)	0.7613(9)	0.042(7)
C325	0.043(2)	0.5395(14)	0.7500(12)	0.063(10)
C326	0.0929(17)	0.5240(10)	0.7166(8)	0.032(6)
C331	0.1553(16)	0.6792(9)	0.5333(8)	0.030(6)
C332	0.228(2)	0.6440(12)	0.5292(11)	0.051(9)
C333	0.305(2)	0.6700(12)	0.5219(10)	0.050(8)
C334	0.3156(19)	0.7062(11)	0.5466(9)	0.042(7)
C335	0.251(2)	0.7410(12)	0.5510(10)	0.051(9)
C336	0.175(2)	0.7155(14)	0.5625(12)	0.067(11)
C341	0.320(2)	0.5000(14)	0.5939(13)	0.067(11)
C342	0.336(2)	0.5388(14)	0.5700(12)	0.064(10)
C343	0.392(3)	0.5692(16)	0.5896(14)	0.080(13)
C344	0.461(2)	0.5413(13)	0.6051(12)	0.059(10)
C345	0.443(2)	0.4984(14)	0.6302(12)	0.066(11)
C346	0.387(2)	0.4681(12)	0.6083(11)	0.052(9)
C351	0.3531(15)	0.3816(9)	0.4490(7)	0.025(6)
C352	0.4279(18)	0.3719(11)	0.4719(9)	0.039(7)
C353	0.451(3)	0.3233(14)	0.4711(12)	0.069(11)
C354	0.465(3)	0.3094(19)	0.4311(15)	0.091(15)
C355	0.391(3)	0.3190(15)	0.4073(14)	0.075(12)
C356	0.365(2)	0.3720(12)	0.4090(10)	0.048(8)
C361	0.0952(18)	0.3786(10)	0.3691(9)	0.038(7)
C362	0.1214(18)	0.3506(10)	0.4039(9)	0.039(7)
C363	0.118(3)	0.2969(15)	0.3991(13)	0.071(11)
C364	0.166(3)	0.2854(17)	0.3651(14)	0.081(13)
C365	0.145(2)	0.3151(14)	0.3286(12)	0.065(11)
C366	0.147(2)	0.3665(13)	0.3363(11)	0.058(10)