Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics


# Chemically Synthesised Atomically Precise Gold Clusters Deposited and Activated on Titania

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## Electronic supplementary information (ESI)

### I. Preparation of the ligand stabilised gold cluster

All basic laboratory chemicals (solvents *etc.*, AR grade) have been purchased from established suppliers, (e.g. Sigma-Aldrich), and used without further purification. Evonik $TiO_2$ P-25 aeroxide (CAS-No 13463-67-7) was purchased from Chemiplas NZ. Tetrachloroauric acid was prepared using 99.99% pure gold following the procedure detailed by Brauer.[1] Unless otherwise specified, reactions have been carried out under air.

**$AuPPh_3(Cl)$** The synthesis protocol was adapted from the procedure described by Bruce *et al.*[2] Triphenylphosphine (2.65 g, 10.10 mmol) in ethanol (75 mL) was added rapidly to a stirred (500 rpm) solution of tetrachloroauric acid (2.010 g, 5.102 mmol) in ethanol (20 mL). The yellow colour of solution disappeared immediately upon addition of triphenylphosphine to form a white precipitate. The resulting solution was stirred vigorously (1000 rpm) for a further 15 minutes. The reaction mixture was centrifuged (5 min, 5000 rpm) and the white product collected, then washed 3 times with hot ethanol (3 × 20 mL) on a sintered glass funnel filter (porosity 3). The remaining solid was dissolved in chloroform (30 mL), filtered and the solvent removed under reduced pressure. The crude product was dried in a vacuum desiccator. The product was recrystallized from a mixture of dichloromethane and methanol using vapour diffusion resulting in needle-like white crystals.

Yield: 2.250 g, 90 %. $^{31}P$ NMR (chloroform, 25 °C); δ 33.5 ppm referenced to $H_3PO_4$

**$AuPPh_3(NO_3)$** was synthesised according to a protocol described by Mueting *et al.*[3] A solution of $AgNO_3$ (3.430g, 20.191 mmol) in ethanol (130 mL) was added rapidly to a solution of $AuPPh_3(Cl)$ (3.973g, 8.042 mmol) in chloroform (50 mL). The reaction was left to stir for 1 hour with the reaction vessel covered with aluminium foil. The precipitate of AgCl was removed by filtering on a sintered glass funnel filter (porosity 3) and the filtrate was then dried in a rotary evaporator without heating. The crude product was washed with ethanol (3 × 50 mL). The solid was then dissolved in the dichloromethane (50 mL) to which ethanol

(150 mL) was added. The solution was then bubbled through with a flow of nitrogen for 2 hours to remove the dichloromethane. The resulting white crystals were collected by filtration, washed with cold ethanol (3 × 5 mL) and cold diethyl ether (3 × 5 mL). The product was stored in a freezer in the absence of light.

Yield: 3.648g, 87 %. $^{31}$P NMR (chloroform, 25 °C); δ 25.2 ppm referenced to $H_3PO_4$

**1.5 nm Au clusters, "$Au_{101}$"** or $Au_{101}[P(C_6H_5)_3]_{21}Cl_5$ stabilized by triphenylphosphine were prepared according to a protocol described by Hutchison *et al.*[4,4] Tetraoctylammonium bromide (1.40 g, 2.56 mmol) was added to a solution of tetrachloroauric acid (1 g, 2.54 mmol) in ultrapure water (60 mL) and toluene (60 mL). After 5 minutes of vigorous stirring at 1000 rpm, triphenylphosphine (2.3 g, 8.76 mmol) is added to the biphasic system. After 10 minutes of vigorous stirring, a solution of freshly dissolved sodium borohydride (2.0 g, 52.9 mmol) in ultrapure water was rapidly added to the reaction mixture. The reaction mixture was left to stir at 600 rpm for a further 3 hours, after which point the organic layer was separated and washed with saturated solution of NaCl in ultrapure water (2 × 50 mL) and then ultrapure water (3 × 50 mL). The organic layer was separated, filtered and dried under reduced pressure. The resulting solid was redissolved in chloroform (35ml mL) to which pentane (300 mL) was added slowly with gentle swirling and the mixture allowed to stand overnight. The precipitate was collected by filtration on a sintered glass funnel filter (porosity 4) and washed with series of solvent mixtures as follows:

2 ×100 mL hexanes followed by 100 mL 2: 3 MeOH: $H_2O$)

2 ×100 mL hexanes followed by 100 mL 1: 1 MeOH: $H_2O$)

2 x 150 mL 3: 1 pentane: chloroform

2 x 150 mL 2: 1 pentane: chloroform

2 x 150 mL 1: 1 pentane: chloroform

The solvent washes are used to remove by-product $AuPPh_3(Cl)$ and the phase transfer reagent. The effectiveness of the purification steps was monitored by $^1$H NMR. The remaining solid was dissolved in dichloromethane (30 mL) and filtered through to recover the product. Removal of solvent under reduced pressure (rotary evaporator) afforded pure product as a fine black powder.

Yield: 200 – 250 mg.

This cluster was characterised by HRTEM (Fig. S1) and its purity was confirmed by $^1$H NMR in $CDCl_3$

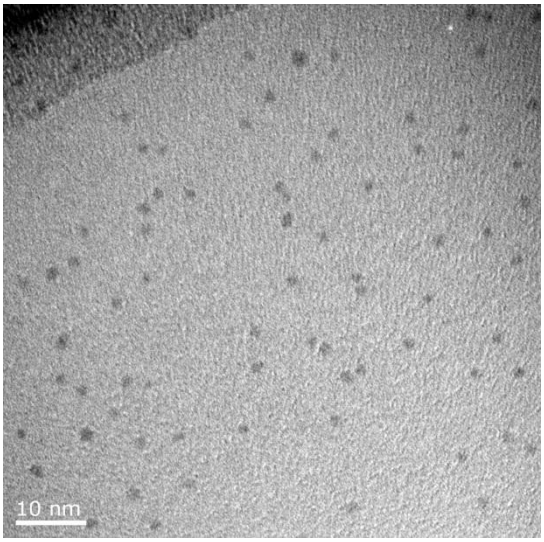


Figure SI 1: A representative HRTEM image of $Au_{101}$ particles deposited onto carbon film of TEM grid (obtained using Philips CM200 high resolution analytical transmission electron microscope).

**$Au_{11}(PPh_3)_8Cl_3$** was synthesised according to a modified protocol described by Hutchison *et al.*[5,6]

A solution of $NaBH_4$ (0.075 g, 1.97 mmol) in ethanol (5 mL) was added dropwise to a stirred suspension of $Au(PPh_3)Cl$ (1.0 g, 2.02 mmol) in ethanol (50 mL). The reaction mixture was left to stir for 2 hours, after which time it was poured into hexanes (1 L) and the product was allowed to precipitate overnight. The precipitate was collected using a sintered glass filter funnel (porosity 4). It was then washed with hexanes (4 × 15 mL), 1:1 (v/v) mixture of $CH_2Cl_2$: hexanes (4 ×15 mL), and 3:1 (v/v) mixture of $CH_2Cl_2$: hexanes (1 × 10 mL). The solid remaining on the filter was dissolved in dichloromethane (20 mL) and filtered through to remove any insoluble by-products. The crude product was obtained upon removal of solvent in vacuum. It was recrystallized from a mixture of dichloromethane and diethyl ether by vapour diffusion at 4°C resulting in deep red platelets.

Yield: 155 mg, 17.5%

$^{31}P$ NMR (chloroform, 25 °C); δ 52.2 ppm referenced to $H_3PO_4$

Mass spectrometry (MS) was performed using Bruker maXis UHR-TOF MS with an electrospray ionisation (ESI) source and positive-ion polarity.

Isotopic distribution modelling was completed by the molecular weight calculator kindly distributed by PNNl http://ncrr.pnl.gov/software/

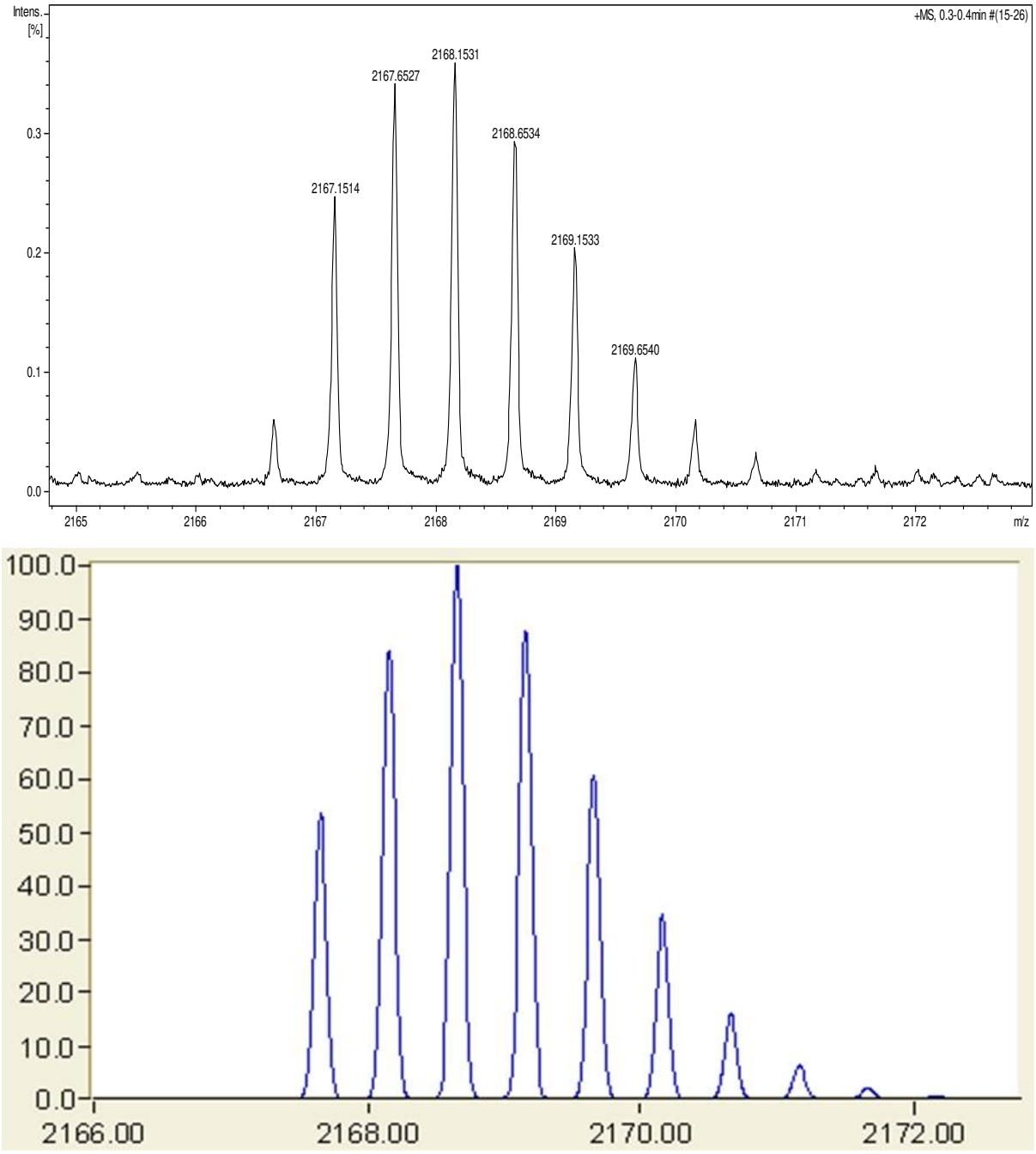


Figure SI 2: Top: Molecular ion peak for the $[Au_{11}(PPh_3)_8Cl_2]^{2+}$, bottom: the isotopic distribution and simulated spectra pattern for the molecular ion.

Table SI 1: Values of m/z, fraction and intensity for the simulated high resolution MS for $Au_{11}$.

| Mass/Charge | Fraction | Intensity |
|---|---|---|
| 2167.657 | 0.119819 | 53.42 |
| 2168.157 | 0.18877 | 84.17 |
| 2168.657 | 0.224282 | 100 |
| 2169.157 | 0.197174 | 87.91 |
| 2169.657 | 0.136167 | 60.71 |
| 2170.157 | 0.077238 | 34.44 |
| 2170.657 | 0.036252 | 16.16 |
| 2171.157 | 0.014096 | 6.28 |
| 2171.657 | 0.004576 | 2.04 |
| 2172.157 | 0.001257 | 0.56 |
| 2172.657 | 0.000298 | 0.13 |
| 2173.157 | 6.05E-05 | 0.03 |
| 2173.657 | 1.22E-05 | 0.01 |
| 2174.157 | 1.6E-06 | 0 |

**$Au_9(PPh_3)_8(NO_3)_3$** was synthesised following protocol described by Wen *et al*.[7]

A solution of $NaBH_4$ (0.072 g, 1.92 mmol) in ethanol (92 mL) was added to the magnetically stirred solution of $AuPPh_3(NO_3)$ (4.0 g, 7.6 mmol) in ethanol (160 mL). The solution became deep red within two hours, after which point the solution was filtered to remove insoluble impurities and solvent removed *in vacuo*. The solid obtained was dissolved in 20 mL $CH_2Cl_2$ and filtered through sintered glass filter funnel (porosity 3). Removal of solvent on rotary evaporator yield product as black precipitate, which was washed with 50 mL of THF. Upon washing, the solid becomes dark-green. The solid was further washed with THF (3 x 50 ml) and hexanes (3 x 50 ml). The precipitate was crystallized from a methanol solution by slow diffusion of diethyl ether at 4°C. Dark green crystals formed within *ca.* 5 days.

Yield 1.24 g, 36 %.

$^{31}P$ NMR (chloroform, 25 °C); δ 56.8 ppm referenced to $H_3PO_4$

Mass spectrometry (MS) was performed using Bruker maXis UHR-TOF MS with an electrospray ionisation (ESI) source and positive-ion polarity.

Isotopic distribution modelling was completed by the molecular weight calculator kindly distributed by PNNl http://ncrr.pnl.gov/software/

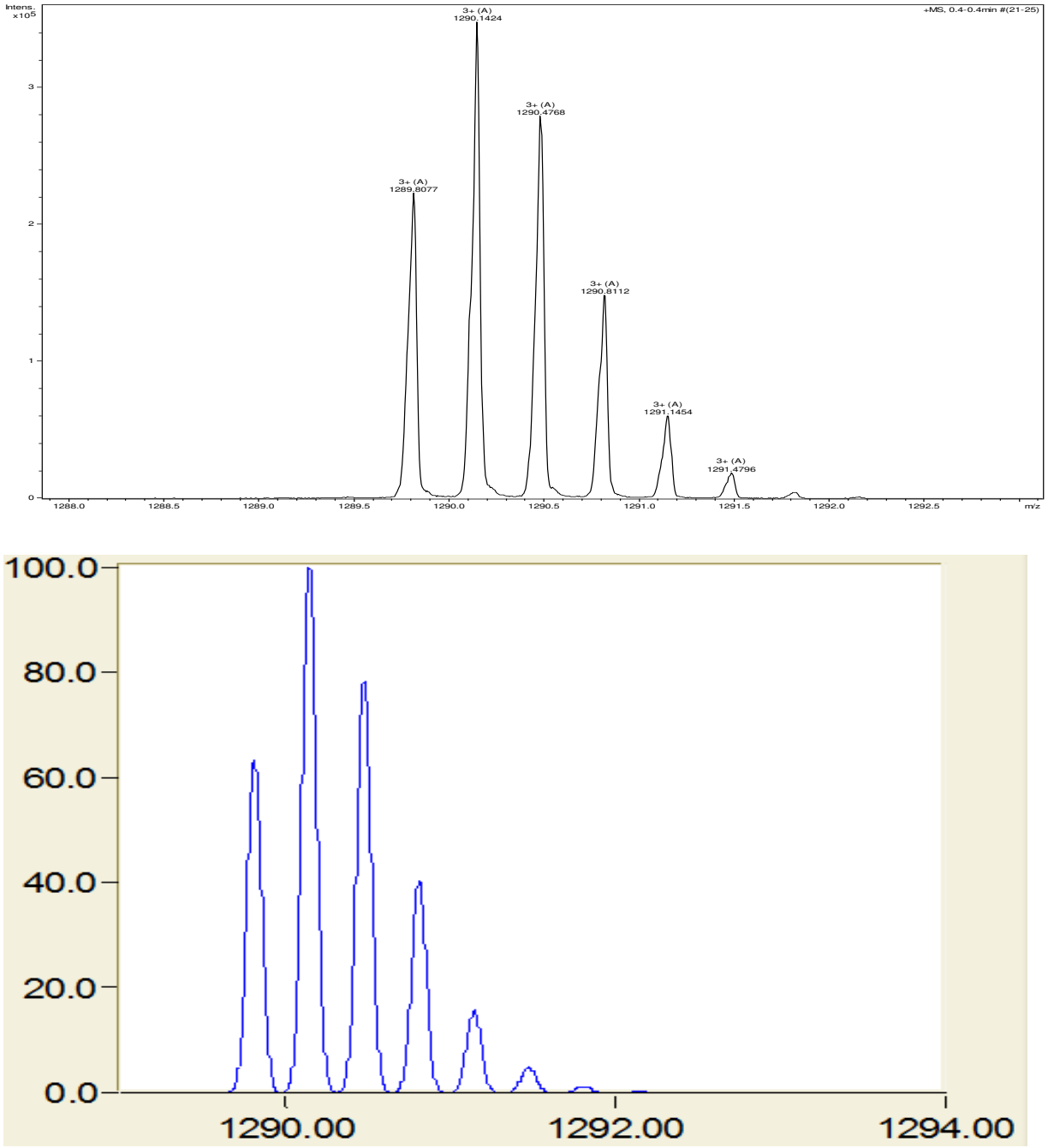


Figure SI 3: Top: Molecular ion peak for the $[Au_9(PPh_3)_8]^{3+}$, bottom: the isotopic distribution and simulated spectra pattern for the molecular ion.

Table SI 2: Values of m/z, fraction and intensity for the simulated high resolution MS for $Au_9$.

| Mass/Charge | Fraction | Intensity |
|---|---|---|
| 1289.80877 | 0.2087423 | 63.49 |
| 1290.1421 | 0.3287728 | 100 |
| 1290.47543 | 0.257153 | 78.22 |
| 1290.80877 | 0.1331733 | 40.51 |
| 1291.1421 | 0.0513696 | 15.62 |
| 1291.47543 | 0.0157422 | 4.79 |
| 1291.80877 | 0.0039922 | 1.21 |
| 1292.1421 | 0.0008617 | 0.26 |
| 1292.47543 | 0.0001616 | 0.05 |
| 1292.80877 | 0.0000267 | 0.01 |
| 1293.1421 | 0.0000075 | 0 |

**$Au_8(PPh_3)_8(NO_3)_2$** was synthesised following the protocol described by Van der Velden *et al.*[8]

$[Au_9(PPh_3)_8](NO_3)_3$ (1.48 g, 0.36 mmol) and $PPh_3$ (0.96 g, 3.66 mmol, 10-fold excess) were mixed in 20 mL of $CH_2Cl_2$. The resulting deep red solution was stirred a further 30 minutes. After that the red product was precipitated by addition of 200 mL of toluene, isolated by filtration on a glass frit (porosity 3), washed alternately with toluene (3 x 20 mL) and hot hexanes (3 x 20 mL) and dried. The red product was crystallized from $CH_2Cl_2$ solution by slow diffusion of diethyl ether at 4°C. Deep red crystals formed within *ca.* 4 days. The crystallization was repeated several times to remove excess of triphenylphosphine.

Yield: 1.38 g, 88 %.

$^{31}P$ NMR (chloroform, 25 °C); δ 58.2 ppm referenced to $H_3PO_4$

Mass spectrometry (MS) was performed using Bruker maXis UHR-TOF MS with an electrospray ionisation (ESI) source and positive-ion polarity.

Isotopic distribution modelling was completed by the molecular weight calculator kindly distributed by PNNl http://ncrr.pnl.gov/software/

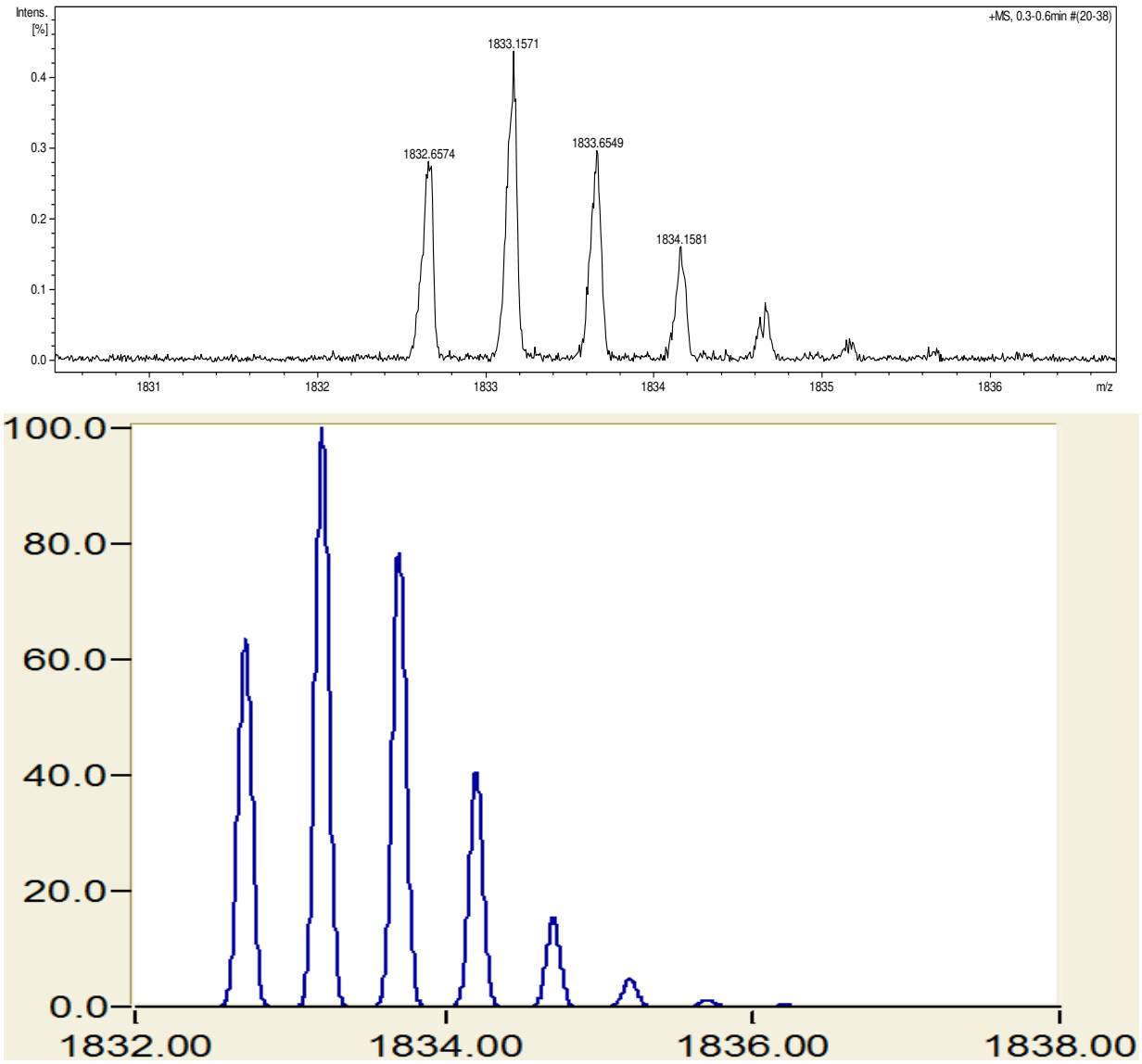


Figure SI 4: Top: Molecular ion peak for the $[Au_8(PPh_3)_8]^{2+}$, bottom: the isotopic distribution and simulated spectra pattern for the molecular ion.

| Mass/Charge | Fraction | Intensity |
|---|---|---|
| 1832.703 | 0.20893 | 63.53 |
| 1833.203 | 0.328881 | 100 |
| 1833.703 | 0.257089 | 78.17 |
| 1834.203 | 0.133062 | 40.46 |
| 1834.703 | 0.051296 | 15.6 |
| 1835.203 | 0.01571 | 4.78 |
| 1835.703 | 0.003982 | 1.21 |
| 1836.203 | 0.000859 | 0.26 |
| 1836.703 | 0.000161 | 0.05 |
| 1837.203 | 2.66E-05 | 0.01 |

Table SI 3: Values of

| | | |
|---|---|---|
| 1837.703 | 7.4E-06 | 0 |

m/z, fraction and intensity for the simulated high resolution MS for $Au_8$.

**Acid washed Evonik P-25 $TiO_2$** was fabricated following the protocol described by Lopez-Sanchez *et al* [9] Evonik P-25 $TiO_2$ (*ca.* 10 g) was acid washed with aqueous $H_2SO_4$ (1 mol/L, 100 ml) with stirring (600 rpm) over 5 hours. The solid was separated by centrifugation (10 min, 5000 rpm). It was then washed with distilled water (50 ml) and methanol (50 ml) by forming a suspension using a Vortex agitator followed by centrifugation (10 min, 5000 rpm) to recover the solid each time. Finally, washed $TiO_2$ was dried at 100 °C under vacuum for 4 hours.

## II. Preparation of the reference samples and recording of the reference spectra

Samples for measuring photoelectron reference spectra of each gold cluster were prepared by drop casting two droplets from a 1 mg/cm$^3$ isopropanol solution of the $Au_n$ cluster on a silicon wafer covered with 10 nm of atomic layer deposited titania. The solution was left drying in air. The photoelectron spectra of the reference samples were recorded using a non-monochromatic Mg-K$\alpha$ radiation and a Phoibos 100 electron energy analyser from SPECS in a vacuum chamber with a base pressure of a few $10^{-10}$ mbar.

## III. Normalisation of the gold intensity

The gold signal was normalised against the silicon dioxide signal according to

$$I_{Au}^{norm} = I_{Au} / \left(1 - \left(I_{Si,Si} + I_{Si,SiO_2} + I_{O,SiO_2}\right)\right) \qquad \text{Eq. 1}$$

where $I_{Au}^{norm}$ is the normalised gold intensity, $I_{Au}$ is the relative gold intensity, $I_{Si,Si}$ the relative intensity of silicon of the silicon substrate, $I_{Si,SiO_2}$ the relative intensity of silicon in the native

$SiO_2$ layer at the surface of Si wafers and $I_{O,SiO_2}$ the relative intensity of oxygen of the silicon dioxide layer covering the silicon substrate. Relative intensity means the intensity of the respective element is normalised by its photo-ionisation cross section and divided by the sum of the intensities of all elements detected. Thus $\left(I_{Si,Si} + I_{Si,SiO_2} + I_{O,SiO_2}\right)$ represents the fraction of the sample not covered by titania particles and $\left(1 - \left(I_{Si,Si} + I_{Si,SiO_2} + I_{O,SiO_2}\right)\right)$. The fraction of the surface covered by titania particles. The uncertainty of the normalisation procedure is the largest contribution to the error bar of the gold intensity in **Error! Reference source not found.**.

## IV. Relative intensity of the phosphorous spectra

For the quantitative analysis of the phosphorous intensity only the phosphorous to gold ratio has been considered. The ratio is calculated as

$$I_{P-Au}^{ratio} = I_P / I_{Au} \qquad \text{Eq. 2}$$

where $I_{P-Au}^{ratio}$ is the phosphorous to gold ratio, $I_P$ is the phosphorous intensity and $I_{Au}$ the gold intensity.

## V. Fitting of the $Au_9$ spectra

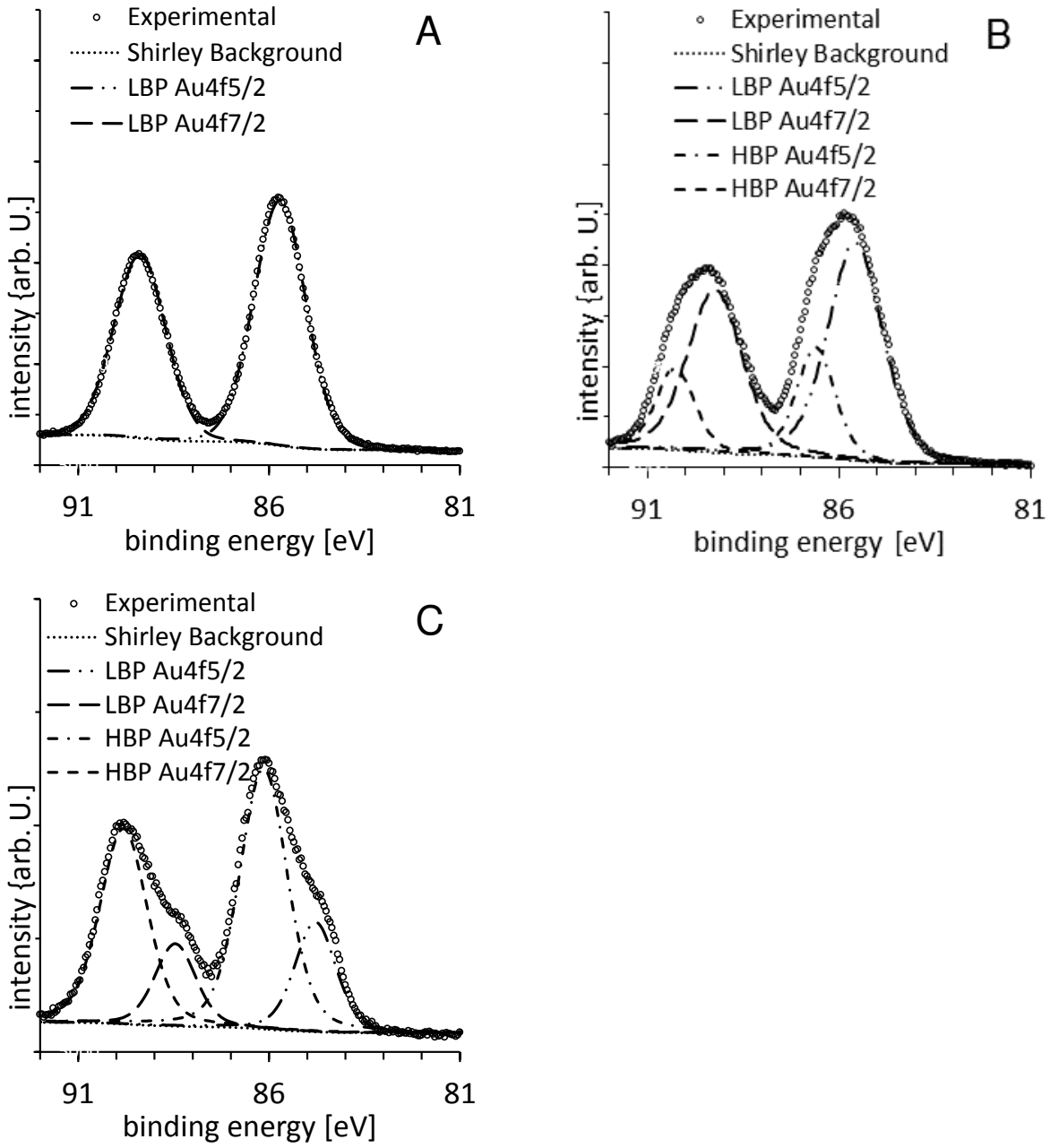


Figure SI 5: fit of the $Au_9$ spectra. A) untreated clusters, B) washed clusters and C) calcined clusters.

## VI. Structure Determination for $Au_8$ and $Au_{11}$ clusters

X-Ray crystal data was collected on a Bruker-Nonius APEX II system using graphite monochromatised Mo Ka (l = 0.71073 Å) radiation. The crystals were kept at 113 K during data collection. The data collection, cell determination and data reduction were all performed with the APEX software. All structures had intensities corrected for Lorentz and polarisation effects and for absorption using SAINT. Absorption corrections were made using SADABS. All structures were solved by direct methods using the XS[10] structure solution program and

refined on F2 using all data by full-matrix least squares procedures using and using Olex2[11], it was refined with the XH[10] refinement package using Least Squares minimisation. All non-hydrogen atoms were refined anisotropically, and all hydrogen atoms were placed as riding atoms with displacement parameters 1.2 times the isotropic equivalent of their carrier carbon atoms. Details of the structures are available from Cambridge Crystallographic Database (CCDC) under reference numbers 907704 for $Au_{11}$ and 907703 for $Au_8$.

**$Au_{11}$ Crystal Data.** $C_{144.5}H_{121}Au_{11}Cl_4P_8$, $M$ =4413.60, monoclinic, $a$ = 22.5484(8) Å, $b$ = 18.1152(6) Å, $c$ = 34.6185(12) Å, $\beta$ = 95.997(2)°, $V$ = 14063.2(8) Å$^3$, $T$ = 113, space group $P2_1/c$ (no. 14), $Z$ = 4, μ(Mo Kα) = 11.640, 244873 reflections measured, 24902 unique ($R_{int}$ = 0.1616) which were used in all calculations. The final $wR_2$ was 0.1612 (all data) and $R_1$ was 0.0570 (>2sigma(I)).

In the Au11 structure similar issues were seen with the phenyl rings, again giving spurious Hirshfeld difference warnings and poor C-C bond accuracies. The counter ion chloride (as opposed to the covalently bound chlorides which were well behaved) was equally disordered over four sites. A half molecule of dichloromethane was also included in the structure.

**$Au_8$ Crystal Data.** $C_{148}H_{128}N_2O_6P_8Au_8Cl_8$, $M$ =4137.62, triclinic, $a$ = 16.8008(5) Å, $b$ = 17.0945(5) Å, $c$ = 28.2942(10) Å, $\alpha$ = 83.338(2)°, $\beta$ = 84.698(2)°, $\gamma$ = 62.656(2)°, $V$ = 7162.4(4) Å$^3$, $T$ = 113, space group P-1 (no. 2), $Z$ = 2, μ(Mo Kα) = 8.453, 96342 reflections measured, 25320 unique ($R_{int}$ = 0.1170) which were used in all calculations. The final $wR_2$ was 0.1447 (all data) and $R_1$ was 0.0634 (>2sigma(I)).

In the $Au_8$ structure, four molecules of dichloromethane were disordered over five sites. Both nitrate anions were poorly ordered with the second nitrate requiring significant restraints. The phenyl rings of the phosphine ligands tend to move in the plane of the ring, meaning the thermal ellipsoids are elongated along some of the bonds. This leads to spurious Hirshfeld difference warnings (that the thermal ellipsoids are elongated towards another atom)[12] and poor C-C bond accuracies.

**Table SI 4: Crystal data and structure refinement for $Au_8(PPh_3)_8(NO_3)_2 \cdot 4CH_2Cl_2$ and $Au_{11}(PPh_3)_8Cl_3 \cdot 0.5CH_2Cl_2$**

| | | |
|---|---|---|
| Empirical formula | $C_{144.5}H_{121}Au_{11}Cl_4P_8$ | $C_{148}H_{128}N_2O_6P_8Au_8Cl_8$ |
| Formula weight | 4413.60 | 4137.62 |
| Temperature/K | 113 (2) | 113 (2) |
| Crystal system | monoclinic | triclinic |
| Space group | $P2_1/c$ | P-1 |

| | | |
|---|---|---|
| a/Å | 22.5484(8) | 16.8008(5) |
| b/Å | 18.1152(6) | 17.0945(5) |
| c/Å | 34.6185(12) | 28.2942(10) |
| α/° | 90.00 | 83.338(2) |
| β/° | 95.997(2) | 84.698(2) |
| γ/° | 90.00 | 62.656(2) |
| Volume/Å$^3$ | 14063.2(8) | 7162.4(4) |
| Z | 4 | 2 |
| $\rho_{calc}$mg/mm$^3$ | 2.085 | 1.919 |
| m/mm$^{-1}$ | 11.640 | 8.453 |
| F(000) | 8180.0 | 3932.0 |
| Crystal size/mm$^3$ | 0.40 × 0.25 × 0.02 | 0.31 × 0.21 × 0.2 |
| 2Θ range for data collection | 4.34 to 50.1° | 3.14 to 50.1° |
| Index ranges | -26 ≤ h ≤ 26, -21 ≤ k ≤ 21, -41 ≤ l ≤ 41 | -18 ≤ h ≤ 20, -19 ≤ k ≤ 20, -33 ≤ l ≤ 33 |
| Reflections collected | 244873 | 96342 |
| Independent reflections | 24902[R(int) = 0.1616] | 25320[R(int) = 0.1170] |
| Data/restraints/parameters | 24902/66/1549 | 25320/145/1675 |
| Goodness-of-fit on F$^2$ | 1.024 | 0.946 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0570, $wR_2$ = 0.1319 | $R_1$ = 0.0634, $wR_2$ = 0.1305 |
| Final R indexes [all data] | $R_1$ = 0.1329, $wR_2$ = 0.1614 | $R_1$ = 0.1241, $wR_2$ = 0.1447 |
| Largest diff. peak/hole / e Å$^{-3}$ | 3.30/-3.03 | 3.31/-2.14 |

**Table SI 5: Bond Lengths for $Au_{11}$**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| Au1 | Au2 | 2.7075(9) | P7 | C67 | 1.83(2) |
| Au1 | Au3 | 2.7199(9) | C55 | C56 | 1.30(3) |
| Au1 | Au4 | 2.7312(10) | C55 | C60 | 1.38(3) |
| Au1 | Au5 | 2.7067(10) | C56 | C57 | 1.39(3) |
| Au1 | Au6 | 2.6919(9) | C57 | C58 | 1.39(3) |
| Au1 | Au7 | 2.7055(9) | C58 | C59 | 1.43(3) |
| Au1 | Au8 | 2.6511(10) | C59 | C60 | 1.35(3) |
| Au1 | Au9 | 2.6437(9) | C61 | C62 | 1.40(2) |
| Au1 | Au10 | 2.6814(9) | C61 | C66 | 1.38(3) |
| Au1 | Au11 | 2.6906(9) | C62 | C63 | 1.37(3) |
| Au2 | Au3 | 2.8870(9) | C63 | C64 | 1.35(3) |
| Au2 | Au4 | 2.8816(9) | C64 | C65 | 1.38(3) |
| Au2 | Au5 | 3.0334(10) | C65 | C66 | 1.37(3) |

| | | | | | |
|---|---|---|---|---|---|
| Au2 | Au6 | 2.9810(10) | C67 | C68 | 1.42(3) |
| Au2 | Au7 | 3.0243(10) | C67 | C72 | 1.36(3) |
| Au2 | P2 | 2.270(5) | C68 | C69 | 1.40(3) |
| Au3 | Au4 | 2.8445(10) | C69 | C70 | 1.37(3) |
| Au3 | Au7 | 2.8904(10) | C70 | C71 | 1.42(4) |
| Au3 | Au9 | 2.8942(10) | C71 | C72 | 1.36(3) |
| Au3 | Cl3 | 2.353(5) | P8 | C73 | 1.79(2) |
| Au4 | Au5 | 2.9064(10) | P8 | C79 | 1.851(19) |
| Au4 | Au10 | 2.8586(10) | P8 | C85 | 1.836(18) |
| Au4 | P4 | 2.286(5) | C73 | C74 | 1.41(3) |
| Au5 | Au6 | 2.9470(10) | C73 | C78 | 1.35(2) |
| Au5 | Au10 | 3.1479(10) | C74 | C75 | 1.42(3) |
| Au5 | Au11 | 2.9447(11) | C75 | C76 | 1.38(3) |
| Au5 | Cl5 | 2.361(5) | C76 | C77 | 1.39(3) |
| Au6 | Au7 | 3.0043(10) | C77 | C78 | 1.40(3) |
| Au6 | Au8 | 3.3647(10) | C79 | C80 | 1.40(3) |
| Au6 | Au11 | 3.0735(10) | C79 | C84 | 1.38(3) |
| Au6 | P6 | 2.298(5) | C80 | C81 | 1.37(3) |
| Au7 | Au8 | 2.9545(10) | C81 | C82 | 1.44(3) |
| Au7 | P7 | 2.312(5) | C82 | C83 | 1.36(3) |
| Au8 | Au9 | 3.1274(10) | C83 | C84 | 1.42(3) |
| Au8 | Au11 | 2.9026(10) | C85 | C86 | 1.34(3) |
| Au8 | P8 | 2.297(6) | C85 | C90 | 1.39(3) |
| Au9 | Au10 | 3.0465(10) | C86 | C87 | 1.43(3) |
| Au9 | P9 | 2.300(5) | C87 | C88 | 1.35(3) |
| Au10 | Au11 | 2.8637(10) | C88 | C89 | 1.34(3) |
| Au10 | P10 | 2.297(5) | C89 | C90 | 1.40(3) |
| Au11 | P11 | 2.298(4) | P9 | C91 | 1.82(2) |
| P2 | C1 | 1.835(19) | P9 | C97 | 1.81(2) |
| P2 | C7 | 1.83(2) | P9 | C103 | 1.81(2) |
| P2 | C13 | 1.832(18) | C91 | C92 | 1.41(3) |

| | | | | | |
|---|---|---|---|---|---|
| C1 | C2 | 1.35(3) | C91 | C96 | 1.41(3) |
| C1 | C6 | 1.40(3) | C92 | C93 | 1.48(4) |
| C2 | C3 | 1.39(3) | C93 | C94 | 1.38(4) |
| C3 | C4 | 1.38(3) | C94 | C95 | 1.38(4) |
| C4 | C5 | 1.33(3) | C95 | C96 | 1.39(4) |
| C5 | C6 | 1.40(3) | C97 | C98 | 1.33(3) |
| C7 | C8 | 1.38(3) | C97 | C102 | 1.43(3) |
| C7 | C12 | 1.37(2) | C98 | C99 | 1.40(3) |
| C8 | C9 | 1.37(3) | C99 | C100 | 1.36(3) |
| C9 | C10 | 1.43(3) | C100 | C101 | 1.36(4) |
| C10 | C11 | 1.35(3) | C101 | C102 | 1.35(3) |
| C11 | C12 | 1.40(3) | C103 | C104 | 1.38(3) |
| C13 | C14 | 1.37(2) | C103 | C108 | 1.41(3) |
| C13 | C18 | 1.38(2) | C104 | C105 | 1.39(3) |
| C14 | C15 | 1.38(3) | C105 | C106 | 1.42(3) |
| C15 | C16 | 1.40(3) | C106 | C107 | 1.35(3) |
| C16 | C17 | 1.37(3) | C107 | C108 | 1.42(3) |
| C17 | C18 | 1.41(2) | P10 | C109 | 1.82(2) |
| P4 | C19 | 1.801(18) | P10 | C115 | 1.842(17) |
| P4 | C25 | 1.842(17) | P10 | C121 | 1.823(18) |
| P4 | C31 | 1.822(19) | C109 | C110 | 1.35(2) |
| C19 | C20 | 1.35(2) | C109 | C114 | 1.38(3) |
| C19 | C24 | 1.46(3) | C110 | C111 | 1.36(3) |
| C20 | C21 | 1.43(3) | C111 | C112 | 1.36(3) |
| C21 | C22 | 1.34(3) | C112 | C113 | 1.41(3) |
| C22 | C23 | 1.37(3) | C113 | C114 | 1.35(3) |
| C23 | C24 | 1.40(3) | C115 | C116 | 1.37(2) |
| C25 | C26 | 1.39(2) | C115 | C120 | 1.37(3) |
| C25 | C30 | 1.35(3) | C116 | C117 | 1.41(3) |
| C26 | C27 | 1.42(3) | C117 | C118 | 1.36(3) |
| C27 | C28 | 1.32(3) | C118 | C119 | 1.39(3) |

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|---|---|---|---|---|---|
| C28 | C29 | 1.35(3) | C119 | C120 | 1.38(3) |
| C29 | C30 | 1.40(3) | C121 | C122 | 1.31(3) |
| C31 | C32 | 1.32(3) | C121 | C126 | 1.40(3) |
| C31 | C36 | 1.40(3) | C122 | C123 | 1.36(4) |
| C32 | C33 | 1.40(3) | C123 | C124 | 1.38(4) |
| C33 | C34 | 1.37(3) | C124 | C125 | 1.43(4) |
| C34 | C35 | 1.37(3) | C125 | C126 | 1.35(3) |
| C35 | C36 | 1.37(3) | P11 | C127 | 1.87(2) |
| P6 | C37 | 1.814(19) | P11 | C133 | 1.807(19) |
| P6 | C43 | 1.832(19) | P11 | C139 | 1.818(18) |
| P6 | C49 | 1.802(19) | C127 | C128 | 1.39(3) |
| C37 | C38 | 1.35(2) | C127 | C132 | 1.34(3) |
| C37 | C42 | 1.37(2) | C128 | C129 | 1.41(3) |
| C38 | C39 | 1.41(3) | C129 | C130 | 1.35(3) |
| C39 | C40 | 1.39(3) | C130 | C131 | 1.40(3) |
| C40 | C41 | 1.40(3) | C131 | C132 | 1.39(3) |
| C41 | C42 | 1.41(3) | C133 | C134 | 1.41(3) |
| C43 | C44 | 1.35(3) | C133 | C138 | 1.37(3) |
| C43 | C48 | 1.39(3) | C134 | C135 | 1.45(3) |
| C44 | C45 | 1.36(3) | C135 | C136 | 1.38(3) |
| C45 | C46 | 1.37(4) | C136 | C137 | 1.40(3) |
| C46 | C47 | 1.37(4) | C137 | C138 | 1.37(3) |
| C47 | C48 | 1.38(3) | C139 | C140 | 1.38(2) |
| C49 | C50 | 1.37(3) | C139 | C144 | 1.39(3) |
| C49 | C54 | 1.42(3) | C140 | C141 | 1.36(3) |
| C50 | C51 | 1.41(3) | C141 | C142 | 1.36(3) |
| C51 | C52 | 1.34(3) | C142 | C143 | 1.37(3) |
| C52 | C53 | 1.42(3) | C143 | C144 | 1.39(3) |
| C53 | C54 | 1.40(3) | C500 | Cl50 | 1.59(5) |
| P7 | C55 | 1.825(19) | C500 | Cl51 | 1.53(5) |
| P7 | C61 | 1.858(18) | | | |

**Table SI 6: Bond Angles for $Au_{11}$.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| Au2 | Au1 | Au3 | 64.27(3) | C9 | C8 | C7 | 123.1(18) |
| Au2 | Au1 | Au4 | 63.99(3) | C8 | C9 | C10 | 117.0(18) |
| Au3 | Au1 | Au4 | 62.91(3) | C11 | C10 | C9 | 120.0(18) |
| Au5 | Au1 | Au2 | 68.15(3) | C10 | C11 | C12 | 120.8(19) |
| Au5 | Au1 | Au3 | 120.02(3) | C7 | C12 | C11 | 119.7(19) |
| Au5 | Au1 | Au4 | 64.62(3) | C14 | C13 | P2 | 117.8(14) |
| Au6 | Au1 | Au2 | 67.02(3) | C14 | C13 | C18 | 120.2(17) |
| Au6 | Au1 | Au3 | 120.82(3) | C18 | C13 | P2 | 122.0(14) |
| Au6 | Au1 | Au4 | 119.77(3) | C13 | C14 | C15 | 118.9(19) |
| Au6 | Au1 | Au5 | 66.17(3) | C14 | C15 | C16 | 122(2) |
| Au6 | Au1 | Au7 | 67.64(3) | C17 | C16 | C15 | 119.1(19) |
| Au7 | Au1 | Au2 | 67.93(3) | C16 | C17 | C18 | 118.9(18) |
| Au7 | Au1 | Au3 | 64.38(3) | C13 | C18 | C17 | 120.7(17) |
| Au7 | Au1 | Au4 | 119.49(3) | C19 | P4 | Au4 | 109.7(6) |
| Au7 | Au1 | Au5 | 125.26(3) | C19 | P4 | C25 | 102.9(7) |
| Au8 | Au1 | Au2 | 130.58(3) | C19 | P4 | C31 | 110.7(8) |
| Au8 | Au1 | Au3 | 111.11(3) | C25 | P4 | Au4 | 117.4(6) |
| Au8 | Au1 | Au4 | 162.08(3) | C31 | P4 | Au4 | 113.3(7) |
| Au8 | Au1 | Au5 | 127.35(3) | C31 | P4 | C25 | 102.1(9) |
| Au8 | Au1 | Au6 | 78.06(3) | C20 | C19 | P4 | 122.6(14) |
| Au8 | Au1 | Au7 | 66.94(3) | C20 | C19 | C24 | 116.1(17) |
| Au8 | Au1 | Au10 | 105.15(3) | C24 | C19 | P4 | 121.2(14) |
| Au8 | Au1 | Au11 | 65.82(3) | C19 | C20 | C21 | 124(2) |
| Au9 | Au1 | Au2 | 129.44(3) | C22 | C21 | C20 | 118(2) |
| Au9 | Au1 | Au3 | 65.29(3) | C21 | C22 | C23 | 122(2) |
| Au9 | Au1 | Au4 | 90.12(3) | C22 | C23 | C24 | 120(2) |
| Au9 | Au1 | Au5 | 140.24(3) | C23 | C24 | C19 | 119.3(19) |
| Au9 | Au1 | Au6 | 149.51(4) | C26 | C25 | P4 | 116.8(13) |
| Au9 | Au1 | Au7 | 93.45(3) | C30 | C25 | P4 | 121.4(14) |

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|---|---|---|---|---|---|---|---|
| Au9 | Au1 | Au8 | 72.41(3) | C30 | C25 | C26 | 121.8(17) |
| Au9 | Au1 | Au10 | 69.79(3) | C25 | C26 | C27 | 116.5(18) |
| Au9 | Au1 | Au11 | 103.95(3) | C28 | C27 | C26 | 122(2) |
| Au10 | Au1 | Au2 | 123.53(3) | C27 | C28 | C29 | 120(2) |
| Au10 | Au1 | Au3 | 107.66(3) | C28 | C29 | C30 | 121(2) |
| Au10 | Au1 | Au4 | 63.75(3) | C25 | C30 | C29 | 119(2) |
| Au10 | Au1 | Au5 | 71.49(3) | C32 | C31 | P4 | 125.6(16) |
| Au10 | Au1 | Au6 | 126.70(3) | C32 | C31 | C36 | 117.0(19) |
| Au10 | Au1 | Au7 | 163.19(3) | C36 | C31 | P4 | 117.0(14) |
| Au10 | Au1 | Au11 | 64.43(3) | C31 | C32 | C33 | 122(2) |
| Au11 | Au1 | Au2 | 126.20(3) | C34 | C33 | C32 | 119(2) |
| Au11 | Au1 | Au3 | 168.94(3) | C35 | C34 | C33 | 121(2) |
| Au11 | Au1 | Au4 | 116.50(3) | C34 | C35 | C36 | 118(2) |
| Au11 | Au1 | Au5 | 66.13(3) | C35 | C36 | C31 | 123(2) |
| Au11 | Au1 | Au6 | 69.64(3) | C37 | P6 | Au6 | 114.3(6) |
| Au11 | Au1 | Au7 | 120.91(3) | C37 | P6 | C43 | 101.2(9) |
| Au1 | Au2 | Au3 | 58.07(2) | C43 | P6 | Au6 | 115.6(6) |
| Au1 | Au2 | Au4 | 58.41(2) | C49 | P6 | Au6 | 114.2(7) |
| Au1 | Au2 | Au5 | 55.91(2) | C49 | P6 | C37 | 105.5(8) |
| Au1 | Au2 | Au6 | 56.24(2) | C49 | P6 | C43 | 104.6(10) |
| Au1 | Au2 | Au7 | 56.00(2) | C38 | C37 | P6 | 120.3(14) |
| Au3 | Au2 | Au5 | 105.07(3) | C38 | C37 | C42 | 116.1(18) |
| Au3 | Au2 | Au6 | 106.63(3) | C42 | C37 | P6 | 123.6(16) |
| Au3 | Au2 | Au7 | 58.49(2) | C37 | C38 | C39 | 123.5(18) |
| Au4 | Au2 | Au3 | 59.09(2) | C40 | C39 | C38 | 119(2) |
| Au4 | Au2 | Au5 | 58.79(2) | C39 | C40 | C41 | 119(2) |
| Au4 | Au2 | Au6 | 106.29(3) | C40 | C41 | C42 | 117.6(18) |
| Au4 | Au2 | Au7 | 105.32(3) | C37 | C42 | C41 | 124(2) |
| Au6 | Au2 | Au5 | 58.67(2) | C44 | C43 | P6 | 125.5(16) |
| Au6 | Au2 | Au7 | 60.03(2) | C44 | C43 | C48 | 120.5(18) |
| Au7 | Au2 | Au5 | 105.01(3) | C48 | C43 | P6 | 113.6(17) |

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|---|---|---|---|---|---|---|---|
| P2 | Au2 | Au1 | 176.14(13) | C43 | C44 | C45 | 123(2) |
| P2 | Au2 | Au3 | 122.63(12) | C44 | C45 | C46 | 117(2) |
| P2 | Au2 | Au4 | 118.25(13) | C45 | C46 | C47 | 122(2) |
| P2 | Au2 | Au5 | 121.12(12) | C46 | C47 | C48 | 120(2) |
| P2 | Au2 | Au6 | 125.20(12) | C47 | C48 | C43 | 118(2) |
| P2 | Au2 | Au7 | 127.83(13) | C50 | C49 | P6 | 124.1(17) |
| Au1 | Au3 | Au2 | 57.66(2) | C50 | C49 | C54 | 116.7(18) |
| Au1 | Au3 | Au4 | 58.74(2) | C54 | C49 | P6 | 119.1(14) |
| Au1 | Au3 | Au7 | 57.57(2) | C49 | C50 | C51 | 124(2) |
| Au1 | Au3 | Au9 | 56.08(2) | C52 | C51 | C50 | 118(2) |
| Au2 | Au3 | Au7 | 63.13(2) | C51 | C52 | C53 | 122(2) |
| Au2 | Au3 | Au9 | 113.65(3) | C54 | C53 | C52 | 118(2) |
| Au4 | Au3 | Au2 | 60.36(2) | C55 | P7 | Au7 | 113.6(6) |
| Au4 | Au3 | Au7 | 109.94(3) | C55 | P7 | C61 | 102.9(8) |
| Au4 | Au3 | Au9 | 83.06(3) | C55 | P7 | C67 | 108.2(9) |
| Au7 | Au3 | Au9 | 84.65(3) | C61 | P7 | Au7 | 112.5(6) |
| Cl3 | Au3 | Au1 | 178.19(14) | C67 | P7 | Au7 | 117.6(6) |
| Cl3 | Au3 | Au2 | 120.73(14) | C67 | P7 | C61 | 100.3(8) |
| Cl3 | Au3 | Au4 | 121.54(16) | C53 | C54 | C49 | 120.9(19) |
| Cl3 | Au3 | Au7 | 121.25(15) | C56 | C55 | P7 | 118.6(14) |
| Cl3 | Au3 | Au9 | 125.58(14) | C56 | C55 | C60 | 118.5(19) |
| Au1 | Au4 | Au2 | 57.61(2) | C60 | C55 | P7 | 122.7(17) |
| Au1 | Au4 | Au3 | 58.35(2) | C55 | C56 | C57 | 126(2) |
| Au1 | Au4 | Au5 | 57.28(2) | C58 | C57 | C56 | 115(2) |
| Au1 | Au4 | Au10 | 57.28(2) | C57 | C58 | C59 | 119.1(19) |
| Au2 | Au4 | Au5 | 63.21(2) | C60 | C59 | C58 | 120(2) |
| Au3 | Au4 | Au2 | 60.55(2) | C59 | C60 | C55 | 120(2) |
| Au3 | Au4 | Au5 | 109.62(3) | C62 | C61 | P7 | 119.5(13) |
| Au3 | Au4 | Au10 | 99.74(3) | C66 | C61 | P7 | 119.9(14) |
| Au10 | Au4 | Au2 | 111.60(3) | C66 | C61 | C62 | 120.6(17) |
| Au10 | Au4 | Au5 | 66.18(2) | C63 | C62 | C61 | 118.0(18) |

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|---|---|---|---|---|---|---|---|
| P4 | Au4 | Au1 | 171.57(12) | C64 | C63 | C62 | 122(2) |
| P4 | Au4 | Au2 | 130.80(12) | C63 | C64 | C65 | 120(2) |
| P4 | Au4 | Au3 | 123.20(12) | C66 | C65 | C64 | 121(2) |
| P4 | Au4 | Au5 | 124.79(12) | C65 | C66 | C61 | 118.8(19) |
| P4 | Au4 | Au10 | 115.09(11) | C68 | C67 | P7 | 116.8(14) |
| Au1 | Au5 | Au2 | 55.94(2) | C72 | C67 | P7 | 122.0(17) |
| Au1 | Au5 | Au4 | 58.10(2) | C72 | C67 | C68 | 121(2) |
| Au1 | Au5 | Au6 | 56.67(2) | C69 | C68 | C67 | 118(2) |
| Au1 | Au5 | Au10 | 53.88(2) | C70 | C69 | C68 | 120(2) |
| Au1 | Au5 | Au11 | 56.67(2) | C69 | C70 | C71 | 122(2) |
| Au2 | Au5 | Au10 | 100.35(3) | C72 | C71 | C70 | 118(2) |
| Au4 | Au5 | Au2 | 57.99(2) | C73 | P8 | Au8 | 116.1(6) |
| Au4 | Au5 | Au6 | 106.54(3) | C73 | P8 | C79 | 101.8(8) |
| Au4 | Au5 | Au10 | 56.18(2) | C73 | P8 | C85 | 101.0(8) |
| Au4 | Au5 | Au11 | 103.99(3) | C79 | P8 | Au8 | 114.8(7) |
| Au6 | Au5 | Au2 | 59.78(2) | C85 | P8 | Au8 | 114.5(6) |
| Au6 | Au5 | Au10 | 103.94(3) | C85 | P8 | C79 | 107.0(8) |
| Au11 | Au5 | Au2 | 107.26(3) | C71 | C72 | C67 | 122(2) |
| Au11 | Au5 | Au6 | 62.89(2) | C74 | C73 | P8 | 118.6(15) |
| Au11 | Au5 | Au10 | 55.95(2) | C78 | C73 | P8 | 125.4(15) |
| Cl5 | Au5 | Au1 | 178.94(13) | C78 | C73 | C74 | 115.7(19) |
| Cl5 | Au5 | Au2 | 125.12(12) | C73 | C74 | C75 | 122(2) |
| Cl5 | Au5 | Au4 | 122.23(14) | C76 | C75 | C74 | 121(2) |
| Cl5 | Au5 | Au6 | 123.63(14) | C75 | C76 | C77 | 115(2) |
| Cl5 | Au5 | Au10 | 125.30(13) | C76 | C77 | C78 | 123(2) |
| Cl5 | Au5 | Au11 | 122.40(12) | C73 | C78 | C77 | 122(2) |
| Au1 | Au6 | Au2 | 56.74(2) | C80 | C79 | P8 | 115.8(15) |
| Au1 | Au6 | Au5 | 57.16(2) | C84 | C79 | P8 | 123.1(15) |
| Au1 | Au6 | Au7 | 56.39(2) | C84 | C79 | C80 | 121.1(18) |
| Au1 | Au6 | Au8 | 50.43(2) | C81 | C80 | C79 | 120(2) |
| Au1 | Au6 | Au11 | 55.16(2) | C80 | C81 | C82 | 119(2) |

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|---|---|---|---|---|---|---|---|
| Au2 | Au6 | Au7 | 60.70(2) | C83 | C82 | C81 | 122(2) |
| Au2 | Au6 | Au8 | 100.02(3) | C82 | C83 | C84 | 118(2) |
| Au2 | Au6 | Au11 | 105.32(3) | C79 | C84 | C83 | 120(2) |
| Au5 | Au6 | Au2 | 61.55(2) | C86 | C85 | P8 | 123.0(15) |
| Au5 | Au6 | Au7 | 107.72(3) | C86 | C85 | C90 | 120.0(18) |
| Au5 | Au6 | Au8 | 98.86(3) | C90 | C85 | P8 | 116.7(14) |
| Au5 | Au6 | Au11 | 58.52(2) | C85 | C86 | C87 | 120(2) |
| Au7 | Au6 | Au8 | 54.92(2) | C88 | C87 | C86 | 119(2) |
| Au7 | Au6 | Au11 | 101.13(3) | C89 | C88 | C87 | 121(2) |
| Au11 | Au6 | Au8 | 53.36(2) | C88 | C89 | C90 | 121(2) |
| P6 | Au6 | Au1 | 175.04(14) | C91 | P9 | Au9 | 114.2(7) |
| P6 | Au6 | Au2 | 121.31(13) | C97 | P9 | Au9 | 115.9(7) |
| P6 | Au6 | Au5 | 117.92(13) | C97 | P9 | C91 | 103.8(11) |
| P6 | Au6 | Au7 | 127.50(13) | C103 | P9 | Au9 | 114.3(7) |
| P6 | Au6 | Au8 | 133.69(14) | C103 | P9 | C91 | 105.4(10) |
| P6 | Au6 | Au11 | 123.76(12) | C103 | P9 | C97 | 101.8(9) |
| Au1 | Au7 | Au2 | 56.06(2) | C85 | C90 | C89 | 119(2) |
| Au1 | Au7 | Au3 | 58.05(2) | C92 | C91 | P9 | 119.7(19) |
| Au1 | Au7 | Au6 | 55.96(2) | C92 | C91 | C96 | 121(2) |
| Au1 | Au7 | Au8 | 55.65(2) | C96 | C91 | P9 | 120(2) |
| Au3 | Au7 | Au2 | 58.38(2) | C91 | C92 | C93 | 118(3) |
| Au3 | Au7 | Au6 | 105.93(3) | C94 | C93 | C92 | 118(3) |
| Au3 | Au7 | Au8 | 98.54(3) | C95 | C94 | C93 | 122(3) |
| Au6 | Au7 | Au2 | 59.27(2) | C94 | C95 | C96 | 120(3) |
| Au8 | Au7 | Au2 | 109.02(3) | C95 | C96 | C91 | 120(3) |
| Au8 | Au7 | Au6 | 68.75(2) | C98 | C97 | P9 | 117.4(18) |
| P7 | Au7 | Au1 | 166.70(13) | C98 | C97 | C102 | 117(2) |
| P7 | Au7 | Au2 | 123.43(13) | C102 | C97 | P9 | 124.9(19) |
| P7 | Au7 | Au3 | 109.45(13) | C97 | C98 | C99 | 124(2) |
| P7 | Au7 | Au6 | 136.83(12) | C100 | C99 | C98 | 116(3) |
| P7 | Au7 | Au8 | 127.52(13) | C99 | C100 | C101 | 123(3) |

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|---|---|---|---|---|---|---|---|
| Au1 | Au8 | Au6 | 51.51(2) | C102 | C101 | C100 | 120(2) |
| Au1 | Au8 | Au7 | 57.41(2) | C101 | C102 | C97 | 120(2) |
| Au1 | Au8 | Au9 | 53.69(2) | C104 | C103 | P9 | 119.3(15) |
| Au1 | Au8 | Au11 | 57.74(2) | C104 | C103 | C108 | 119.9(18) |
| Au7 | Au8 | Au6 | 56.33(2) | C108 | C103 | P9 | 120.9(15) |
| Au7 | Au8 | Au9 | 79.59(3) | C103 | C104 | C105 | 120.9(18) |
| Au9 | Au8 | Au6 | 104.86(3) | C104 | C105 | C106 | 120(2) |
| Au11 | Au8 | Au6 | 58.18(2) | C107 | C106 | C105 | 120(2) |
| Au11 | Au8 | Au7 | 106.55(3) | C106 | C107 | C108 | 121.5(19) |
| Au11 | Au8 | Au9 | 88.28(3) | C109 | P10 | Au10 | 116.3(6) |
| P8 | Au8 | Au1 | 178.20(13) | C109 | P10 | C115 | 103.6(8) |
| P8 | Au8 | Au6 | 127.49(13) | C109 | P10 | C121 | 103.5(9) |
| P8 | Au8 | Au7 | 123.68(13) | C115 | P10 | Au10 | 112.3(6) |
| P8 | Au8 | Au9 | 127.47(13) | C121 | P10 | Au10 | 112.8(7) |
| P8 | Au8 | Au11 | 120.53(13) | C121 | P10 | C115 | 107.4(8) |
| Au1 | Au9 | Au3 | 58.62(2) | C103 | C108 | C107 | 118.4(19) |
| Au1 | Au9 | Au8 | 53.91(2) | C110 | C109 | P10 | 118.9(16) |
| Au1 | Au9 | Au10 | 55.69(2) | C110 | C109 | C114 | 117(2) |
| Au3 | Au9 | Au8 | 94.64(3) | C114 | C109 | P10 | 123.6(15) |
| Au3 | Au9 | Au10 | 94.41(3) | C109 | C110 | C111 | 121(2) |
| Au10 | Au9 | Au8 | 86.61(3) | C110 | C111 | C112 | 123(2) |
| P9 | Au9 | Au1 | 175.81(14) | C111 | C112 | C113 | 117(2) |
| P9 | Au9 | Au3 | 117.36(14) | C114 | C113 | C112 | 119(2) |
| P9 | Au9 | Au8 | 127.24(15) | C113 | C114 | C109 | 123(2) |
| P9 | Au9 | Au10 | 127.41(14) | C116 | C115 | P10 | 120.9(14) |
| Au1 | Au10 | Au4 | 58.97(2) | C120 | C115 | P10 | 118.3(14) |
| Au1 | Au10 | Au5 | 54.63(2) | C120 | C115 | C116 | 120.6(17) |
| Au1 | Au10 | Au9 | 54.52(2) | C115 | C116 | C117 | 120.8(18) |
| Au1 | Au10 | Au11 | 57.94(2) | C118 | C117 | C116 | 118.3(19) |
| Au4 | Au10 | Au5 | 57.64(2) | C117 | C118 | C119 | 121(2) |
| Au4 | Au10 | Au9 | 80.17(3) | C120 | C119 | C118 | 120(2) |

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|---|---|---|---|---|---|---|---|
| Au4 | Au10 | Au11 | 107.36(3) | C115 | C120 | C119 | 119(2) |
| Au9 | Au10 | Au5 | 108.63(3) | C122 | C121 | P10 | 116.6(16) |
| Au11 | Au10 | Au5 | 58.43(2) | C122 | C121 | C126 | 122.2(19) |
| Au11 | Au10 | Au9 | 90.58(3) | C126 | C121 | P10 | 121.1(16) |
| P10 | Au10 | Au1 | 174.64(12) | C121 | C122 | C123 | 122(3) |
| P10 | Au10 | Au4 | 122.50(13) | C122 | C123 | C124 | 117(3) |
| P10 | Au10 | Au5 | 121.05(13) | C123 | C124 | C125 | 122(3) |
| P10 | Au10 | Au9 | 130.16(13) | C126 | C125 | C124 | 117(3) |
| P10 | Au10 | Au11 | 117.59(12) | C127 | P11 | Au11 | 116.5(6) |
| Au1 | Au11 | Au5 | 57.20(2) | C133 | P11 | Au11 | 116.3(7) |
| Au1 | Au11 | Au6 | 55.20(2) | C133 | P11 | C127 | 105.9(9) |
| Au1 | Au11 | Au8 | 56.43(2) | C133 | P11 | C139 | 102.1(9) |
| Au1 | Au11 | Au10 | 57.63(2) | C139 | P11 | Au11 | 112.4(6) |
| Au5 | Au11 | Au6 | 58.59(2) | C139 | P11 | C127 | 101.7(9) |
| Au8 | Au11 | Au5 | 110.42(3) | C125 | C126 | C121 | 119(2) |
| Au8 | Au11 | Au6 | 68.46(2) | C128 | C127 | P11 | 116.3(16) |
| Au10 | Au11 | Au5 | 65.62(3) | C132 | C127 | P11 | 121.9(17) |
| Au10 | Au11 | Au6 | 107.92(3) | C132 | C127 | C128 | 122(2) |
| Au10 | Au11 | Au8 | 94.51(3) | C127 | C128 | C129 | 118(2) |
| P11 | Au11 | Au1 | 177.27(13) | C130 | C129 | C128 | 121(2) |
| P11 | Au11 | Au5 | 124.96(13) | C129 | C130 | C131 | 119(2) |
| P11 | Au11 | Au6 | 127.02(13) | C132 | C131 | C130 | 121(2) |
| P11 | Au11 | Au8 | 122.14(13) | C127 | C132 | C131 | 119(2) |
| P11 | Au11 | Au10 | 121.09(13) | C134 | C133 | P11 | 115.6(14) |
| C1 | P2 | Au2 | 111.6(6) | C138 | C133 | P11 | 124.8(17) |
| C7 | P2 | Au2 | 113.8(6) | C138 | C133 | C134 | 119.5(18) |
| C7 | P2 | C1 | 106.3(8) | C133 | C134 | C135 | 117.8(17) |
| C7 | P2 | C13 | 103.2(9) | C136 | C135 | C134 | 121(2) |
| C13 | P2 | Au2 | 116.7(6) | C135 | C136 | C137 | 118(2) |
| C13 | P2 | C1 | 104.2(8) | C138 | C137 | C136 | 122(2) |
| C2 | C1 | P2 | 118.5(14) | C137 | C138 | C133 | 121(2) |

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|---|---|---|---|---|---|---|---|
| C2 | C1 | C6 | 119.8(18) | C140 | C139 | P11 | 119.8(15) |
| C6 | C1 | P2 | 121.8(16) | C140 | C139 | C144 | 119.7(17) |
| C1 | C2 | C3 | 120.6(19) | C144 | C139 | P11 | 120.2(14) |
| C4 | C3 | C2 | 120(2) | C141 | C140 | C139 | 119.3(18) |
| C5 | C4 | C3 | 119.6(19) | C140 | C141 | C142 | 121.4(19) |
| C4 | C5 | C6 | 121.4(19) | C141 | C142 | C143 | 121(2) |
| C1 | C6 | C5 | 118.5(19) | C142 | C143 | C144 | 119.2(19) |
| C8 | C7 | P2 | 122.8(14) | C143 | C144 | C139 | 119.7(18) |
| C12 | C7 | P2 | 118.2(14) | Cl51 | C500 | Cl50 | 121(3) |
| C12 | C7 | C8 | 119.0(18) | | | | |

**Table SI 7: Bond Lengths for $Au_8$.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| Au1 | Au2 | 2.8748(6) | C57 | C58 | 1.387(19) |
| Au1 | Au3 | 2.8701(6) | C58 | C59 | 1.391(16) |
| Au1 | Au4 | 2.8852(6) | C59 | C60 | 1.393(15) |
| Au1 | Au6 | 2.7318(5) | C61 | C62 | 1.444(16) |
| Au1 | P7 | 2.322(3) | C61 | C66 | 1.422(17) |
| Au2 | Au6 | 2.7290(5) | C62 | C63 | 1.343(17) |
| Au2 | Au7 | 2.8882(6) | C63 | C64 | 1.383(19) |
| Au2 | P5 | 2.317(3) | C64 | C65 | 1.326(18) |
| Au3 | Au5 | 2.8664(5) | C65 | C66 | 1.377(18) |
| Au3 | Au6 | 2.6828(6) | C67 | C68 | 1.374(16) |
| Au3 | P3 | 2.290(3) | C67 | C72 | 1.391(13) |
| Au4 | Au5 | 2.8777(6) | C68 | C69 | 1.412(13) |
| Au4 | Au6 | 2.5827(6) | C69 | C70 | 1.365(15) |
| Au4 | Au7 | 2.8925(7) | C70 | C71 | 1.408(18) |
| Au4 | P4 | 2.260(3) | C71 | C72 | 1.348(13) |
| Au5 | Au6 | 2.7950(6) | C73 | C74 | 1.402(12) |
| Au5 | Au8 | 2.8723(7) | C73 | C78 | 1.416(15) |
| Au5 | P2 | 2.339(3) | C74 | C75 | 1.370(14) |

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|---|---|---|---|---|---|
| Au6 | Au7 | 2.7352(6) | C75 | C76 | 1.410(17) |
| Au6 | Au8 | 2.6783(5) | C76 | C77 | 1.379(14) |
| Au6 | P1 | 2.382(3) | C77 | C78 | 1.389(15) |
| Au7 | Au8 | 2.8453(6) | C79 | C80 | 1.391(15) |
| Au7 | P6 | 2.316(3) | C79 | C84 | 1.355(14) |
| Au8 | P8 | 2.290(3) | C80 | C81 | 1.360(14) |
| P1 | C73 | 1.833(10) | C81 | C82 | 1.370(15) |
| P1 | C79 | 1.860(9) | C82 | C83 | 1.367(16) |
| P1 | C85 | 1.841(10) | C83 | C84 | 1.397(14) |
| P2 | C37 | 1.764(12) | C85 | C86 | 1.389(15) |
| P2 | C43 | 1.850(10) | C85 | C90 | 1.392(14) |
| P2 | C49 | 1.843(11) | C86 | C87 | 1.365(16) |
| P3 | C55 | 1.818(12) | C87 | C88 | 1.385(15) |
| P3 | C61 | 1.760(12) | C88 | C89 | 1.400(16) |
| P3 | C67 | 1.845(9) | C89 | C90 | 1.379(15) |
| P4 | C126 | 1.794(9) | C91 | C92 | 1.378(16) |
| P4 | C132 | 1.853(11) | C91 | C96 | 1.376(16) |
| P4 | C137 | 1.826(12) | C92 | C93 | 1.371(16) |
| P5 | C91 | 1.814(11) | C93 | C94 | 1.392(18) |
| P5 | C97 | 1.804(12) | C94 | C95 | 1.378(18) |
| P5 | C103 | 1.833(11) | C95 | C96 | 1.383(17) |
| P6 | C1 | 1.857(10) | C97 | C98 | 1.399(16) |
| P6 | C7 | 1.822(11) | C97 | C102 | 1.358(14) |
| P6 | C13 | 1.805(11) | C98 | C99 | 1.400(17) |
| P7 | C109 | 1.784(11) | C99 | C100 | 1.350(16) |
| P7 | C115 | 1.792(10) | C100 | C101 | 1.36(2) |
| P7 | C121 | 1.810(13) | C101 | C102 | 1.419(18) |
| P8 | C19 | 1.831(12) | C103 | C104 | 1.402(16) |
| P8 | C30 | 1.793(12) | C103 | C108 | 1.390(15) |
| P8 | C31 | 1.790(11) | C104 | C105 | 1.393(15) |
| C1 | C2 | 1.316(15) | C105 | C106 | 1.330(17) |

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|---|---|---|---|---|---|
| C1 | C6 | 1.386(14) | C106 | C107 | 1.396(17) |
| C2 | C3 | 1.358(14) | C107 | C108 | 1.348(16) |
| C3 | C4 | 1.442(16) | C109 | C110 | 1.341(14) |
| C4 | C5 | 1.315(17) | C109 | C114 | 1.439(13) |
| C5 | C6 | 1.396(15) | C110 | C111 | 1.398(17) |
| C7 | C8 | 1.439(15) | C111 | C112 | 1.422(15) |
| C7 | C12 | 1.332(17) | C112 | C113 | 1.368(15) |
| C8 | C9 | 1.376(16) | C113 | C114 | 1.385(17) |
| C9 | C10 | 1.388(18) | C115 | C116 | 1.430(13) |
| C10 | C11 | 1.408(18) | C115 | C120 | 1.403(16) |
| C11 | C12 | 1.395(17) | C116 | C117 | 1.350(15) |
| C13 | C14 | 1.424(16) | C117 | C118 | 1.394(19) |
| C13 | C18 | 1.368(14) | C118 | C119 | 1.378(15) |
| C14 | C15 | 1.360(16) | C119 | C120 | 1.368(15) |
| C15 | C16 | 1.352(14) | C121 | C122 | 1.319(17) |
| C16 | C17 | 1.408(18) | C121 | C142 | 1.377(17) |
| C17 | C18 | 1.348(17) | C122 | C123 | 1.377(19) |
| C19 | C20 | 1.402(16) | C123 | C124 | 1.38(2) |
| C19 | C24 | 1.381(17) | C124 | C125 | 1.336(18) |
| C20 | C21 | 1.347(17) | C125 | C142 | 1.381(19) |
| C21 | C22 | 1.336(18) | C126 | C127 | 1.358(16) |
| C22 | C23 | 1.351(18) | C126 | C131 | 1.428(13) |
| C23 | C24 | 1.423(19) | C127 | C128 | 1.397(14) |
| C25 | C26 | 1.438(17) | C128 | C129 | 1.400(15) |
| C25 | C30 | 1.401(15) | C129 | C130 | 1.381(17) |
| C26 | C27 | 1.352(17) | C130 | C131 | 1.379(14) |
| C27 | C28 | 1.412(17) | C132 | C133 | 1.353(17) |
| C28 | C29 | 1.399(17) | C132 | C136 | 1.364(16) |
| C29 | C30 | 1.398(16) | C133 | C134 | 1.376(17) |
| C31 | C32 | 1.418(13) | C134 | C143 | 1.380(18) |
| C31 | C36 | 1.360(16) | C135 | C136 | 1.404(17) |

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|---|---|---|---|---|---|
| C32 | C33 | 1.374(16) | C135 | C143 | 1.35(2) |
| C33 | C34 | 1.36(2) | C137 | C138 | 1.385(15) |
| C34 | C35 | 1.385(15) | C137 | C144 | 1.386(15) |
| C35 | C36 | 1.420(16) | C138 | C139 | 1.324(16) |
| C37 | C38 | 1.416(17) | C139 | C140 | 1.392(15) |
| C37 | C42 | 1.426(16) | C140 | C141 | 1.351(19) |
| C38 | C39 | 1.293(18) | C141 | C144 | 1.379(19) |
| C39 | C40 | 1.413(19) | N11 | O11 | 1.3827(13) |
| C40 | C41 | 1.32(2) | N11 | O12 | 1.0899(12) |
| C41 | C42 | 1.461(19) | N11 | O13 | 1.2000(9) |
| C43 | C44 | 1.395(16) | N21 | O21 | 1.3831(13) |
| C43 | C48 | 1.342(15) | N21 | O22 | 1.0896(13) |
| C44 | C45 | 1.436(15) | N21 | O23 | 1.2000(2) |
| C45 | C46 | 1.356(16) | C550 | Cl50 | 1.611(10) |
| C46 | C47 | 1.368(18) | C550 | Cl51 | 1.709(9) |
| C47 | C48 | 1.372(15) | C510 | Cl10 | 1.588(13) |
| C49 | C50 | 1.359(12) | C510 | Cl11 | 1.698(11) |
| C49 | C54 | 1.316(15) | C520 | Cl20 | 1.95(2) |
| C50 | C51 | 1.387(17) | C520 | Cl21 | 1.51(2) |
| C51 | C52 | 1.408(18) | C530 | Cl30 | 1.562(13) |
| C52 | C53 | 1.319(15) | C530 | Cl31 | 1.677(14) |
| C53 | C54 | 1.500(18) | C540 | Cl40 | 1.609(11) |
| C55 | C56 | 1.377(14) | C540 | Cl41 | 1.714(12) |
| C55 | C60 | 1.342(15) | C560 | Cl60 | 1.64(2) |
| C56 | C57 | 1.410(17) | C560 | Cl61 | 1.79(2) |

**Table SI 8: Bond Angles for $Au_8$.**

| Atom | Atom | Atom | Angle/˚ | Atom | Atom | Atom | Angle/˚ |
|---|---|---|---|---|---|---|---|
| Au2 | Au1 | Au4 | 87.525(17) | C29 | C28 | C27 | 121.9(12) |
| Au3 | Au1 | Au2 | 108.069(19) | C30 | C29 | C28 | 119.3(11) |
| Au3 | Au1 | Au4 | 79.629(15) | C25 | C30 | P8 | 117.6(9) |

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|---|---|---|---|---|---|---|---|
| Au6 | Au1 | Au2 | 58.188(14) | C29 | C30 | P8 | 122.2(9) |
| Au6 | Au1 | Au3 | 57.164(14) | C29 | C30 | C25 | 120.2(11) |
| Au6 | Au1 | Au4 | 54.666(14) | C32 | C31 | P8 | 121.2(9) |
| P7 | Au1 | Au2 | 118.95(8) | C36 | C31 | P8 | 121.0(7) |
| P7 | Au1 | Au3 | 124.81(8) | C36 | C31 | C32 | 117.8(10) |
| P7 | Au1 | Au4 | 127.03(8) | C33 | C32 | C31 | 120.1(12) |
| P7 | Au1 | Au6 | 177.06(8) | C34 | C33 | C32 | 122.1(11) |
| Au1 | Au2 | Au7 | 92.824(17) | C33 | C34 | C35 | 119.3(12) |
| Au6 | Au2 | Au1 | 58.282(14) | C34 | C35 | C36 | 119.1(12) |
| Au6 | Au2 | Au7 | 58.196(15) | C31 | C36 | C35 | 121.5(9) |
| P5 | Au2 | Au1 | 130.37(7) | C38 | C37 | P2 | 120.4(9) |
| P5 | Au2 | Au6 | 163.41(8) | C38 | C37 | C42 | 117.3(11) |
| P5 | Au2 | Au7 | 127.92(8) | C42 | C37 | P2 | 121.5(9) |
| Au5 | Au3 | Au1 | 99.995(19) | C39 | C38 | C37 | 120.8(13) |
| Au6 | Au3 | Au1 | 58.823(15) | C38 | C39 | C40 | 124.1(14) |
| Au6 | Au3 | Au5 | 60.379(15) | C41 | C40 | C39 | 118.5(14) |
| P3 | Au3 | Au1 | 126.12(6) | C40 | C41 | C42 | 120.7(15) |
| P3 | Au3 | Au5 | 126.77(6) | C37 | C42 | C41 | 118.4(12) |
| P3 | Au3 | Au6 | 164.34(8) | C44 | C43 | P2 | 120.7(8) |
| Au1 | Au4 | Au7 | 92.518(17) | C48 | C43 | P2 | 119.6(9) |
| Au5 | Au4 | Au1 | 99.372(19) | C48 | C43 | C44 | 119.6(10) |
| Au5 | Au4 | Au7 | 100.303(18) | C43 | C44 | C45 | 115.6(11) |
| Au6 | Au4 | Au1 | 59.642(15) | C46 | C45 | C44 | 123.5(12) |
| Au6 | Au4 | Au5 | 61.295(16) | C45 | C46 | C47 | 118.2(10) |
| Au6 | Au4 | Au7 | 59.624(17) | C46 | C47 | C48 | 119.4(12) |
| P4 | Au4 | Au1 | 118.51(7) | C43 | C48 | C47 | 123.6(12) |
| P4 | Au4 | Au5 | 118.73(8) | C50 | C49 | P2 | 120.8(9) |
| P4 | Au4 | Au6 | 177.85(8) | C54 | C49 | P2 | 116.9(8) |
| P4 | Au4 | Au7 | 122.13(9) | C54 | C49 | C50 | 122.1(11) |
| Au3 | Au5 | Au4 | 79.815(15) | C49 | C50 | C51 | 122.7(11) |
| Au3 | Au5 | Au8 | 109.697(18) | C50 | C51 | C52 | 116.9(10) |

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|---|---|---|---|---|---|---|---|
| Au6 | Au5 | Au3 | 56.554(14) | C53 | C52 | C51 | 120.6(13) |
| Au6 | Au5 | Au4 | 54.142(14) | C52 | C53 | C54 | 120.9(12) |
| Au6 | Au5 | Au8 | 56.386(14) | C49 | C54 | C53 | 116.2(9) |
| Au8 | Au5 | Au4 | 78.043(17) | C56 | C55 | P3 | 123.7(9) |
| P2 | Au5 | Au3 | 119.03(8) | C60 | C55 | P3 | 116.6(8) |
| P2 | Au5 | Au4 | 131.77(8) | C60 | C55 | C56 | 119.7(10) |
| P2 | Au5 | Au6 | 173.29(9) | C55 | C56 | C57 | 119.0(11) |
| P2 | Au5 | Au8 | 125.34(7) | C58 | C57 | C56 | 120.4(12) |
| Au1 | Au6 | Au5 | 105.321(19) | C57 | C58 | C59 | 119.0(12) |
| Au1 | Au6 | Au7 | 99.553(18) | C58 | C59 | C60 | 118.5(12) |
| Au2 | Au6 | Au1 | 63.530(15) | C55 | C60 | C59 | 122.8(10) |
| Au2 | Au6 | Au5 | 161.69(2) | C62 | C61 | P3 | 125.1(9) |
| Au2 | Au6 | Au7 | 63.817(15) | C66 | C61 | P3 | 121.0(9) |
| Au3 | Au6 | Au1 | 64.013(16) | C66 | C61 | C62 | 113.9(11) |
| Au3 | Au6 | Au2 | 118.447(17) | C63 | C62 | C61 | 121.7(12) |
| Au3 | Au6 | Au5 | 63.067(15) | C62 | C63 | C64 | 121.1(13) |
| Au3 | Au6 | Au7 | 154.28(2) | C65 | C64 | C63 | 120.3(13) |
| Au4 | Au6 | Au1 | 65.692(16) | C64 | C65 | C66 | 120.8(13) |
| Au4 | Au6 | Au2 | 97.149(19) | C65 | C66 | C61 | 122.2(13) |
| Au4 | Au6 | Au3 | 88.81(2) | C68 | C67 | P3 | 121.6(7) |
| Au4 | Au6 | Au5 | 64.563(17) | C68 | C67 | C72 | 120.5(9) |
| Au4 | Au6 | Au7 | 65.828(18) | C72 | C67 | P3 | 117.8(8) |
| Au4 | Au6 | Au8 | 86.945(18) | C67 | C68 | C69 | 118.7(10) |
| Au7 | Au6 | Au5 | 106.457(18) | C70 | C69 | C68 | 120.3(12) |
| Au8 | Au6 | Au1 | 152.34(2) | C69 | C70 | C71 | 119.7(10) |
| Au8 | Au6 | Au2 | 119.34(2) | C72 | C71 | C70 | 120.0(10) |
| Au8 | Au6 | Au3 | 122.144(19) | C71 | C72 | C67 | 120.7(11) |
| Au8 | Au6 | Au5 | 63.265(15) | C74 | C73 | P1 | 119.5(8) |
| Au8 | Au6 | Au7 | 63.406(16) | C74 | C73 | C78 | 119.2(9) |
| P1 | Au6 | Au1 | 120.15(6) | C78 | C73 | P1 | 121.3(7) |
| P1 | Au6 | Au2 | 87.68(6) | C75 | C74 | C73 | 120.8(11) |

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|---|---|---|---|---|---|---|---|
| P1 | Au6 | Au3 | 92.25(7) | C74 | C75 | C76 | 119.4(9) |
| P1 | Au6 | Au4 | 173.84(6) | C77 | C76 | C75 | 120.7(10) |
| P1 | Au6 | Au5 | 110.62(6) | C76 | C77 | C78 | 120.2(11) |
| P1 | Au6 | Au7 | 113.42(7) | C77 | C78 | C73 | 119.6(9) |
| P1 | Au6 | Au8 | 87.35(6) | C80 | C79 | P1 | 117.9(8) |
| Au2 | Au7 | Au4 | 87.132(17) | C84 | C79 | P1 | 123.3(8) |
| Au6 | Au7 | Au2 | 57.987(14) | C84 | C79 | C80 | 118.6(9) |
| Au6 | Au7 | Au4 | 54.548(16) | C81 | C80 | C79 | 120.2(10) |
| Au6 | Au7 | Au8 | 57.322(14) | C80 | C81 | C82 | 121.9(11) |
| Au8 | Au7 | Au2 | 108.98(2) | C83 | C82 | C81 | 117.9(10) |
| Au8 | Au7 | Au4 | 78.236(17) | C82 | C83 | C84 | 120.9(11) |
| P6 | Au7 | Au2 | 122.46(7) | C79 | C84 | C83 | 120.4(12) |
| P6 | Au7 | Au4 | 122.16(9) | C86 | C85 | P1 | 120.8(8) |
| P6 | Au7 | Au6 | 176.62(9) | C86 | C85 | C90 | 117.5(10) |
| P6 | Au7 | Au8 | 123.91(6) | C90 | C85 | P1 | 121.6(8) |
| Au6 | Au8 | Au5 | 60.350(15) | C87 | C86 | C85 | 122.4(11) |
| Au6 | Au8 | Au7 | 59.271(15) | C86 | C87 | C88 | 119.7(12) |
| Au7 | Au8 | Au5 | 101.572(18) | C87 | C88 | C89 | 119.3(11) |
| P8 | Au8 | Au5 | 126.15(8) | C90 | C89 | C88 | 119.8(10) |
| P8 | Au8 | Au6 | 166.88(9) | C89 | C90 | C85 | 121.1(11) |
| P8 | Au8 | Au7 | 124.23(8) | C92 | C91 | P5 | 119.6(9) |
| C73 | P1 | Au6 | 118.0(3) | C96 | C91 | P5 | 123.9(9) |
| C73 | P1 | C79 | 100.1(5) | C96 | C91 | C92 | 116.5(11) |
| C73 | P1 | C85 | 102.9(5) | C93 | C92 | C91 | 121.9(12) |
| C79 | P1 | Au6 | 117.7(3) | C92 | C93 | C94 | 119.8(13) |
| C85 | P1 | Au6 | 113.9(4) | C95 | C94 | C93 | 120.0(13) |
| C85 | P1 | C79 | 101.8(5) | C94 | C95 | C96 | 117.7(13) |
| C37 | P2 | Au5 | 115.2(3) | C91 | C96 | C95 | 123.9(12) |
| C37 | P2 | C43 | 101.5(5) | C98 | C97 | P5 | 118.8(8) |
| C37 | P2 | C49 | 106.6(5) | C102 | C97 | P5 | 122.9(10) |
| C43 | P2 | Au5 | 119.4(4) | C102 | C97 | C98 | 118.3(11) |

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|---|---|---|---|---|---|---|---|
| C49 | P2 | Au5 | 111.7(3) | C97 | C98 | C99 | 118.5(10) |
| C49 | P2 | C43 | 100.7(5) | C100 | C99 | C98 | 123.4(13) |
| C55 | P3 | Au3 | 113.8(4) | C99 | C100 | C101 | 117.9(13) |
| C55 | P3 | C67 | 102.9(5) | C100 | C101 | C102 | 120.5(12) |
| C61 | P3 | Au3 | 115.7(4) | C97 | C102 | C101 | 121.2(12) |
| C61 | P3 | C55 | 105.8(5) | C104 | C103 | P5 | 122.7(9) |
| C61 | P3 | C67 | 104.2(5) | C108 | C103 | P5 | 118.7(9) |
| C67 | P3 | Au3 | 113.1(3) | C108 | C103 | C104 | 118.3(10) |
| C126 | P4 | Au4 | 112.8(4) | C105 | C104 | C103 | 119.2(11) |
| C126 | P4 | C132 | 104.4(5) | C106 | C105 | C104 | 121.4(12) |
| C126 | P4 | C137 | 104.7(5) | C105 | C106 | C107 | 119.6(11) |
| C132 | P4 | Au4 | 112.5(4) | C108 | C107 | C106 | 120.6(12) |
| C137 | P4 | Au4 | 116.8(4) | C107 | C108 | C103 | 120.7(12) |
| C137 | P4 | C132 | 104.5(5) | C110 | C109 | P7 | 123.6(8) |
| C91 | P5 | Au2 | 114.4(3) | C110 | C109 | C114 | 115.7(10) |
| C91 | P5 | C103 | 102.8(5) | C114 | C109 | P7 | 120.6(8) |
| C97 | P5 | Au2 | 114.4(4) | C109 | C110 | C111 | 124.9(10) |
| C97 | P5 | C91 | 105.1(6) | C110 | C111 | C112 | 117.9(10) |
| C97 | P5 | C103 | 103.6(5) | C113 | C112 | C111 | 118.8(11) |
| C103 | P5 | Au2 | 115.1(4) | C112 | C113 | C114 | 121.0(10) |
| C1 | P6 | Au7 | 112.8(4) | C113 | C114 | C109 | 121.2(10) |
| C7 | P6 | Au7 | 118.4(4) | C116 | C115 | P7 | 122.9(9) |
| C7 | P6 | C1 | 98.3(5) | C120 | C115 | P7 | 119.6(7) |
| C13 | P6 | Au7 | 113.8(4) | C120 | C115 | C116 | 117.0(9) |
| C13 | P6 | C1 | 107.9(5) | C117 | C116 | C115 | 120.5(12) |
| C13 | P6 | C7 | 104.0(5) | C116 | C117 | C118 | 121.0(11) |
| C109 | P7 | Au1 | 117.4(3) | C119 | C118 | C117 | 119.6(11) |
| C109 | P7 | C115 | 104.7(5) | C120 | C119 | C118 | 120.2(13) |
| C109 | P7 | C121 | 103.1(5) | C119 | C120 | C115 | 121.6(10) |
| C115 | P7 | Au1 | 110.8(4) | C122 | C121 | P7 | 126.1(11) |
| C115 | P7 | C121 | 104.4(5) | C122 | C121 | C142 | 115.4(13) |

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|---|---|---|---|---|---|---|---|
| C121 | P7 | Au1 | 115.1(3) | C142 | C121 | P7 | 118.4(9) |
| C19 | P8 | Au8 | 111.2(4) | C121 | C122 | C123 | 125.6(13) |
| C30 | P8 | Au8 | 116.6(3) | C124 | C123 | C122 | 117.9(13) |
| C30 | P8 | C19 | 105.7(5) | C125 | C124 | C123 | 118.3(13) |
| C31 | P8 | Au8 | 115.0(4) | C124 | C125 | C142 | 121.6(14) |
| C31 | P8 | C19 | 103.9(5) | C127 | C126 | P4 | 123.5(8) |
| C31 | P8 | C30 | 103.2(5) | C127 | C126 | C131 | 118.4(9) |
| C2 | C1 | P6 | 124.2(7) | C131 | C126 | P4 | 118.0(8) |
| C2 | C1 | C6 | 119.2(9) | C126 | C127 | C128 | 122.3(10) |
| C6 | C1 | P6 | 116.5(9) | C127 | C128 | C129 | 119.0(11) |
| C1 | C2 | C3 | 120.4(10) | C130 | C129 | C128 | 119.2(10) |
| C2 | C3 | C4 | 119.9(12) | C131 | C130 | C129 | 121.5(10) |
| C5 | C4 | C3 | 119.8(10) | C130 | C131 | C126 | 119.5(11) |
| C4 | C5 | C6 | 117.7(11) | C133 | C132 | P4 | 118.0(8) |
| C1 | C6 | C5 | 122.4(11) | C133 | C132 | C136 | 119.5(11) |
| C8 | C7 | P6 | 121.3(9) | C136 | C132 | P4 | 122.4(10) |
| C12 | C7 | P6 | 120.6(8) | C132 | C133 | C134 | 122.8(12) |
| C12 | C7 | C8 | 118.1(11) | C133 | C134 | C143 | 117.8(13) |
| C9 | C8 | C7 | 119.3(12) | C143 | C135 | C136 | 121.0(13) |
| C8 | C9 | C10 | 120.9(12) | C132 | C136 | C135 | 118.7(13) |
| C9 | C10 | C11 | 119.7(13) | C138 | C137 | P4 | 123.9(8) |
| C12 | C11 | C10 | 117.5(13) | C138 | C137 | C144 | 119.2(11) |
| C7 | C12 | C11 | 124.0(12) | C144 | C137 | P4 | 116.8(9) |
| C14 | C13 | P6 | 121.6(8) | C139 | C138 | C137 | 121.2(10) |
| C18 | C13 | P6 | 119.0(9) | C138 | C139 | C140 | 120.8(12) |
| C18 | C13 | C14 | 119.0(10) | C141 | C140 | C139 | 118.3(13) |
| C15 | C14 | C13 | 119.7(10) | C140 | C141 | C144 | 122.3(12) |
| C16 | C15 | C14 | 120.7(12) | C121 | C142 | C125 | 121.1(13) |
| C15 | C16 | C17 | 119.6(11) | C135 | C143 | C134 | 120.2(13) |
| C18 | C17 | C16 | 120.5(11) | C141 | C144 | C137 | 118.0(12) |
| C17 | C18 | C13 | 120.5(12) | O12 | N11 | O11 | 116.07(12) |

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|---|---|---|---|---|---|---|---|
| C20 | C19 | P8 | 118.8(9) | O12 | N11 | O13 | 138.71(14) |
| C24 | C19 | P8 | 122.3(10) | O13 | N11 | O11 | 102.55(11) |
| C24 | C19 | C20 | 118.8(12) | O22 | N21 | O21 | 116.04(14) |
| C21 | C20 | C19 | 121.5(12) | O22 | N21 | O23 | 138.79(19) |
| C22 | C21 | C20 | 120.8(13) | O23 | N21 | O21 | 102.51(12) |
| C21 | C22 | C23 | 119.9(13) | Cl50 | C550 | Cl51 | 119.9(7) |
| C22 | C23 | C24 | 122.2(14) | Cl10 | C510 | Cl11 | 119.9(8) |
| C19 | C24 | C23 | 116.7(13) | Cl21 | C520 | Cl20 | 109.7(11) |
| C30 | C25 | C26 | 118.3(11) | Cl30 | C530 | Cl31 | 125.1(10) |
| C27 | C26 | C25 | 122.4(12) | Cl40 | C540 | Cl41 | 118.8(9) |
| C26 | C27 | C28 | 117.9(12) | Cl60 | C560 | Cl61 | 114.4(13) |

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