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Supporting Information

for

A stable Cerberus tris(*malo*NHC) and its coinage metal complexes

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General Considerations: All reactions, unless otherwise noted, were performed using standard Schlenk techniques under an atmosphere of argon or in a nitrogen-filled gloxebox. Glassware was dried at 100 °C in an oven for at least 12 hours. THF was distilled from sodium/benzophenone. Dry dichloromethane was purchased from Aldrich and used as received. Known methods were followed to synthesize 1,3,5-tris(4-bromo-phenyl)benzene[1] and *N*,*N'*-bis(2,6-diisopropylphenyl)formamidine.[2] Column chromatography was performed using the indicated solvent systems on silica gel (40-75 µm). ^{1}H, ^{13}C and ^{31}P NMR spectra were recorded using a Bruker Ascend 400 MHz spectrometer. Chemical shifts were reported in ppm and are referenced to internal $SiMe_4$ (^{1}H and ^{13}C NMR) or external 85% H_3PO_4 (^{31}P NMR). FT- IR spectra were obtained using a Perkin Elmer Spectrum One FT-IR Spectrometer. Elemental analyses were performed by

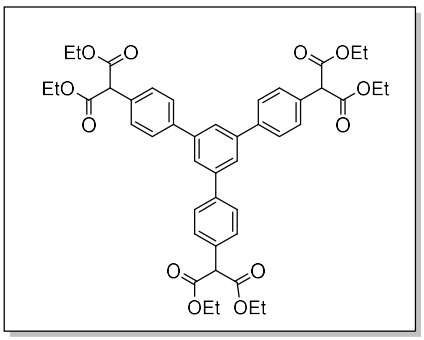
[1] R. Z. Lange, G. Hofer, T. Weber and A. D. Schlüter,. *J. Am. Chem. Soc.* 2017, **139** (5), 2053–2059.
[2] K. M. Kuhn and R. H. Grubbs *Org. Lett.* 2008, **10**, 2075–2077.

Atlantic Microlab (Norcross, GA). Single crystal X-ray diffraction measurements were performed using a Bruker D8 Venture diffractometer with an Incoatec microfocus source and a Photon 100 detector, and a Bruker D8 Quest diffractometer with a sealed tube X-ray source and a Photon 2 detector. Diffraction data for compound **11** were collected under nitrogen at 173 K using Cu Ka (λ= 1.54178 Å) radiation, and the diffraction data for compounds **12** and **13** were collected under nitrogen at 100 K using Mo Ka (λ= 0.71073 Å) radiation. Data were collected using phi and omega scans in 0.5° oscillations. Data were processed using the Apex 3 software suite utilizing SAINT and SADABS for integration and scaling.[3] The structures were solved by direct methods and refined using full-matrix least squares techniques on F2 using the SHELXTL (SHELXT-2014, SHELXL-2014) software package.[4] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in calculated positions using the appropriate riding models. Co-crystallized solvent molecules were also present in each of the crystal structures. These were identified from the difference electron density map and included in the structure refinements using appropriate restraints. On a formula unit basis there were three toluene solvent molecules in **11**, 2.5 benzene solvent molecules in **12**, and two benzene solvent molecules in **13**. In the case of **13**, one of the $AgPPh_3$ ligands was found to exist in half-occupied general positions disordered across a 2-fold rotation axis.

1. Synthesis and characterization of compounds

1.1 Synthesis of compound 8

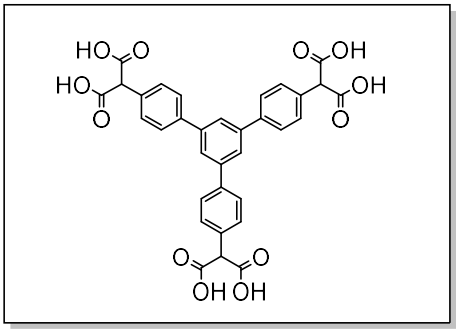
A pressure flask was charged under inert conditions with bis(dibenzylideneacetone)palladium(0) (67 mg, 0.12 mmol), di-*tert*-butylneopentylphosphine (53 µL, 0.21 mmol), sodium hydride (215 mg, 8.96 mmol), and 1,3,5-tribromo(4-phenyl)benzene (1.39 g, 2.56 mmol) in toluene (12 mL). Diethyl malonate (1.40 mL, 9.18 mmol) was added slowly, and the reaction was stirred at 70 °C for six days. The resulting mixture was filtered through a Celite plug and the volatiles was evaporated under reduced pressure. Compound **8** was purified on silica gel using 4:1 hexane-EtOAc to afford **8** as a translucent oil in 50% yield (1.01 g); mp 96-99 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.77 (s, 3H, Ar-C*H*), 7.68 (d, *J* = 8.3 Hz, 6H, Ar-C*H*), 7.53 (d, *J* = 8.3 Hz, 6H, Ar-C*H*), 4.69 (s, 3H, C*H*(CO_2Et)$_2$), 4.26 (m, 12H, C*H*$_2$CH$_3$), 1.30 (t, *J* = 7.1 Hz, 18H, C*H*$_3$). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.6 MHz): *δ* 168.1 (*C*O_2Et), 141.8, 140.9, 132.2, 129.8, 127.5, 125.3, 61.9 (*C*H$_2$CH$_3$), 57.7 (*C*H(CO_2Et)$_2$), 14.1 (*C*H$_3$). FT-IR (solid ATR): 2982, 2938, 1745, 1730 (CO), 1265, 1296, 1217, 1143, 1028, 1018, 862, 839, 757, 719, 700, 609 cm^{-1}. Anal. Calcd for $C_{45}H_{48}O_{12}$: C, 69.22; H, 6.20. Found: C, 69.02; H, 6.27.



[3] Apex3; Bruker AXS Inc.: Madison, WI, 2015.
[4] G. M. Sheldrick, Crystal structure refinement with SHELXL. *Acta Crystallogr. Sect. C: Struct. Chem*. 2015, **71**, 3-8.

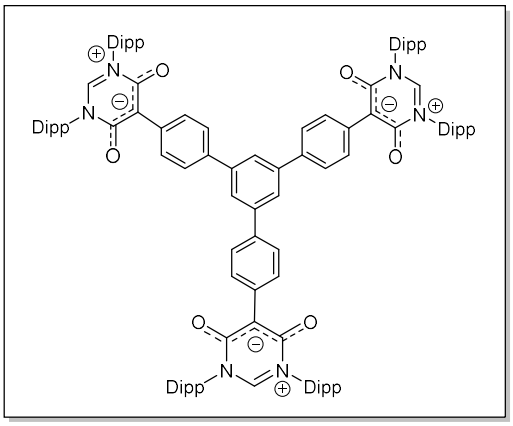
1.2 Synthesis of 9

Ester **8** (128 mg, 0.164 mmol) and potassium hydroxide (115 mg, 2.05 mmol) were dissolved in 50% v/v ethanol/water (1 mL) in ambient conditions. The mixture was stirred at 60°C for 1 hour. After cooling at room temperature, the reaction mixture was extracted twice with diethyl ether. The aqueous layer was acidified with concentrated HCl to pH = 1 and extracted with ethyl acetate. The organic layer was dried with Na_2SO_4, filtered, and concentrated under vacuum to give the carboxylic acid **9** as a white solid in 98% yield (99 mg). *Note*: the carboxylic acid decarboxylates when heated above 100 °C. ^{1}H NMR (CD_3OD, 400 MHz): δ 7.88 (s, 3H, Ar-C*H*), 7.78 (d, *J* = 8.3 Hz, 6H, Ar-C*H*), 7.58 (d, *J* = 8.3 Hz, 6H, Ar-C*H*), 4.75 (s, 3H, C*H*(COOH)$_2$, COO*H* proton not observed due to H-D exchange. ^{13}C{^{1}H} NMR (CD_3OD, 100.6 MHz): δ 170.5 (*C*OOH), 141.8, 140.5, 133.3, 129.6, 129.6, 126.9, 124.5, 57.3 (*C*(CO)). FT-IR (solid ATR): 2978, 1725, 1696 (CO), 1396, 1269, 1193, 1173, 1018, 821, 759, 698, 676, 607 cm^{-1}. Anal. Calcd for $C_{33}H_{24}O_{12} \cdot 3\ H_2O$: C, 59.46; H, 4.54. Found: C, 59.64; H, 4.14.



1.3 Synthesis of 11

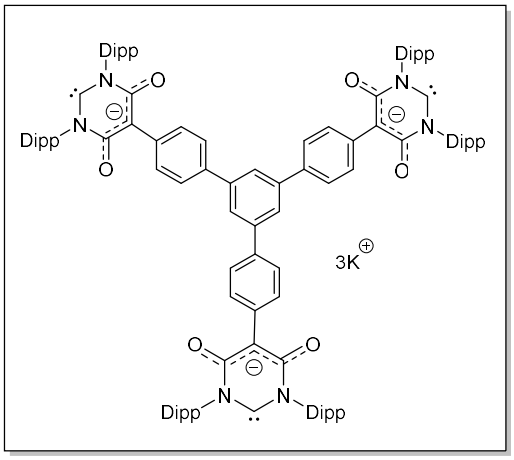
A mixture of carboxylic acid **9** (1.00 g, 1.63 mmol) and *N*,*N*-dimethylformamide (26.5 µL, 0.342 mmol) in 23 mL dichloromethane was cooled at 0 °C under argon. Oxalyl chloride (1.07 mL, 12.4 mmol) was added dropwise to the reaction mixture. After the addition of oxalyl chloride, the reaction mixture was removed from the ice bath and allowed to stir for 2.5 h at room temperature. The volatiles were evaporated *in vacuo* leaving a yellow oil containing the acyl chloride **10**. The crude oil was redissolved in dichloromethane (23 mL) and cooled to 0 °C. This mixture was transferred under argon to a stirring solution of *N*,*N*′-bis(2,6-diisopropylphenyl)formamidine (1.88 g, 5.15 mmol) and Et_3N (1.16 mL, 8.32 mmol) in dichloromethane (23 mL) at 0 °C. The reaction mixture was stirred overnight at room temperature and the volatiles were evaporated. The residue was triturated with water, filtered, and dried. The resulting solid was purified by flash column chromatography on silica gel using 1:25 ethylacetate-dichloromethane to afford the bright-yellow zwitterion **11** in 47% yield (1.23 g). Crystals of **11** were obtained by slow evaporation of a chloroform-toluene solution of **11** at room temperature under ambient conditions. ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.15 (s, 3H, NC*H*N), 8.14 (d, *J* = 8.5 Hz, 6H, Ar-C*H*), 7.78 (s, 3H, Ar-C*H*), 7.65 (d, *J* = 8.5 Hz, 6H, Ar-C*H*), 7.46 (t, *J* = 7.8 Hz,



6H, Ar-C*H*), 7.28 (d, *J* = 7.8 Hz, 12H, Ar-C*H*), 2.90 (sept, *J* = 6.8 Hz, 12H, C*H*(CH_3)$_3$, 1.33 (d, *J* = 6.8 Hz, 36H, C*H*$_3$), 1.23 (d, *J* = 6.8 Hz, 36H, C*H*$_3$). ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.87 (s, 3H, NC*H*N), 7.88 (d, *J* = 8.5 Hz, 6H, Ar-C*H*), 7.84 (s, 3H, Ar-C*H*), 7.75 (d, *J* = 8.5 Hz, 6H, Ar-C*H*), 7.51 (t, *J* = 7.8 Hz, 6H, Ar-C*H*), 7.37 (d, *J* = 7.8 Hz, 12H, Ar-C*H*), 2.77 (sept, *J* = 6.7 Hz, 12H, C*H*(CH_3)$_3$), 1.21 (d, *J* = 6.7 Hz, 36H, C*H*$_3$), 1.20 (d, *J* = 6.7 Hz, 36H, C*H*$_3$). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.6 MHz): δ 158.4 (*C*O), 147.4 (N(*C*H)N), 145.8, 142.4, 138.9, 133.2, 132.1, 130.9, 130.4, 126.4, 124.7, 124.3, 98.2 (*C*(CO)), 29.20 (*C*H(CH_3)$_2$), 24.16 (*C*H$_3$). FT-IR (solid ATR): 2962, 2932, 2867, 1665 (CO), 1596, 1324, 1219, 1142, 1057, 934, 834, 803, 763 cm^{-1}. Anal. Calcd for $C_{108}H_{120}N_6O_6 \cdot 3\ H_2O$: C, 78.51; H, 7.68; N, 5.09. Found: C, 78.67; H, 7.54; N, 5.05.

1.4 Synthesis of carbene 7

In a dried NMR tube, zwitterion **11** (21 mg, 0.013 mmol) and potassium bis(trimethylsilyl)amide (KHMDS) (12 mg, 0.060 mmol) were dissolved in DMSO-d_6 (0.6 mL) under nitrogen. The NMR tube was sealed. The resulting solution was subjected to ^{1}H and ^{13}C NMR measurements, which indicated the formation of the carbene **7** within minutes. This solution did not show major decomposition overnight.



In a vial, zwitterion **11** (39 mg, 0.024 mmol) was dissolved in DMSO-d_6 (0.5 mL). KHMDS (26 mg, 0.13 mmol) was added to the vial. After 30 minutes of stirring and complete conversion (as determined by ^{1}H NMR), the solvent was removed *in vacuo* at 36 ºC. The residue was triturated with anhydrous toluene to produce carbene **7** in quantitative yield as a yellow-orange powder. ^{1}H NMR (DMSO-d_6, 400 MHz, ppm): δ 8.08 (d, *J* = 8.5 Hz, 6H, Ar-C*H*), 7.70 (s, 3H, Ar-C*H*), 7.56 (d, *J* = 8.5 Hz, 6H, Ar-C*H*), 7.23 (t, *J* = 7.6 Hz, 6H, Ar-C*H*), 7.14 (d, *J* = 7.6 Hz, 12H, Ar-C*H*), 3.05 (sept, *J* = 6.8 Hz, 12H, C*H*(CH_3)$_2$), 1.15 (d, *J* = 6.8 Hz, 36H, C*H*$_3$), 1.08 (d, *J* = 6.8 Hz, 36H, C*H*$_3$). ^{13}C{^{1}H} NMR (DMSO-d_6, 100.6 MHz, ppm): δ 242.5 (N*C*N), 160.8 (*C*O), 144.9, 142.0, 141.7, 138.4, 134.5, 130.2, 126.5, 124.6, 122.4, 92.9 (*C*(CO)), 27.7 (*C*H(CH_3)$_2$), 23.7 (*C*H$_3$), 23.3 (*C*H$_3$).

1.5 Synthesis of 12

A solution of KHMDS (133 mg, 0.667 mmol) in THF (6 mL) was added dropwise to a stirring suspension of zwitterion **11** (150 mg, 0.094 mmol) in THF (3 mL). The reaction mixture was stirred for 45 min at ambient temperature. AuCl(SMe_2) (137 mg, 0.46 mmol) and PPh_3 (125 mg, 0.477 mmol) were placed in a separate flask and stirred for 45 min in THF (2 mL) to ensure precoordination of PPh_3 on the gold center. The latter solution was added dropwise to the *in situ* generated carbene suspension. The reaction mixture was stirred for

24 h at room temperature. The volatiles were removed *in vacuo* and the residue was redissolved in dichloromethane and filtered through a Celite plug. The filtrate was triturated with hexane and then passed through a short silica column using a 1:40 methanol-dichloromethane mixture. The resulting solid was dissolved in minimal dichloromethane and precipitated with 70 mL of a 1:1 toluene-Et_2O mixture to afford, after filtration, the title compound as a bright-yellow solid (160 mg, 58% yield); mp > 250 °C. Crystals of **12** were obtained by slow evaporation of a saturated dichlorometane-benzene solution of **12** at room temperature under ambient conditions. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.24 (d, 6H, J = 8.6 Hz, Ar-C*H*), 7.74 (s, 3H, Ar-C*H*), 7.59 (d, 6H, J = 8.6 Hz, Ar-C*H*), 7.45 (td, 9H, J = 7.5 Hz, J =1.8 Hz, Ar-C*H*), 7.30-7.38 (m, 24H, CH_{PPh3} & Ar-C*H*), 7.20 (d, J = 7.7 Hz, 12H, Ar-C*H*), 6.86 (dd, 18H, J = 7.7 Hz, J =12.8 Hz, CH_{PPh3}), 3.04 (sept J = 6.7 Hz, 12H, $CH(CH_3)_2$), 1.27 (d, J = 6.8 Hz, 36H, CH_3), 1.09 (d, J = 6.8 Hz, 36H, CH_3). ^{13}C NMR (CD_2Cl_2, 100.6 MHz): δ 201.5 (d, J =119.8 Hz, N*C*N), 160.7 (d, J = 2.1 Hz), 146.6, 142.3, 138.2, 137.6, 135.4, 133.8 (d, J =13.8 Hz), 131.8 (d, J = 2.1 Hz), 130.9, 129.2, 129.1 (d, J = 11.6 Hz), 128.2 (d, J = 57.1 Hz), 125.8, 124.1, 123.8, 96.7 (*C*-CO), 28.8 ($CH(CH_3)_2$), 24.1 (CH_3), 23.7 (CH_3). ^{31}P NMR ($CDCl_3$, 161.9 MHz, ppm): δ 39.3. FT-IR (solid ATR): 2959, 2932, 2865, 1726, 1614 (CO), 1510, 1436, 1361, 1328, 1269, 1224, 1149, 1100, 1057, 1027, 997, 837, 801, 745, 691, 618 cm^{-1}. Anal. Calcd for $C_{162}H_{162}N_6O_6Au_3P_3 \cdot 1.5\ CHCl_3$: C, 62.3; H, 5.23; N 2.67. Found: C, 62.31; H, 5.51; N, 2.87.

1.6 Synthesis of 13

Under inert conditions , a solution of KHMDS (152 mg, 0.762 mmol) in THF (2 mL) was added dropwise to a stirring suspension of zwitterion **11** (152 mg, 0.095 mmol) in THF (6 mL). The reaction mixture was stirred for 1 hr. In a separate vial, silver triflate (144 mg, 0.560 mmol) and triphenylphosphine (150 mg, 0.572 mmol) were stirred in THF (2 mL) for one hour. The latter solution was added dropwise to the *in situ* generated carbene and the reaction was stirred for four days inside the glovebox. After the volatiles were evaporated, the residue was redissolved in dichlorometane and filtered through a Celite plug. The resulting mixture was purified by column chromatography using gradient elution (1:80

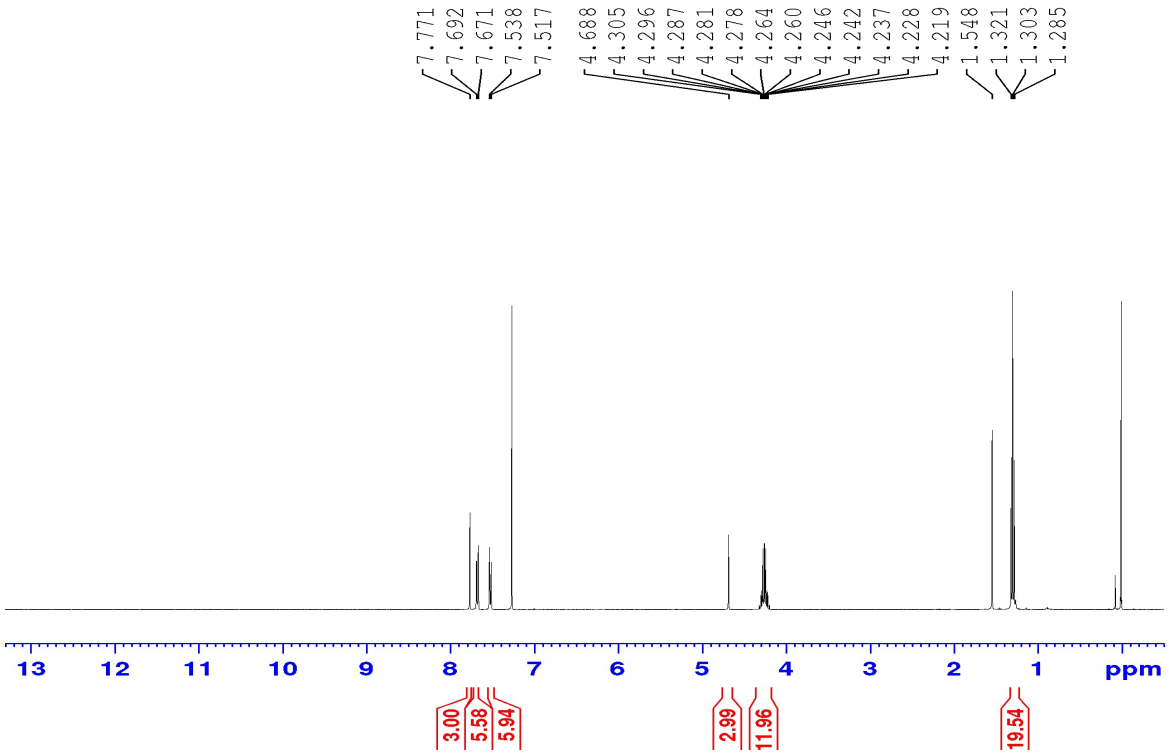
to 1:60 methanol-dichlorometane). The silver complex **13** was obtained as a bright-yellow solid in 71% yield (182 mg); mp > 250 °C. Crystals of **13** were obtained by slow evaporation of a saturated dichlorometane-benzene solution of **13** at room temperature under ambient conditions.

^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.26 (d, 6H, J = 8.3 Hz, Ar-C*H*), 7.74 (s, 3H, Ar-C*H*), 7.59 (d, 6H, J = 8.3 Hz, Ar-C*H*), 7.44 (t, 9H, J = 7.1 Hz Ar-C*H*), 7.36-7.29 (m, 30H, CH_{PPh3} & Ar-C*H*), 7.20 (d, J = 7.7 Hz, 6H, Ar-C*H*), 6.8 (dd, 18H, J = 7.5 Hz, J =12.5 Hz, CH_{PPh3}), 3.11 (sept, J = 6.7 Hz, 12H, $CH(CH_3)_2$), 1.29 (d, J = 6.7 Hz, 36H, CH_3), 1.08 (d, J = 6.7 Hz, 36H, CH_3). ^{13}C{^{1}H} NMR (CD_2Cl_2, 100.6 MHz, ppm): δ 200.9 (dd + dd, J(^{13}C - ^{109}Ag) = 231.1 Hz, J(^{13}C - ^{107}Ag) = 201.2 Hz), J_{C-P} = 63.7 Hz, N*C*N), 160.8 (d, J = 6.0 Hz), 146.4, 142.3, 140.3, 137.4, 135.6, 133.5 (d, J = 15.9 Hz), 131.5, 130.9, 129.2 (d, J = 10.9 Hz), 129.0, 128.4 (d, J = 42.2 Hz), 125.7, 124.0, 123.9, 96.5 (*C*-CO), 28.7 ($CH(CH_3)_2$), 24.1 (CH_3), 24.0 (CH_3). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.9 MHz, ppm): δ 18.2 (d + d, J(^{31}P - ^{109}Ag) = 536.5 Hz, J(^{31}P - ^{107}Ag) = 464.9 Hz).

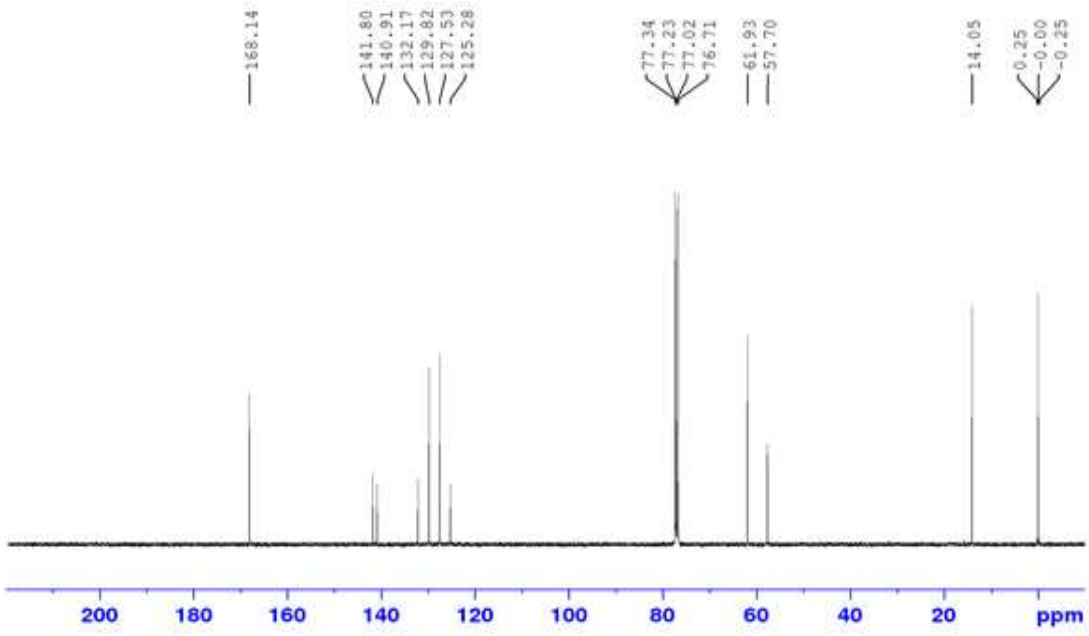
FT-IR (solid ATR): 2958, 2921, 2867, 1606 (CO), 1509, 1435, 1382, 1328, 1273, 115 2, 1097, 837, 801, 742, 691, 636 cm^{-1}. Anal. Calcd for $C_{162}H_{162}N_6O_6Ag_3P_3 \cdot 0.5\ CH_2Cl_2$: C, 71.02; H 5.98; N, 3.06. Found: C, 70.94; H, 6.07; N, 3.12.

2. NMR Spectra

2.1 ^{1}H and ^{13}C NMR spectra of **8**

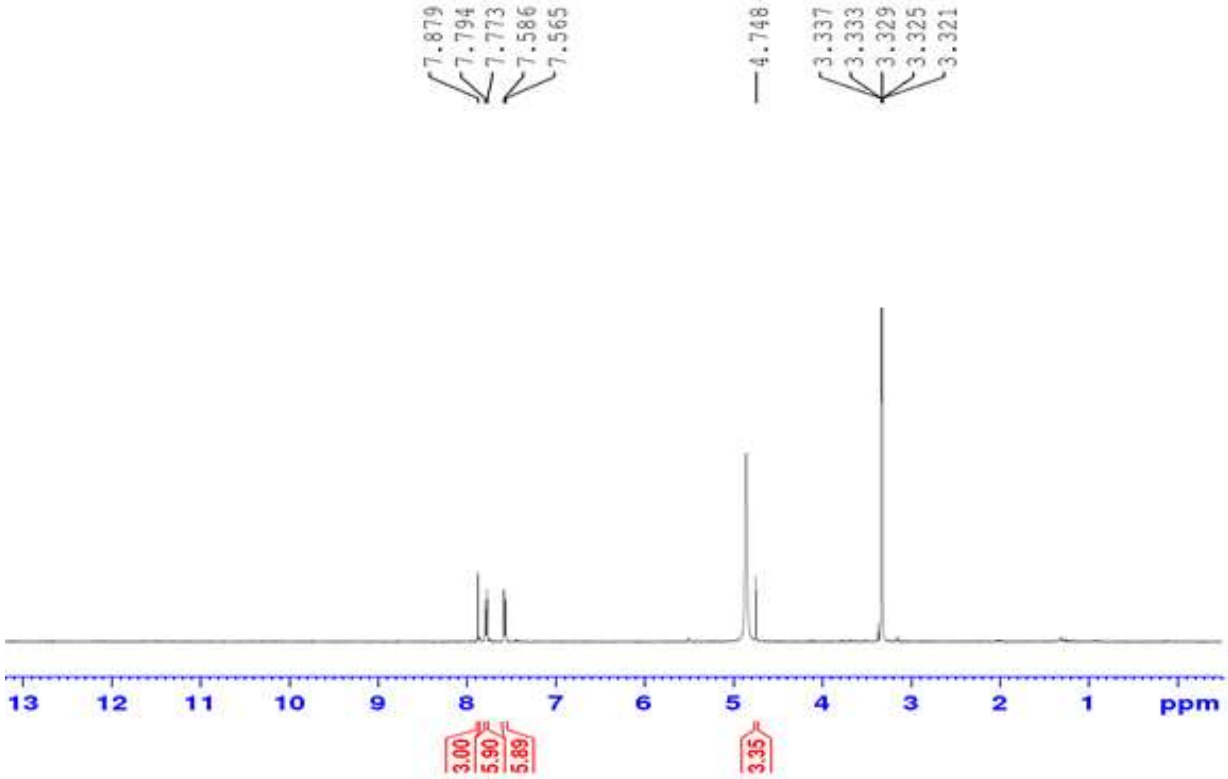


^{1}H NMR spectrum of **8** in $CDCl_3$

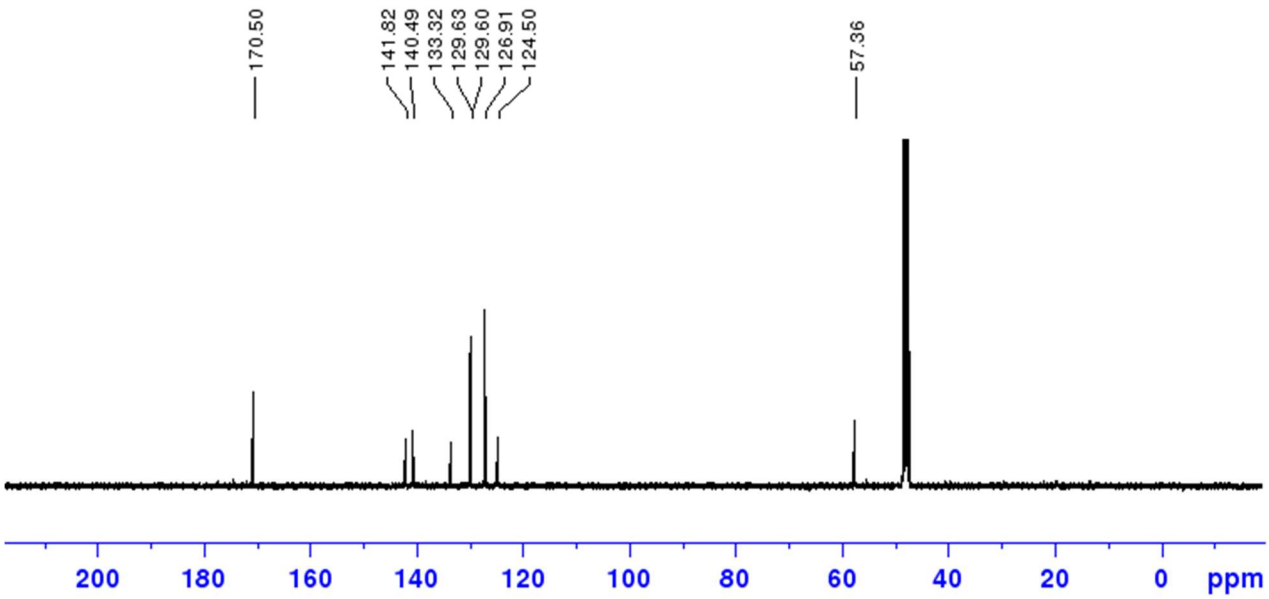


^{13}C NMR spectrum of **8** in $CDCl_3$

2.2 ^{1}H and ^{13}C NMR spectra of **9**

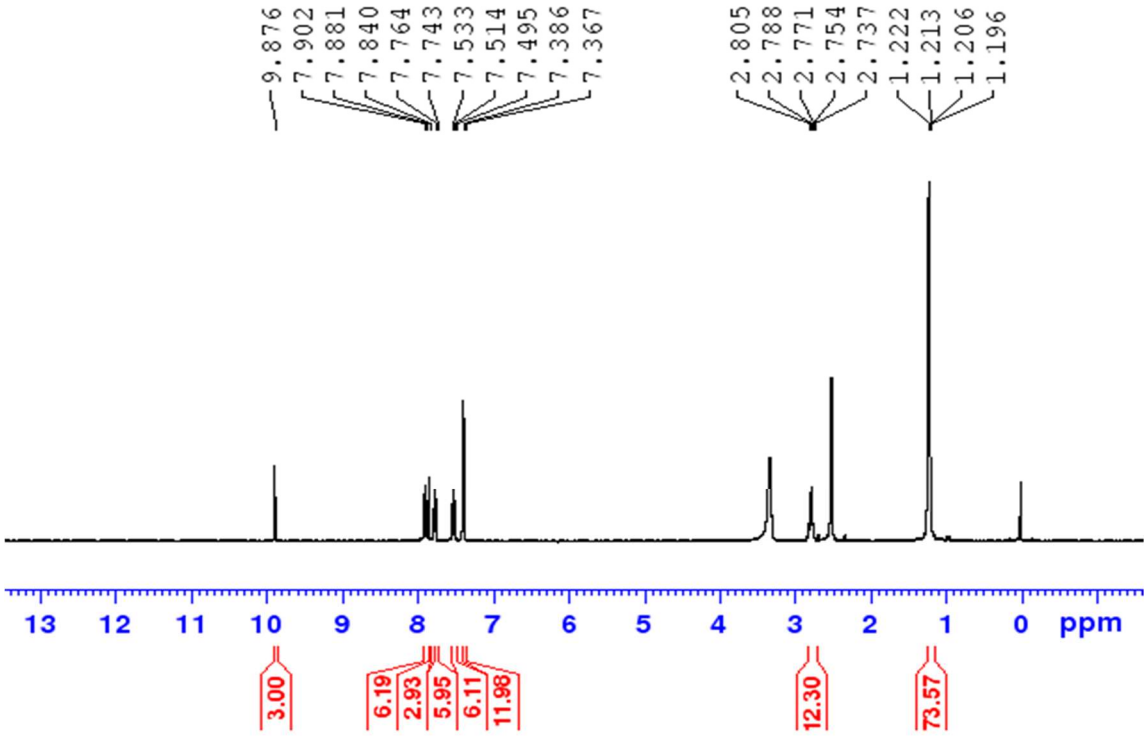


^{1}H NMR spectrum of **9** in CD_3OD

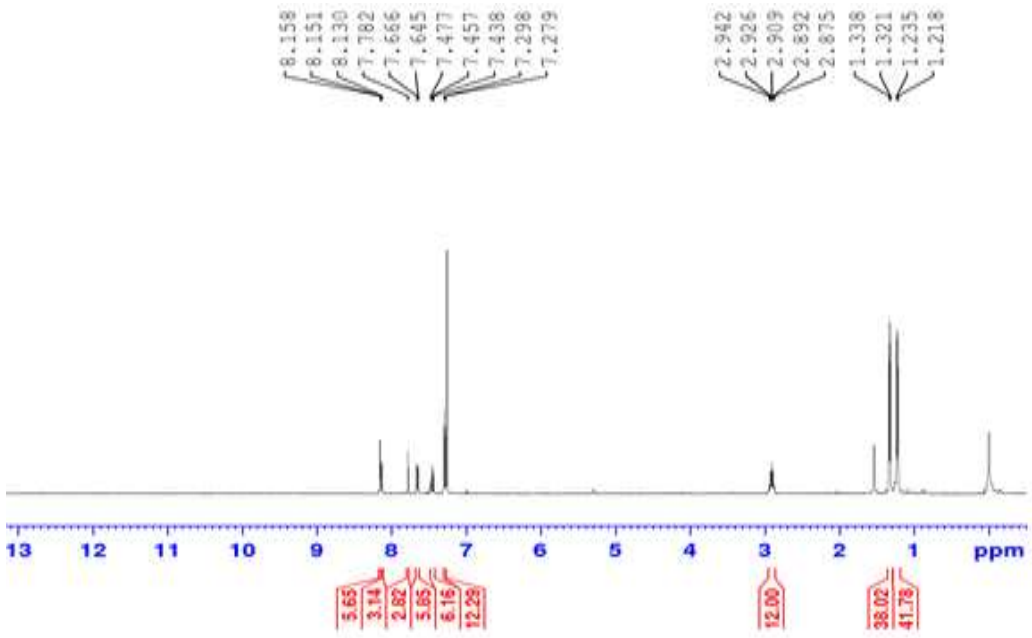


^{13}C NMR spectrum of **9** in CD_3OD

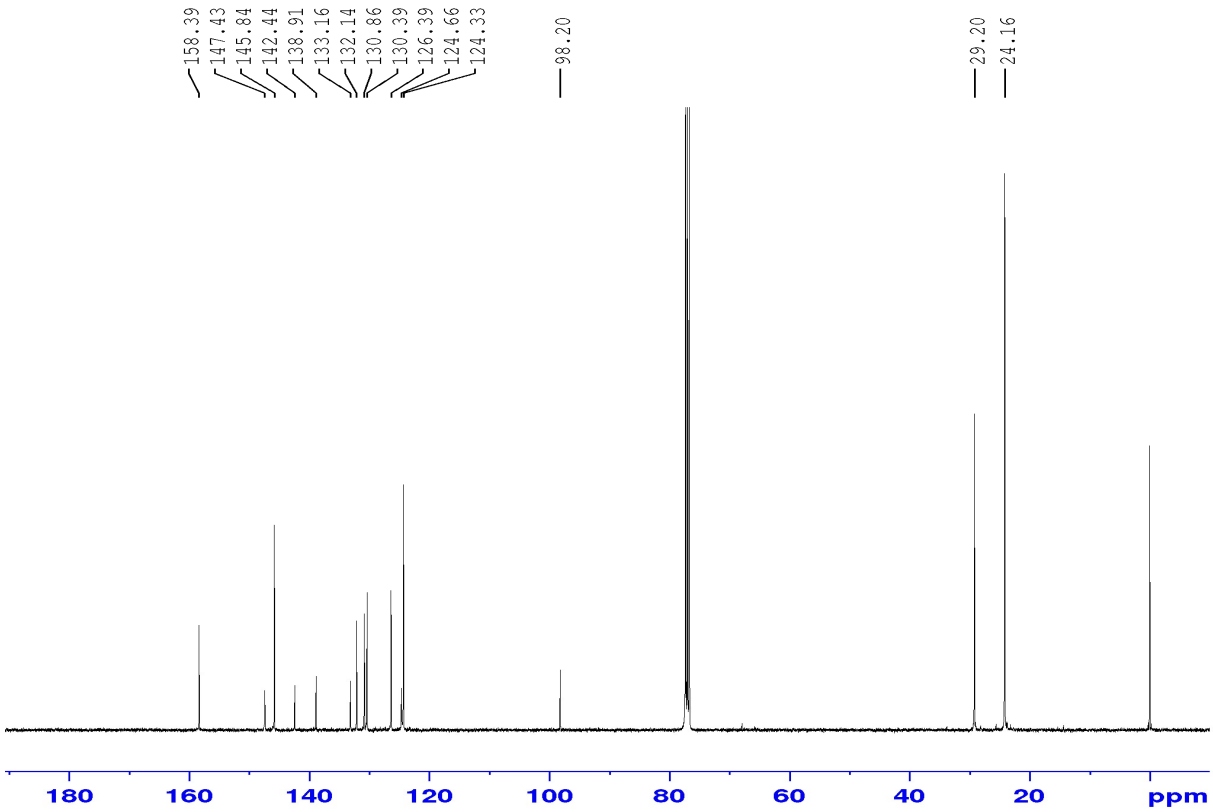
2.3 ^{1}H and ^{13}C NMR spectra of **11**



^{1}H NMR of **11** in DMSO-d_6

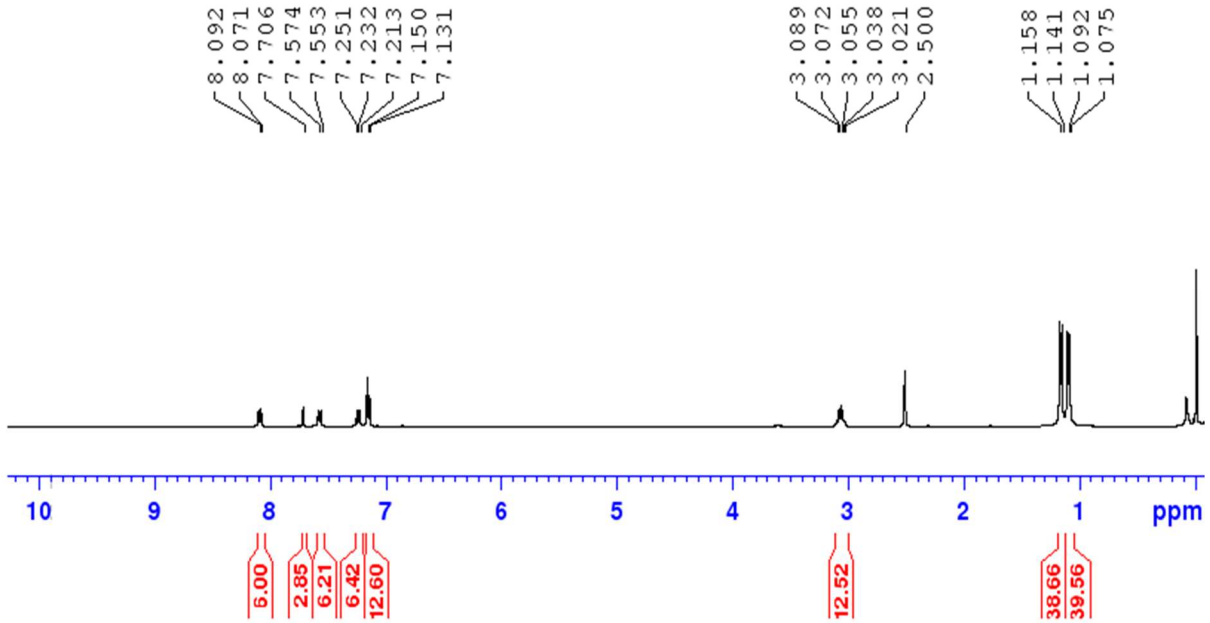


^{1}H NMR spectrum of **11** in $CDCl_3$.

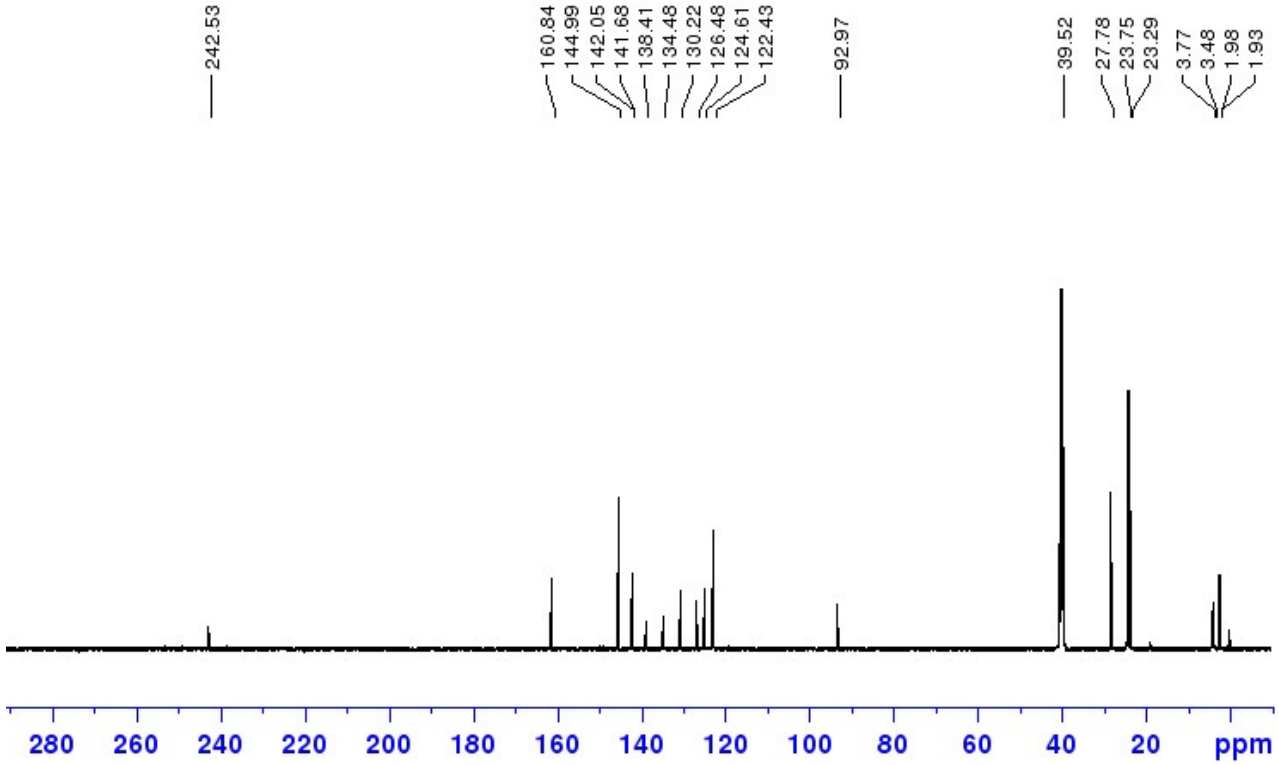


^{13}C NMR spectrum of **11** in $CDCl_3$

2.4 ^{1}H and ^{13}C NMR spectra of **7**

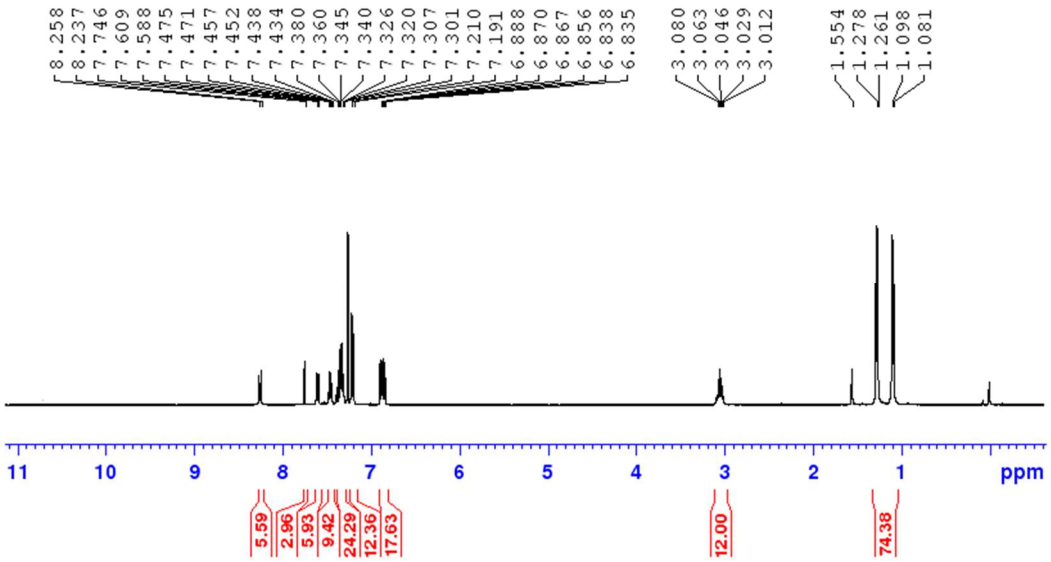


^{1}H NMR of **7** in DMSO-d_6

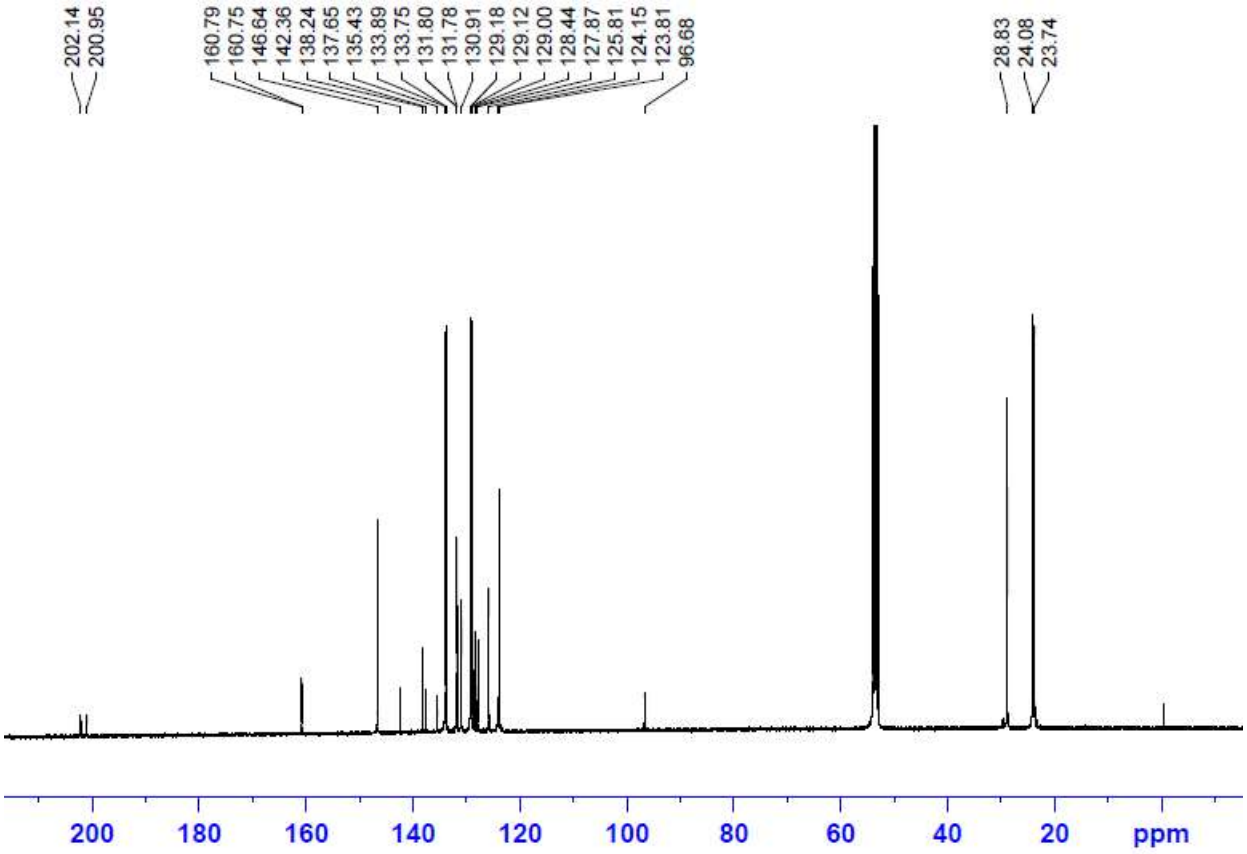


^{13}C NMR of **7** in DMSO-d_6

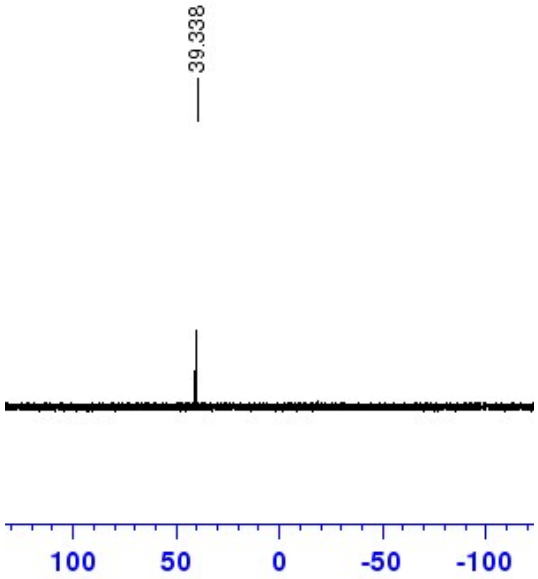
2.5 ^{1}H, ^{13}C NMR and ^{31}P spectra of **12**



^{1}H NMR of **12** in $CDCl_3$

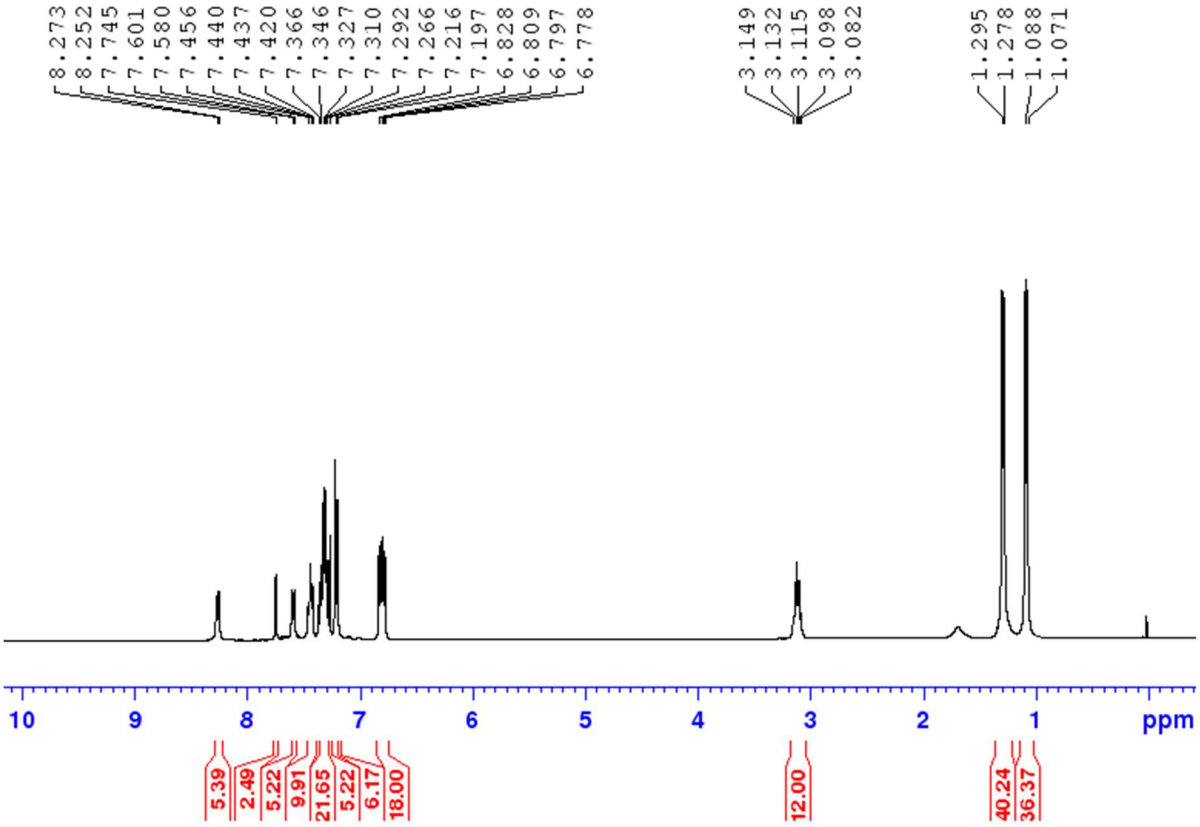


^{13}C NMR of **12** in CD_2Cl_2

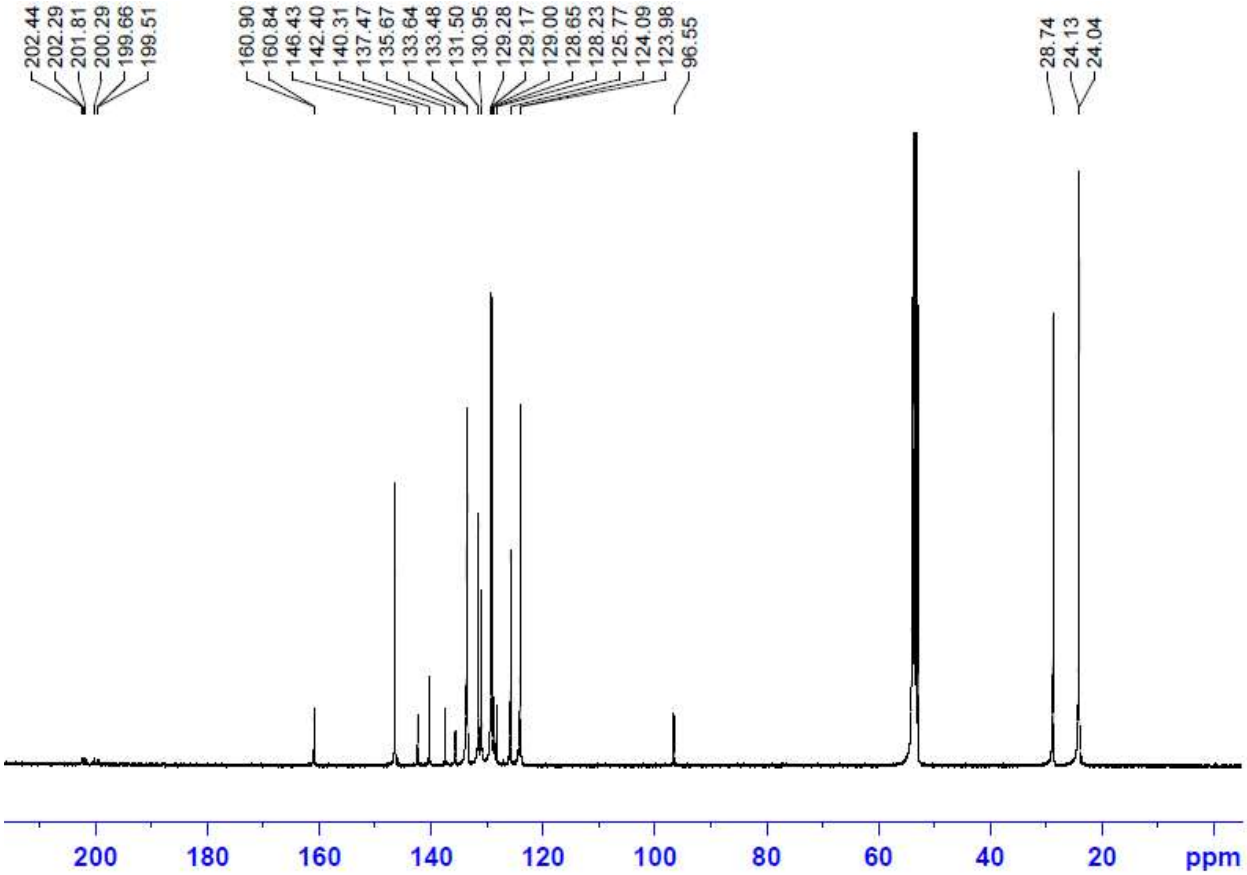


^{31}P NMR of **12** in $CDCl_3$

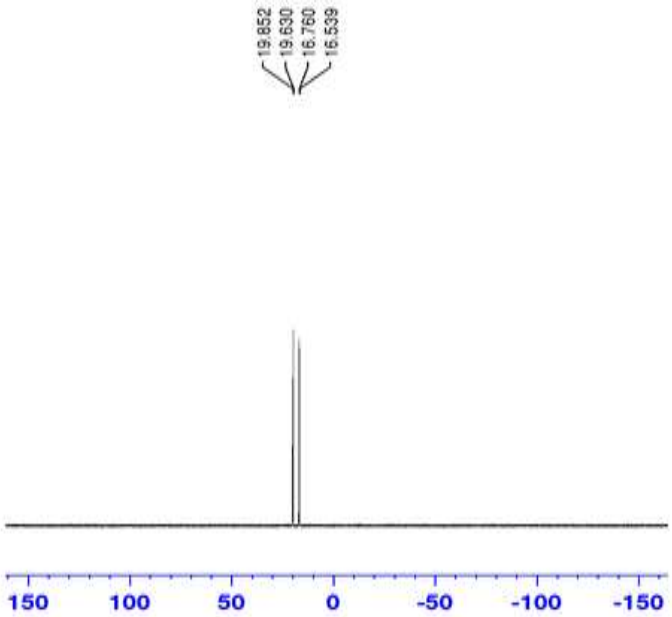
2.6 ^{1}H, ^{13}C NMR and ^{31}P spectra of **13**



^{1}H NMR of **13** in $CDCl_3$



^{13}C NMR of **13** in CD_2Cl_2



^{31}P NMR of **13** in $CDCl_3$

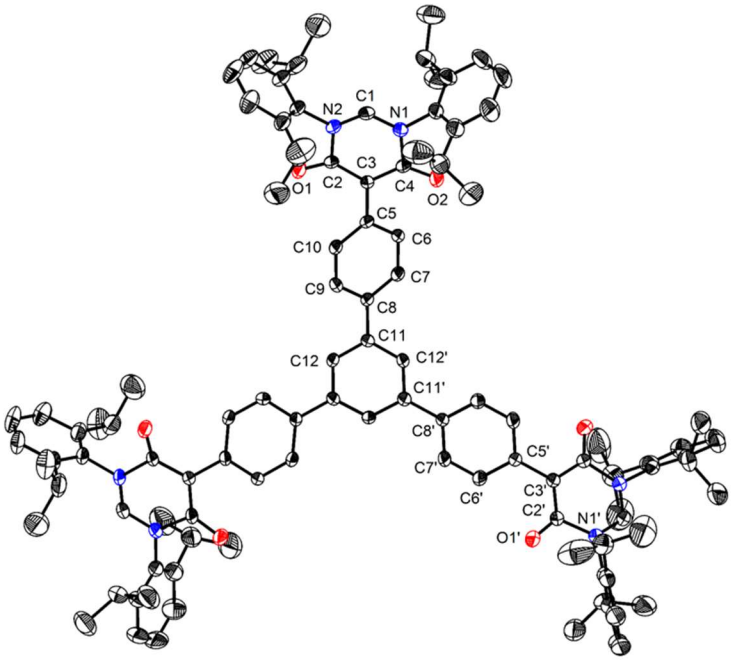
3. X-Ray Crystallography

3.1. X-ray crystallography data for compound 11

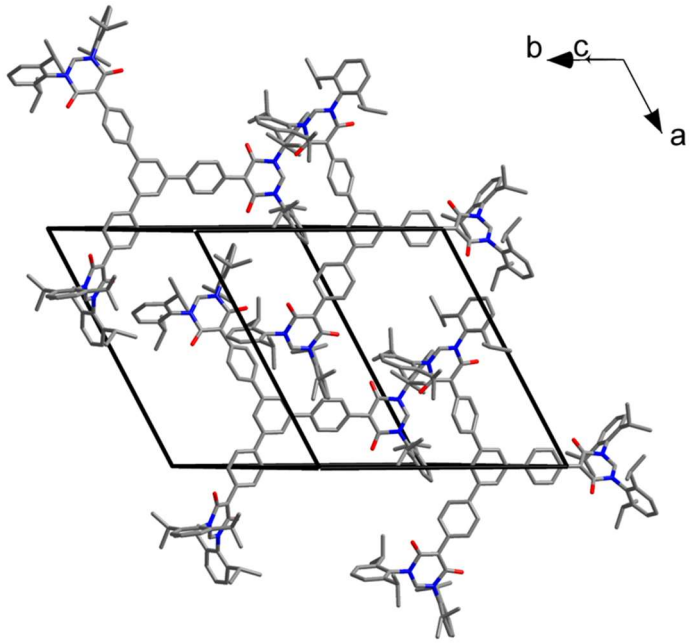
A specimen of $C_{129}H_{144}N_6O_6$, approximate dimensions 0.142 mm x 0.187 mm x 0.339 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using a trigonal unit cell yielded a total of 65897 reflections to a maximum θ angle of 70.15° (0.82 Å resolution), of which 10040 were independent (average redundancy 6.563, completeness = 99.3%, R_{int} = 6.79%, R_{sig} = 4.17%) and 8337 (83.04%) were greater than $2\sigma(F^2)$. The final cell constants of a = 19.6416(3) Å, b = 19.6416(3) Å, c = 23.8212(6) Å, volume = 7958.8(3) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8614 and 1.0000.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 31 2 1, with Z = 3 for the formula unit, $C_{129}H_{144}N_6O_6$. The final anisotropic full-matrix least-squares refinement on F^2 with 651 variables converged at R1 = 6.27%, for the observed data and wR2 = 16.18% for all data. The goodness-of-fit was 1.066. The largest peak in the final difference electron density synthesis was 0.348 $e^-/Å^3$ and the largest hole was -0.451 $e^-/Å^3$ with an RMS deviation of 0.048 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.173 g/cm^3 and F(000), 3024 e^-.



Solid state molecular structure of **11** with 50% probability ellipsoids. Hydrogen atoms and solvent molecules are omitted for clarity. Only half of the atoms are numbered, since the other half of the molecule is completed by inversion symmetry.



Partial packing diagram of the **11** (solvent molecules omitted for clarity).

Table 3.1.1 Sample and crystal data for salt 11.

Chemical formula	$C_{129}H_{144}N_6O_6$	
Formula weight	1874.49 g/mol	
Temperature	173(2) K	
Wavelength	1.54178 Å	
Crystal size	0.142 x 0.187 x 0.339 mm	
Crystal system	trigonal	
Space group	P 31 2 1	
Unit cell dimensions	a = 19.6416(3) Å	α = 90°
	b = 19.6416(3) Å	β = 90°
	c = 23.8212(6) Å	γ = 120°
Volume	7958.8(3) $Å^3$	
Z	3	
Density (calculated)	1.173 g/cm^3	
Absorption coefficient	0.549 mm^{-1}	
F(000)	3024	

Table 3.1.2 Data collection and structure refinement for salt 11.

Theta range for data collection	2.60 to 70.15°
Index ranges	$-23 \leq h \leq 23$, $-20 \leq k \leq 23$, $-28 \leq l \leq 24$
Reflections collected	65897
Independent reflections	10040 [R(int) = 0.0679]
Max. and min. transmission	1.0000 and 0.8614
Structure solution technique	direct methods
Structure solution program	SHELXT-2014 (Sheldrick 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014 (Sheldrick 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	10040 / 81 / 651
Goodness-of-fit on F^2	1.066
Final R indices	8337 data; $I>2\sigma(I)$ R1 = 0.0627, wR2 = 0.1493
	all data R1 = 0.0799, wR2 = 0.1618
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0628P)^2+5.7836P]$ where $P=(F_o^2+2F_c^2)/3$
Absolute structure parameter	0.1(1)
Largest diff. peak and hole	0.348 and -0.451 eÅ^{-3}
R.M.S. deviation from mean	0.048 eÅ^{-3}

Table 3.1.3 Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for salt 11. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
O1	0.68446(16)	0.35109(15)	0.13848(14)	0.0410(7)
O1'	0.89116(17)	0.78239(16)	0.22838(15)	0.0449(8)
O2	0.55802(16)	0.07519(16)	0.11358(16)	0.0457(8)
N1	0.50004(18)	0.14699(19)	0.08960(16)	0.0325(8)
N2	0.56292(18)	0.28139(18)	0.09979(15)	0.0304(7)
C1	0.5023(2)	0.2146(2)	0.08440(18)	0.0308(9)
C1'	0.0	0.7075(3)	0.1667	0.0299(12)
C2	0.6342(2)	0.2863(2)	0.12196(18)	0.0288(8)
C2'	0.9439(2)	0.7854(2)	0.19954(19)	0.0310(9)
C3	0.6351(2)	0.2144(2)	0.12220(17)	0.0262(8)
C3'	0.0	0.8477(3)	0.1667	0.0299(12)
C4	0.5670(2)	0.1413(2)	0.11014(19)	0.0314(9)
C5	0.7098(2)	0.2159(2)	0.13507(17)	0.0263(8)
C5'	0.0	0.9235(3)	0.1667	0.0274(11)
C6	0.7118(2)	0.1536(2)	0.16161(19)	0.0307(9)

	x/a	y/b	z/c	U(eq)
C6'	0.0684(2)	0.9953(2)	0.1680(3)	0.0574(16)
C7	0.7826(2)	0.1548(2)	0.17000(19)	0.0313(9)
C7'	0.0683(2)	0.0656(2)	0.1677(3)	0.0542(15)
C8	0.8537(2)	0.2170(2)	0.15266(18)	0.0273(8)
C8'	0.0	0.0688(3)	0.1667	0.0283(12)
C9	0.8516(2)	0.2799(2)	0.12689(19)	0.0319(9)
C10	0.7819(2)	0.2796(2)	0.11860(18)	0.0305(9)
C11	0.9291(2)	0.2171(2)	0.16009(18)	0.0284(9)
C11'	0.0	0.1448(3)	0.1667	0.0298(12)
C12	0.0	0.2877(3)	0.1667	0.0285(12)
C12'	0.9304(2)	0.1469(2)	0.16017(18)	0.0303(9)
C13	0.5614(2)	0.3535(2)	0.0867(2)	0.0354(9)
C13'	0.8983(2)	0.6477(2)	0.23460(19)	0.0331(9)
C14	0.5346(3)	0.3851(3)	0.1276(2)	0.0425(11)
C14'	0.9094(3)	0.6528(3)	0.2923(2)	0.0430(11)
C15	0.5289(3)	0.4511(3)	0.1111(2)	0.0511(13)
C15'	0.8595(3)	0.5872(3)	0.3244(2)	0.0530(13)
C16	0.5510(4)	0.4817(3)	0.0585(3)	0.0595(14)
C17	0.5793(3)	0.4504(3)	0.0196(2)	0.0524(13)
C18	0.5858(3)	0.3846(2)	0.0332(2)	0.0395(10)
C16'	0.8025(3)	0.5202(3)	0.2988(3)	0.0599(16)
C17'	0.7930(3)	0.5161(3)	0.2421(3)	0.0512(13)
C18'	0.8398(2)	0.5807(2)	0.2074(2)	0.0403(11)
C19	0.5118(3)	0.3534(3)	0.1853(2)	0.0546(13)
C19'	0.9745(3)	0.7259(3)	0.3208(2)	0.0518(12)
C20	0.5485(4)	0.4163(4)	0.2302(3)	0.0716(17)
C20'	0.0414(5)	0.7121(5)	0.3375(4)	0.111(3)
C21	0.4213(4)	0.3090(4)	0.1912(3)	0.085(2)
C22	0.6204(3)	0.3521(3)	0.9914(2)	0.0458(11)
C23	0.7096(4)	0.3979(4)	0.9943(3)	0.080(2)
C24	0.5939(5)	0.3497(5)	0.9323(3)	0.082(2)
C21'	0.9475(6)	0.7529(5)	0.3702(4)	0.123(4)
C22'	0.8268(3)	0.5750(3)	0.1449(2)	0.0503(12)
C23'	0.7423(3)	0.5500(3)	0.1290(3)	0.0659(16)
C24'	0.8511(3)	0.5186(3)	0.1193(3)	0.0723(18)
C25	0.4279(2)	0.0753(2)	0.0751(2)	0.0377(10)
C26	0.3642(2)	0.0501(3)	0.1113(2)	0.0462(12)
C27	0.2959(3)	0.9813(3)	0.0956(3)	0.0615(16)
C28	0.2929(3)	0.9410(3)	0.0484(3)	0.0687(18)
C29	0.3566(3)	0.9677(3)	0.0136(3)	0.0624(15)
C30	0.4267(3)	0.0375(3)	0.0260(2)	0.0478(12)

	x/a	y/b	z/c	U(eq)
C31	0.3683(3)	0.0935(3)	0.1652(2)	0.0526(13)
C32	0.2893(3)	0.0816(4)	0.1849(3)	0.0756(18)
C33	0.4059(3)	0.0705(4)	0.2113(3)	0.0682(16)
C34	0.4950(3)	0.0696(3)	0.9848(2)	0.0525(13)
C35	0.5120(4)	0.0082(4)	0.9617(4)	0.095(2)
C36	0.4831(4)	0.1140(5)	0.9376(3)	0.092(2)
C109	0.7587(5)	0.8691(5)	0.3270(4)	0.096(2)
C110	0.6902(4)	0.8405(4)	0.3540(3)	0.084(2)
C111	0.6363(5)	0.8614(5)	0.3414(4)	0.093(2)
C112	0.6472(6)	0.9109(5)	0.2994(4)	0.117(3)
C113	0.7174(7)	0.9418(5)	0.2688(5)	0.139(4)
C114	0.7735(6)	0.9210(6)	0.2840(4)	0.134(4)
C115	0.8208(7)	0.8486(9)	0.3431(6)	0.183(7)
C123	0.1265(6)	0.0	0.3333	0.095(3)
C124	0.1892(6)	0.0548(5)	0.3624(4)	0.118(3)
C125	0.2601(8)	0.0577(8)	0.3617(5)	0.174(5)
C126	0.2617(10)	0.0	0.3333	0.158(6)
C129	0.0500(9)	0.0	0.3333	0.239(14)
N1'	0.95078(18)	0.71452(18)	0.19966(15)	0.0309(7)

Table 3.1.4 Bond lengths (Å) for salt 11.

O1-C2	1.222(5)	O1'-C2'	1.220(5)
O2-C4	1.223(5)	N1-C1	1.312(5)
N1-C25	1.455(5)	N1-C4	1.459(5)
N2-C1	1.308(5)	N2-C2	1.454(5)
N2-C13	1.465(5)	C1-H1	0.95
C1'-N1'	1.306(4)	C1'-N1'	1.306(4)
C1'-H1'	0.95	C2-C3	1.421(5)
C2'-C3'	1.405(5)	C2'-N1'	1.465(5)
C3-C4	1.419(5)	C3-C5	1.484(5)
C3'-C2'	1.405(5)	C3'-C5'	1.488(7)
C5-C6	1.396(5)	C5-C10	1.397(5)
C5'-C6'	1.379(5)	C5'-C6'	1.379(5)
C6-C7	1.394(5)	C6-H6	0.95
C6'-C7'	1.383(6)	C6'-H6'	0.95
C7-C8	1.382(5)	C7-H7	0.95
C7'-C8'	1.374(5)	C7'-H7'	0.95
C8-C9	1.398(5)	C8-C11	1.489(5)
C8'-C7'	1.374(5)	C8'-C11'	1.492(7)
C9-C10	1.382(5)	C9-H9	0.95

C10-H10	0.95	C11-C12'	1.392(5)
C11-C12	1.399(4)	C11'-C12'	1.396(4)
C11'-C12'	1.396(5)	C12-C11	1.399(4)
C12-H12	0.95	C12'-H12'	0.95
C13-C18	1.390(7)	C13-C14	1.394(6)
C13'-C14'	1.387(7)	C13'-C18'	1.399(6)
C13'-N1'	1.458(5)	C14-C15	1.411(6)
C14-C19	1.482(7)	C14'-C15'	1.394(7)
C14'-C19'	1.524(7)	C15-C16	1.363(8)
C15-H15	0.95	C15'-C16'	1.372(8)
C15'-H15'	0.95	C16-C17	1.374(8)
C16-H16	0.95	C17-C18	1.398(6)
C17-H17	0.95	C18-C22	1.513(7)
C16'-C17'	1.361(8)	C16'-H16'	0.95
C17'-C18'	1.404(6)	C17'-H17'	0.95
C18'-C22'	1.505(7)	C19-C20	1.517(8)
C19-C21	1.546(9)	C19-H19	1.0
C19'-C21'	1.493(9)	C19'-C20'	1.521(9)
C19'-H19'	1.0	C20-H20A	0.98
C20-H20B	0.98	C20-H20C	0.98
C20'-H20D	0.98	C20'-H20E	0.98
C20'-H20F	0.98	C21-H21A	0.98
C21-H21B	0.98	C21-H21C	0.98
C22-C24	1.495(8)	C22-C23	1.520(8)
C22-H22	1.0	C23-H23A	0.98
C23-H23B	0.98	C23-H23C	0.98
C24-H24A	0.98	C24-H24B	0.98
C24-H24C	0.98	C21'-H21D	0.98
C21'-H21E	0.98	C21'-H21F	0.98
C22'-C23'	1.525(7)	C22'-C24'	1.534(8)
C22'-H22'	1.0	C23'-H23D	0.98
C23'-H23E	0.98	C23'-H23F	0.98
C24'-H24D	0.98	C24'-H24E	0.98
C24'-H24F	0.98	C25-C30	1.378(7)
C25-C26	1.391(7)	C26-C27	1.397(7)
C26-C31	1.521(8)	C27-C28	1.359(9)
C27-H27	0.95	C28-C29	1.368(9)
C28-H28	0.95	C29-C30	1.405(7)
C29-H29	0.95	C30-C34	1.522(8)
C31-C33	1.512(8)	C31-C32	1.524(7)
C31-H31	1.0	C32-H32A	0.98
C32-H32B	0.98	C32-H32C	0.98

C33-H33A	0.98	C33-H33B	0.98
C33-H33C	0.98	C34-C35	1.506(8)
C34-C36	1.511(9)	C34-H34	1.0
C35-H35A	0.98	C35-H35B	0.98
C35-H35C	0.98	C36-H36A	0.98
C36-H36B	0.98	C36-H36C	0.98
C109-C110	1.336(9)	C109-C114	1.371(11)
C109-C115	1.512(14)	C110-C111	1.346(9)
C110-H110	0.95	C111-C112	1.337(10)
C111-H111	0.95	C112-C113	1.401(12)
C112-H112	0.95	C113-C114	1.403(11)
C113-H113	0.95	C114-H114	0.95
C115-H11A	0.98	C115-H11B	0.98
C115-H11C	0.98	C123-C124	1.351(10)
C123-C124	1.351(10)	C123-C129	1.503(19)
C124-C125	1.365(12)	C124-H124	0.95
C125-C126	1.334(12)	C125-H125	0.95
C126-C125	1.334(12)	C126-H126	0.95
C129-H12D	0.98	C129-H12E	0.98
C129-H12F	0.98		

Table 3.1.5 Bond angles (°) for 11.

C1-N1-C25	118.8(3)	C1-N1-C4	122.2(3)
C25-N1-C4	119.0(3)	C1-N2-C2	122.1(3)
C1-N2-C13	117.4(3)	C2-N2-C13	119.9(3)
N2-C1-N1	122.8(3)	N2-C1-H1	118.6
N1-C1-H1	118.6	N1'-C1'-N1'	123.2(5)
N1'-C1'-H1'	118.4	N1'-C1'-H1'	118.4
O1-C2-C3	128.9(3)	O1-C2-N2	115.8(3)
C3-C2-N2	115.2(3)	O1'-C2'-C3'	129.3(4)
O1'-C2'-N1'	115.6(3)	C3'-C2'-N1'	115.1(3)
C4-C3-C2	122.0(3)	C4-C3-C5	119.0(3)
C2-C3-C5	119.0(3)	C2'-C3'-C2'	122.9(5)
C2'-C3'-C5'	118.6(2)	C2'-C3'-C5'	118.6(2)
O2-C4-C3	128.6(3)	O2-C4-N1	116.5(3)
C3-C4-N1	114.9(3)	C6-C5-C10	116.9(3)
C6-C5-C3	122.5(3)	C10-C5-C3	120.6(3)
C6'-C5'-C6'	115.2(5)	C6'-C5'-C3'	122.4(3)
C6'-C5'-C3'	122.4(3)	C7-C6-C5	121.0(3)
C7-C6-H6	119.5	C5-C6-H6	119.5
C5'-C6'-C7'	122.3(4)	C5'-C6'-H6'	118.9

C7'-C6'-H6'	118.9	C8-C7-C6	122.1(3)
C8-C7-H7	119.0	C6-C7-H7	119.0
C8'-C7'-C6'	122.4(4)	C8'-C7'-H7'	118.8
C6'-C7'-H7'	118.8	C7-C8-C9	116.7(3)
C7-C8-C11	122.0(3)	C9-C8-C11	121.3(3)
C7'-C8'-C7'	115.4(5)	C7'-C8'-C11'	122.3(3)
C7'-C8'-C11'	122.3(3)	C10-C9-C8	121.8(3)
C10-C9-H9	119.1	C8-C9-H9	119.1
C9-C10-C5	121.5(3)	C9-C10-H10	119.3
C5-C10-H10	119.3	C12'-C11-C12	118.6(3)
C12'-C11-C8	120.7(3)	C12-C11-C8	120.7(3)
C12'-C11'-C12'	117.5(5)	C12'-C11'-C8'	121.3(2)
C12'-C11'-C8'	121.3(2)	C11-C12-C11	120.9(5)
C11-C12-H12	119.6	C11-C12-H12	119.6
C11-C12'-C11'	122.2(3)	C11-C12'-H12'	118.9
C11'-C12'-H12'	118.9	C18-C13-C14	124.7(4)
C18-C13-N2	116.9(4)	C14-C13-N2	118.4(4)
C14'-C13'-C18'	123.5(4)	C14'-C13'-N1'	119.1(4)
C18'-C13'-N1'	117.5(4)	C13-C14-C15	115.8(5)
C13-C14-C19	124.3(4)	C15-C14-C19	119.9(4)
C13'-C14'-C15'	117.6(5)	C13'-C14'-C19'	122.5(4)
C15'-C14'-C19'	119.8(5)	C16-C15-C14	120.5(5)
C16-C15-H15	119.7	C14-C15-H15	119.7
C16'-C15'-C14'	120.2(5)	C16'-C15'-H15'	119.9
C14'-C15'-H15'	119.9	C15-C16-C17	122.2(4)
C15-C16-H16	118.9	C17-C16-H16	118.9
C16-C17-C18	120.1(5)	C16-C17-H17	120.0
C18-C17-H17	120.0	C13-C18-C17	116.6(4)
C13-C18-C22	123.0(4)	C17-C18-C22	120.3(5)
C17'-C16'-C15'	121.3(5)	C17'-C16'-H16'	119.3
C15'-C16'-H16'	119.3	C16'-C17'-C18'	121.4(5)
C16'-C17'-H17'	119.3	C18'-C17'-H17'	119.3
C13'-C18'-C17'	115.9(5)	C13'-C18'-C22'	123.8(4)
C17'-C18'-C22'	120.2(4)	C14-C19-C20	113.1(5)
C14-C19-C21	110.0(5)	C20-C19-C21	109.8(5)
C14-C19-H19	107.9	C20-C19-H19	107.9
C21-C19-H19	107.9	C21'-C19'-C20'	110.5(7)
C21'-C19'-C14'	113.9(5)	C20'-C19'-C14'	110.0(5)
C21'-C19'-H19'	107.4	C20'-C19'-H19'	107.4
C14'-C19'-H19'	107.4	C19-C20-H20A	109.5
C19-C20-H20B	109.5	H20A-C20-H20B	109.5
C19-C20-H20C	109.5	H20A-C20-H20C	109.5

H20B-C20-H20C	109.5	C19'-C20'-H20D	109.5
C19'-C20'-H20E	109.5	H20D-C20'-H20E	109.5
C19'-C20'-H20F	109.5	H20D-C20'-H20F	109.5
H20E-C20'-H20F	109.5	C19-C21-H21A	109.5
C19-C21-H21B	109.5	H21A-C21-H21B	109.5
C19-C21-H21C	109.5	H21A-C21-H21C	109.5
H21B-C21-H21C	109.5	C24-C22-C18	114.2(4)
C24-C22-C23	110.0(5)	C18-C22-C23	110.4(4)
C24-C22-H22	107.3	C18-C22-H22	107.3
C23-C22-H22	107.3	C22-C23-H23A	109.5
C22-C23-H23B	109.5	H23A-C23-H23B	109.5
C22-C23-H23C	109.5	H23A-C23-H23C	109.5
H23B-C23-H23C	109.5	C22-C24-H24A	109.5
C22-C24-H24B	109.5	H24A-C24-H24B	109.5
C22-C24-H24C	109.5	H24A-C24-H24C	109.5
H24B-C24-H24C	109.5	C19'-C21'-H21D	109.5
C19'-C21'-H21E	109.5	H21D-C21'-H21E	109.5
C19'-C21'-H21F	109.5	H21D-C21'-H21F	109.5
H21E-C21'-H21F	109.5	C18'-C22'-C23'	112.7(5)
C18'-C22'-C24'	110.2(5)	C23'-C22'-C24'	110.5(4)
C18'-C22'-H22'	107.7	C23'-C22'-H22'	107.7
C24'-C22'-H22'	107.7	C22'-C23'-H23D	109.5
C22'-C23'-H23E	109.5	H23D-C23'-H23E	109.5
C22'-C23'-H23F	109.5	H23D-C23'-H23F	109.5
H23E-C23'-H23F	109.5	C22'-C24'-H24D	109.5
C22'-C24'-H24E	109.5	H24D-C24'-H24E	109.5
C22'-C24'-H24F	109.5	H24D-C24'-H24F	109.5
H24E-C24'-H24F	109.5	C30-C25-C26	124.3(4)
C30-C25-N1	118.0(4)	C26-C25-N1	117.6(4)
C25-C26-C27	115.9(5)	C25-C26-C31	122.6(4)
C27-C26-C31	121.6(5)	C28-C27-C26	121.6(5)
C28-C27-H27	119.2	C26-C27-H27	119.2
C27-C28-C29	120.9(5)	C27-C28-H28	119.5
C29-C28-H28	119.5	C28-C29-C30	120.6(6)
C28-C29-H29	119.7	C30-C29-H29	119.7
C25-C30-C29	116.7(5)	C25-C30-C34	123.3(4)
C29-C30-C34	120.0(5)	C33-C31-C26	110.1(4)
C33-C31-C32	110.0(5)	C26-C31-C32	114.2(5)
C33-C31-H31	107.4	C26-C31-H31	107.4
C32-C31-H31	107.4	C31-C32-H32A	109.5
C31-C32-H32B	109.5	H32A-C32-H32B	109.5
C31-C32-H32C	109.5	H32A-C32-H32C	109.5

H32B-C32-H32C	109.5	C31-C33-H33A	109.5
C31-C33-H33B	109.5	H33A-C33-H33B	109.5
C31-C33-H33C	109.5	H33A-C33-H33C	109.5
H33B-C33-H33C	109.5	C35-C34-C36	110.5(6)
C35-C34-C30	113.9(5)	C36-C34-C30	111.1(5)
C35-C34-H34	107.0	C36-C34-H34	107.0
C30-C34-H34	107.0	C34-C35-H35A	109.5
C34-C35-H35B	109.5	H35A-C35-H35B	109.5
C34-C35-H35C	109.5	H35A-C35-H35C	109.5
H35B-C35-H35C	109.5	C34-C36-H36A	109.5
C34-C36-H36B	109.5	H36A-C36-H36B	109.5
C34-C36-H36C	109.5	H36A-C36-H36C	109.5
H36B-C36-H36C	109.5	C110-C109-C114	117.8(9)
C110-C109-C115	122.9(10)	C114-C109-C115	119.2(10)
C109-C110-C111	123.1(9)	C109-C110-H110	118.5
C111-C110-H110	118.5	C112-C111-C110	121.6(9)
C112-C111-H111	119.2	C110-C111-H111	119.2
C111-C112-C113	118.1(10)	C111-C112-H112	121.0
C113-C112-H112	121.0	C112-C113-C114	119.0(10)
C112-C113-H113	120.5	C114-C113-H113	120.5
C109-C114-C113	120.3(10)	C109-C114-H114	119.8
C113-C114-H114	119.8	C109-C115-H11A	109.5
C109-C115-H11B	109.5	H11A-C115-H11B	109.5
C109-C115-H11C	109.5	H11A-C115-H11C	109.5
H11B-C115-H11C	109.5	C124-C123-C124	118.4(13)
C124-C123-C129	120.8(7)	C124-C123-C129	120.8(7)
C123-C124-C125	122.1(12)	C123-C124-H124	119.0
C125-C124-H124	119.0	C126-C125-C124	115.3(16)
C126-C125-H125	122.4	C124-C125-H125	122.4
C125-C126-C125	127.(2)	C125-C126-H126	116.6
C125-C126-H126	116.6	C123-C129-H12D	109.5
C123-C129-H12E	109.5	H12D-C129-H12E	109.5
C123-C129-H12F	109.5	H12D-C129-H12F	109.5
H12E-C129-H12F	109.5	C1'-N1'-C13'	118.4(3)
C1'-N1'-C2'	121.6(3)	C13'-N1'-C2'	119.8(3)

Table 3.1.6 Torsion angles (°) for 11.

C2-N2-C1-N1	2.5(7)	C13-N2-C1-N1	174.0(4)
C25-N1-C1-N2	175.6(4)	C4-N1-C1-N2	-3.6(7)
C1-N2-C2-O1	-175.1(4)	C13-N2-C2-O1	13.6(6)
C1-N2-C2-C3	4.0(6)	C13-N2-C2-C3	-167.4(4)

O1-C2-C3-C4	169.3(4)	N2-C2-C3-C4	-9.6(6)
O1-C2-C3-C5	-11.1(7)	N2-C2-C3-C5	170.0(3)
O1'-C2'-C3'-C2'	-177.7(5)	N1'-C2'-C3'-C2'	3.3(2)
O1'-C2'-C3'-C5'	2.3(5)	N1'-C2'-C3'-C5'	-176.7(2)
C2-C3-C4-O2	-173.1(5)	C5-C3-C4-O2	7.4(7)
C2-C3-C4-N1	8.6(6)	C5-C3-C4-N1	-170.9(4)
C1-N1-C4-O2	179.5(4)	C25-N1-C4-O2	0.4(6)
C1-N1-C4-C3	-2.0(6)	C25-N1-C4-C3	178.9(4)
C4-C3-C5-C6	-31.4(6)	C2-C3-C5-C6	149.1(4)
C4-C3-C5-C10	145.9(4)	C2-C3-C5-C10	-33.7(6)
C2'-C3'-C5'-C6'	139.0(4)	C2'-C3'-C5'-C6'	-41.0(4)
C2'-C3'-C5'-C6'	-41.0(4)	C2'-C3'-C5'-C6'	139.0(4)
C10-C5-C6-C7	-1.3(6)	C3-C5-C6-C7	176.0(4)
C6'-C5'-C6'-C7'	-0.4(4)	C3'-C5'-C6'-C7'	179.6(4)
C5-C6-C7-C8	0.0(7)	C5'-C6'-C7'-C8'	0.8(9)
C6-C7-C8-C9	1.0(6)	C6-C7-C8-C11	-178.1(4)
C6'-C7'-C8'-C7'	-0.4(4)	C6'-C7'-C8'-C11'	179.6(4)
C7-C8-C9-C10	-0.6(6)	C11-C8-C9-C10	178.5(4)
C8-C9-C10-C5	-0.7(7)	C6-C5-C10-C9	1.7(6)
C3-C5-C10-C9	-175.7(4)	C7-C8-C11-C12'	29.4(6)
C9-C8-C11-C12'	-149.6(4)	C7-C8-C11-C12	-151.1(4)
C9-C8-C11-C12	29.9(6)	C7'-C8'-C11'-C12'	173.8(4)
C7'-C8'-C11'-C12'	-6.2(4)	C7'-C8'-C11'-C12'	-6.2(4)
C7'-C8'-C11'-C12'	173.8(4)	C12'-C11-C12-C11	0.0(3)
C8-C11-C12-C11	-179.5(4)	C12-C11-C12'-C11'	0.1(6)
C8-C11-C12'-C11'	179.6(3)	C12'-C11'-C12'-C11	0.0(3)
C8'-C11'-C12'-C11	180.0(3)	C1-N2-C13-C18	-84.0(5)
C2-N2-C13-C18	87.8(5)	C1-N2-C13-C14	94.9(5)
C2-N2-C13-C14	-93.4(5)	C18-C13-C14-C15	3.3(7)
N2-C13-C14-C15	-175.4(4)	C18-C13-C14-C19	-177.3(5)
N2-C13-C14-C19	3.9(7)	C18'-C13'-C14'-C15'	0.5(6)
N1'-C13'-C14'-C15'	-178.4(4)	C18'-C13'-C14'-C19'	178.8(4)
N1'-C13'-C14'-C19'	-0.1(6)	C13-C14-C15-C16	-1.9(7)
C19-C14-C15-C16	178.7(5)	C13'-C14'-C15'-C16'	0.8(7)
C19'-C14'-C15'-C16'	-177.6(5)	C14-C15-C16-C17	0.2(9)
C15-C16-C17-C18	0.3(9)	C14-C13-C18-C17	-2.9(7)
N2-C13-C18-C17	175.9(4)	C14-C13-C18-C22	175.2(4)
N2-C13-C18-C22	-6.1(6)	C16-C17-C18-C13	0.9(7)
C16-C17-C18-C22	-177.2(5)	C14'-C15'-C16'-C17'	-0.3(8)
C15'-C16'-C17'-C18'	-1.5(8)	C14'-C13'-C18'-C17'	-2.2(6)
N1'-C13'-C18'-C17'	176.8(4)	C14'-C13'-C18'-C22'	179.3(4)
N1'-C13'-C18'-C22'	-1.8(6)	C16'-C17'-C18'-C13'	2.6(7)

C16'-C17'-C18'-C22'	-178.8(4)	C13-C14-C19-C20	131.6(5)
C15-C14-C19-C20	-49.0(6)	C13-C14-C19-C21	-105.2(5)
C15-C14-C19-C21	74.2(6)	C13'-C14'-C19'-C21'	132.3(6)
C15'-C14'-C19'-C21'	-49.5(7)	C13'-C14'-C19'-C20'	-103.1(6)
C15'-C14'-C19'-C20'	75.2(7)	C13-C18-C22-C24	140.3(5)
C17-C18-C22-C24	-41.7(7)	C13-C18-C22-C23	-95.2(6)
C17-C18-C22-C23	82.8(6)	C13'-C18'-C22'-C23'	-126.3(5)
C17'-C18'-C22'-C23'	55.3(6)	C13'-C18'-C22'-C24'	109.7(5)
C17'-C18'-C22'-C24'	-68.7(5)	C1-N1-C25-C30	106.7(5)
C4-N1-C25-C30	-74.1(5)	C1-N1-C25-C26	-72.4(5)
C4-N1-C25-C26	106.9(4)	C30-C25-C26-C27	0.6(7)
N1-C25-C26-C27	179.5(4)	C30-C25-C26-C31	179.7(4)
N1-C25-C26-C31	-1.4(6)	C25-C26-C27-C28	1.3(8)
C31-C26-C27-C28	-177.8(5)	C26-C27-C28-C29	-1.6(9)
C27-C28-C29-C30	0.0(9)	C26-C25-C30-C29	-2.1(7)
N1-C25-C30-C29	179.0(4)	C26-C25-C30-C34	175.0(4)
N1-C25-C30-C34	-3.9(7)	C28-C29-C30-C25	1.8(8)
C28-C29-C30-C34	-175.4(5)	C25-C26-C31-C33	-81.7(6)
C27-C26-C31-C33	97.4(6)	C25-C26-C31-C32	154.0(5)
C27-C26-C31-C32	-27.0(7)	C25-C30-C34-C35	137.9(6)
C29-C30-C34-C35	-45.1(7)	C25-C30-C34-C36	-96.5(6)
C29-C30-C34-C36	80.5(7)	C114-C109-C110-C111	-1.2(11)
C115-C109-C110-C111	176.8(8)	C109-C110-C111-C112	2.1(12)
C110-C111-C112-C113	-0.8(12)	C111-C112-C113-C114	-1.3(13)
C110-C109-C114-C113	-0.9(13)	C115-C109-C114-C113	-179.0(9)
C112-C113-C114-C109	2.1(14)	C124-C123-C124-C125	2.1(8)
C129-C123-C124-C125	-177.9(8)	C123-C124-C125-C126	-4.0(16)
C124-C125-C126-C125	1.9(8)	N1'-C1'-N1'-C13'	179.8(4)
N1'-C1'-N1'-C2'	3.8(3)	C14'-C13'-N1'-C1'	111.0(4)
C18'-C13'-N1'-C1'	-68.0(4)	C14'-C13'-N1'-C2'	-72.9(5)
C18'-C13'-N1'-C2'	108.2(4)	O1'-C2'-N1'-C1'	173.6(3)
C3'-C2'-N1'-C1'	-7.2(5)	O1'-C2'-N1'-C13'	-2.3(6)
C3'-C2'-N1'-C13'	176.8(3)		

Table 3.1.7 Anisotropic atomic displacement parameters (Å^2) for 11. The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0318(14)	0.0238(14)	0.071(2)	-0.0065(13)	-0.0116(14)	0.0162(12)
O1'	0.0379(16)	0.0301(15)	0.072(2)	0.0098(14)	0.0179(15)	0.0211(13)
O2	0.0274(14)	0.0236(14)	0.085(3)	-0.0027(14)	-0.0149(15)	0.0118(12)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	0.0202(15)	0.0271(16)	0.051(2)	-0.0013(15)	-0.0055(14)	0.0123(13)
N2	0.0255(16)	0.0272(16)	0.045(2)	0.0021(14)	-0.0036(14)	0.0177(14)
C1	0.0234(18)	0.032(2)	0.042(3)	0.0025(17)	-0.0014(16)	0.0178(16)
C1'	0.027(3)	0.0224(18)	0.042(4)	0.0005(12)	0.001(2)	0.0136(13)
C2	0.0198(17)	0.0258(19)	0.045(3)	0.0004(16)	-0.0031(16)	0.0141(15)
C2'	0.0236(19)	0.0239(18)	0.046(3)	0.0002(16)	0.0012(17)	0.0126(15)
C3	0.0198(17)	0.0220(18)	0.038(2)	0.0009(15)	0.0000(15)	0.0113(14)
C3'	0.021(2)	0.0224(19)	0.046(4)	-0.0013(11)	-0.003(2)	0.0105(12)
C4	0.0232(19)	0.0276(19)	0.049(3)	-0.0003(17)	-0.0060(17)	0.0167(16)
C5	0.0222(18)	0.0237(18)	0.037(2)	-0.0022(15)	-0.0019(15)	0.0147(15)
C5'	0.022(2)	0.0204(18)	0.040(3)	0.0012(11)	0.002(2)	0.0111(12)
C6	0.0189(17)	0.0195(17)	0.053(3)	0.0026(16)	0.0013(16)	0.0095(14)
C6'	0.021(2)	0.024(2)	0.129(5)	-0.006(2)	-0.009(3)	0.0129(18)
C7	0.0254(19)	0.0217(18)	0.050(3)	0.0036(16)	-0.0035(17)	0.0144(16)
C7'	0.020(2)	0.019(2)	0.120(5)	-0.009(2)	-0.008(2)	0.0071(16)
C8	0.0202(17)	0.0197(17)	0.043(3)	-0.0029(15)	-0.0028(16)	0.0109(14)
C8'	0.018(2)	0.0198(18)	0.047(4)	-0.0009(11)	-0.002(2)	0.0090(12)
C9	0.0195(18)	0.0205(17)	0.052(3)	0.0028(17)	0.0013(17)	0.0069(15)
C10	0.0261(19)	0.0208(18)	0.048(3)	0.0036(16)	-0.0022(16)	0.0143(16)
C11	0.0175(18)	0.0216(17)	0.046(3)	-0.0024(16)	-0.0016(16)	0.0093(15)
C11'	0.021(2)	0.0223(19)	0.046(4)	-0.0015(12)	-0.003(2)	0.0103(12)
C12	0.022(2)	0.0177(17)	0.047(4)	-0.0013(11)	-0.003(2)	0.0111(12)
C12'	0.0184(18)	0.0179(17)	0.052(3)	-0.0017(16)	-0.0031(16)	0.0069(14)
C13	0.030(2)	0.028(2)	0.055(3)	0.0017(18)	-0.0037(18)	0.0199(17)
C13'	0.0290(19)	0.0262(19)	0.048(3)	0.0091(17)	0.0084(18)	0.0169(17)
C14	0.041(2)	0.037(2)	0.061(3)	-0.001(2)	-0.002(2)	0.028(2)
C14'	0.037(2)	0.045(3)	0.054(3)	0.010(2)	0.008(2)	0.026(2)
C15	0.061(3)	0.049(3)	0.064(4)	0.001(2)	0.000(3)	0.043(3)
C15'	0.051(3)	0.059(3)	0.055(3)	0.021(2)	0.012(2)	0.031(3)
C16	0.084(4)	0.052(3)	0.067(4)	0.002(3)	-0.011(3)	0.053(3)
C17	0.073(3)	0.047(3)	0.049(3)	0.006(2)	-0.007(3)	0.039(3)
C18	0.043(2)	0.033(2)	0.048(3)	-0.0025(19)	-0.009(2)	0.0233(19)
C16'	0.046(3)	0.047(3)	0.087(5)	0.033(3)	0.022(3)	0.024(2)
C17'	0.037(2)	0.031(2)	0.081(4)	0.009(2)	0.007(2)	0.014(2)
C18'	0.031(2)	0.027(2)	0.065(3)	0.0039(19)	0.007(2)	0.0166(17)
C19	0.067(3)	0.055(3)	0.064(4)	0.008(3)	0.011(3)	0.048(3)
C19'	0.053(3)	0.055(3)	0.047(3)	0.006(2)	-0.003(2)	0.027(2)
C20	0.098(5)	0.086(4)	0.063(4)	0.000(3)	-0.001(3)	0.070(4)
C20'	0.097(6)	0.091(5)	0.147(8)	-0.038(5)	-0.070(6)	0.049(5)
C21	0.084(5)	0.076(4)	0.097(6)	0.016(4)	0.036(4)	0.042(4)
C22	0.056(3)	0.040(2)	0.047(3)	0.005(2)	0.004(2)	0.028(2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C23	0.067(4)	0.079(4)	0.094(5)	-0.016(4)	0.010(3)	0.037(3)
C24	0.106(5)	0.107(5)	0.056(4)	-0.013(4)	-0.006(4)	0.071(5)
C21'	0.145(8)	0.068(5)	0.114(7)	-0.019(4)	0.060(6)	0.022(5)
C22'	0.041(2)	0.029(2)	0.070(4)	-0.004(2)	-0.002(2)	0.0094(19)
C23'	0.051(3)	0.047(3)	0.094(5)	-0.012(3)	-0.017(3)	0.021(3)
C24'	0.052(3)	0.049(3)	0.101(5)	-0.021(3)	0.007(3)	0.015(3)
C25	0.0245(19)	0.026(2)	0.061(3)	-0.0017(19)	-0.0083(19)	0.0119(16)
C26	0.025(2)	0.038(2)	0.072(4)	0.010(2)	-0.003(2)	0.0135(18)
C27	0.027(2)	0.049(3)	0.094(5)	0.009(3)	-0.002(3)	0.008(2)
C28	0.036(3)	0.039(3)	0.108(5)	-0.003(3)	-0.020(3)	0.002(2)
C29	0.049(3)	0.048(3)	0.076(4)	-0.020(3)	-0.020(3)	0.014(2)
C30	0.035(2)	0.040(2)	0.067(4)	-0.004(2)	-0.014(2)	0.017(2)
C31	0.033(2)	0.047(3)	0.074(4)	0.011(2)	0.009(2)	0.017(2)
C32	0.050(3)	0.097(5)	0.089(5)	0.018(4)	0.012(3)	0.044(3)
C33	0.045(3)	0.080(4)	0.082(5)	-0.005(3)	-0.009(3)	0.033(3)
C34	0.041(3)	0.047(3)	0.066(4)	-0.015(2)	-0.011(2)	0.019(2)
C35	0.079(5)	0.071(4)	0.141(7)	-0.026(4)	0.014(5)	0.041(4)
C36	0.080(5)	0.124(6)	0.085(6)	0.028(5)	0.012(4)	0.061(5)
C109	0.079(4)	0.094(5)	0.087(5)	-0.035(4)	-0.001(4)	0.022(4)
C110	0.076(4)	0.065(4)	0.086(5)	-0.019(3)	-0.006(4)	0.016(3)
C111	0.081(4)	0.080(5)	0.102(6)	-0.029(4)	-0.020(4)	0.028(4)
C112	0.129(6)	0.073(5)	0.130(7)	-0.032(5)	-0.054(6)	0.037(5)
C113	0.161(8)	0.069(5)	0.115(7)	0.002(5)	-0.033(6)	0.002(6)
C114	0.109(6)	0.106(6)	0.099(6)	-0.024(5)	0.009(5)	-0.011(5)
C115	0.136(9)	0.255(16)	0.204(14)	-0.139(13)	-0.079(9)	0.132(11)
C123	0.100(6)	0.085(7)	0.093(8)	-0.005(6)	-0.002(3)	0.043(3)
C124	0.155(7)	0.079(5)	0.097(6)	0.000(4)	-0.011(6)	0.040(5)
C125	0.154(8)	0.172(10)	0.118(8)	0.044(7)	-0.029(7)	0.024(8)
C126	0.143(8)	0.214(15)	0.139(13)	0.063(11)	0.031(5)	0.107(7)
C129	0.171(12)	0.42(4)	0.21(2)	0.12(3)	0.060(13)	0.21(2)
N1'	0.0244(16)	0.0238(16)	0.044(2)	0.0026(14)	0.0033(14)	0.0114(13)

Table 3.1.8 Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 11.

	x/a	y/b	z/c	U(eq)
H1	-0.5420	0.2151	0.0688	0.037
H1'	0.0000	-0.3409	0.1667	0.036
H6	-0.3359	0.1097	0.1742	0.037
H6'	0.1173	-0.0035	0.1693	0.069

	x/a	y/b	z/c	U(eq)
H7	-0.2181	0.1114	0.1882	0.038
H7'	0.1171	0.1134	0.1682	0.065
H9	-0.1006	0.3240	0.1147	0.038
H10	-0.2170	0.3238	0.1013	0.037
H12	0.0000	0.3360	0.1667	0.034
H12'	-0.1176	0.0988	0.1557	0.036
H15	-0.4905	0.4743	0.1368	0.061
H15'	-0.1351	-0.4111	0.3641	0.064
H16	-0.4532	0.5262	0.0484	0.071
H17	-0.4056	0.4734	-0.0166	0.063
H16'	-0.2309	-0.5242	0.3211	0.072
H17'	-0.2462	-0.5316	0.2256	0.061
H19	-0.4698	0.3149	0.1915	0.065
H19'	-0.0042	-0.2307	0.2925	0.062
H20A	-0.4676	0.3919	0.2674	0.107
H20B	-0.4691	0.4546	0.2252	0.107
H20C	-0.3941	0.4430	0.2272	0.107
H20D	0.0885	-0.2374	0.3458	0.166
H20E	0.0526	-0.3137	0.3066	0.166
H20F	0.0263	-0.3215	0.3709	0.166
H21A	-0.5936	0.2812	0.2272	0.127
H21B	-0.6022	0.2710	0.1605	0.127
H21C	-0.5976	0.3466	0.1897	0.127
H22	-0.3971	0.2968	0.0029	0.055
H23A	-0.2735	0.3992	0.0332	0.12
H23B	-0.2690	0.3723	-0.0294	0.12
H23C	-0.2711	0.4518	-0.0189	0.12
H24A	-0.3814	0.3281	-0.0921	0.123
H24B	-0.4634	0.3164	-0.0698	0.123
H24C	-0.3909	0.4031	-0.0800	0.123
H21D	-0.0074	-0.2017	0.3874	0.184
H21E	-0.0771	-0.2898	0.3977	0.184
H21F	-0.0908	-0.2322	0.3578	0.184
H22'	-0.1384	-0.3717	0.1286	0.06
H23D	-0.2626	-0.4513	0.0881	0.099
H23E	-0.2716	-0.4123	0.1445	0.099
H23F	-0.2932	-0.5024	0.1443	0.099
H24D	-0.1518	-0.4801	0.0783	0.108
H24E	-0.1844	-0.5349	0.1327	0.108
H24F	-0.0949	-0.4652	0.1306	0.108
H27	-0.7496	-0.0378	0.1185	0.074

	x/a	y/b	z/c	U(eq)
H28	-0.7541	-0.1062	0.0394	0.082
H29	-0.6465	-0.0612	-0.0192	0.075
H31	-0.5967	0.1509	0.1579	0.063
H32A	-0.7023	0.1179	0.2159	0.113
H32B	-0.7438	0.0274	0.1978	0.113
H32C	-0.7367	0.0921	0.1538	0.113
H33A	-0.5893	0.1007	0.2453	0.102
H33B	-0.5418	0.0818	0.1992	0.102
H33C	-0.6268	0.0143	0.2192	0.102
H34	-0.4571	0.1084	0.0058	0.063
H35A	-0.4784	-0.0185	-0.0072	0.143
H35B	-0.4414	0.0335	-0.0624	0.143
H35C	-0.5332	-0.0302	-0.0602	0.143
H36A	-0.5234	0.1566	-0.0468	0.138
H36B	-0.5641	0.0781	-0.0837	0.138
H36C	-0.4711	0.1361	-0.0873	0.138
H110	0.6789	0.8037	0.3834	0.101
H111	0.5894	0.8403	0.3629	0.112
H112	0.6085	0.9248	0.2906	0.14
H113	0.7268	0.9764	0.2381	0.167
H114	0.8221	0.9429	0.2643	0.16
H11A	0.7954	0.7951	0.3584	0.275
H11B	0.8556	0.8858	0.3716	0.275
H11C	0.8516	0.8517	0.3099	0.275
H124	-0.8163	0.0925	0.3839	0.142
H125	-0.6949	0.0981	0.3801	0.209
H126	-0.6900	0.0000	0.3333	0.189
H12D	-0.9885	-0.0436	0.3102	0.287
H12E	-0.9697	-0.0062	0.3719	0.287
H12F	-0.9417	0.0498	0.3179	0.287

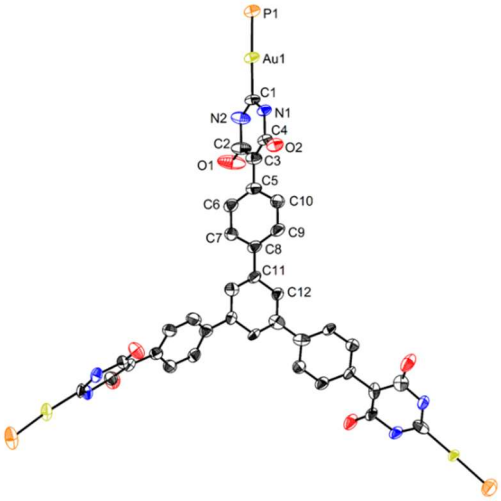
3.2. X-ray crystallography data for compound 12 ($C_{162}H_{162}Au_3N_6O_6P_3 \cdot 2.5C_6H_6$)

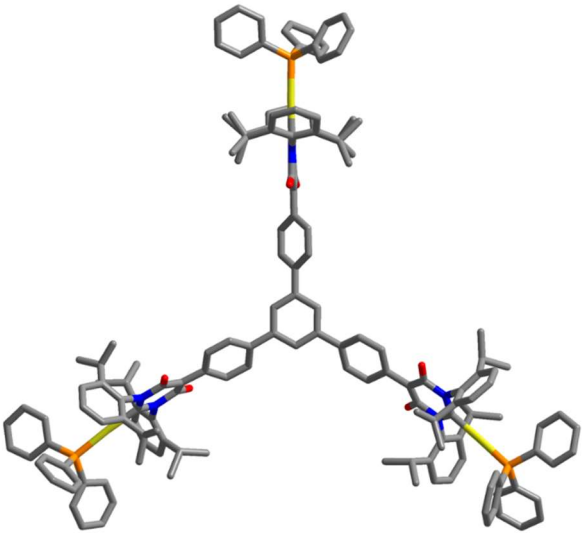
A specimen of $C_{177}H_{177}Au_3N_6O_6P_3$, approximate dimensions 0.067 mm x 0.069 mm x 0.302 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using a triclinic unit cell yielded a total of 240728 reflections to a maximum θ angle of 25.50° (0.83 Å resolution), of which 28689 were independent (average redundancy 8.391, completeness = 99.7%, R_{int} = 5.24%, R_{sig} = 3.11%) and 24617 (85.81%) were greater than $2\sigma(F^2)$. The final cell constants of a = 21.1658(11) Å, b = 21.5918(11) Å, c = 22.3912(12) Å, α = 62.407(2)°, β = 66.748(2)°, γ = 60.859(2)°, volume = 7729.5(7) $Å^3$, are based

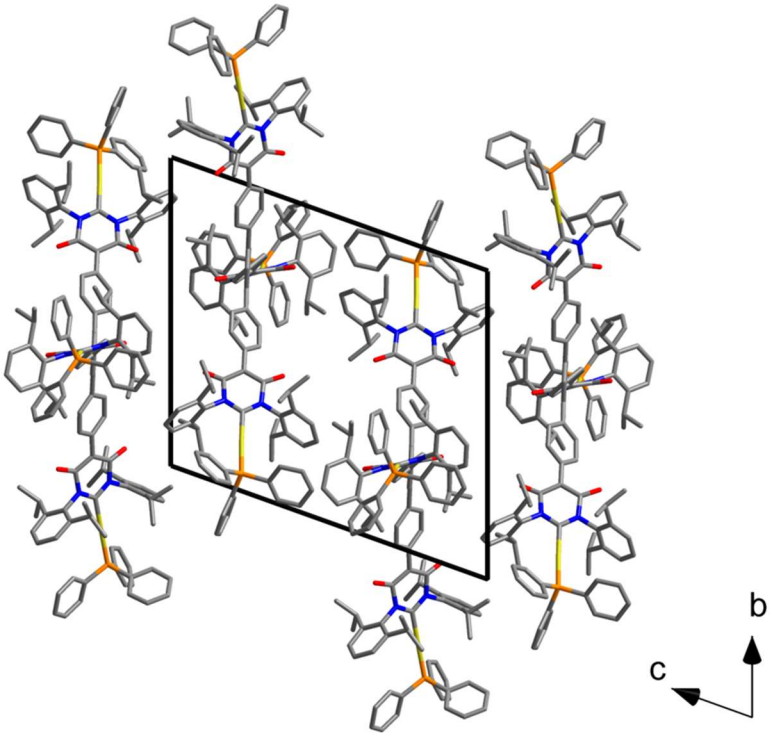
upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7903 and 1.0000.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 2 for the formula unit, $C_{177}H_{177}Au_3N_6O_6P_3$. The final anisotropic full-matrix least-squares refinement on F^2 with 1793 variables converged at R1 = 7.96%, for the observed data and wR2 = 19.59% for all data. The goodness-of-fit was 1.172. The largest peak in the final difference electron density synthesis was 4.765 $e^-/Å^3$ and the largest hole was -4.166 $e^-/Å^3$ with an RMS deviation of 0.199 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.361 g/cm^3 and F(000), 3222 e^-.





Solid state molecular structure of **12** with 50% probability ellipsoids. Hydrogen atoms and solvent molecules are omitted for clarity. Only half of the atoms are numbered, since the other half of the molecule is completed by inversion symmetry.



Partial packing diagram of the Au complex (solvent molecules omitted for clarity).

Table 3.2.1 Sample and crystal data for 12.

Chemical formula	$C_{177}H_{177}Au_3N_6O_6P_3$	
Formula weight	3168.04 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.067 x 0.069 x 0.302 mm	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 21.1658(11) Å	α = 62.407(2)°
	b = 21.5918(11) Å	β = 66.748(2)°
	c = 22.3912(12) Å	γ = 60.859(2)°
Volume	7729.5(7) $Å^3$	
Z	2	
Density (calculated)	1.361 g/cm^3	
Absorption coefficient	2.929 mm^{-1}	
F(000)	3222	

Table 3.2.2 Data collection and structure refinement for 12

Theta range for data collection	2.60 to 25.50°	
Index ranges	$-25 \leq h \leq 25$, $-26 \leq k \leq 26$, $-27 \leq l \leq 27$	
Reflections collected	240728	
Independent reflections	28689 [R(int) = 0.0524]	
Max. and min. transmission	1.0000 and 0.7903	
Structure solution technique	direct methods	
Structure solution program	SHELXT-2014 (Sheldrick 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014 (Sheldrick 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	28689 / 193 / 1793	
Goodness-of-fit on F^2	1.172	
Δ/σ_{max}	0.001	
Final R indices	24617 data; $I>2\sigma(I)$	R1 = 0.0796, wR2 = 0.1873
	all data	R1 = 0.0919, wR2 = 0.1959
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0080P)^2+208.5209P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	4.765 and -4.166 eÅ^{-3}	
R.M.S. deviation from mean	0.199 eÅ^{-3}	

Table 3.2.3 Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 12. 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	0.19920(2)	0.83930(2)	0.22381(2)	0.02492(11)
P1	0.09274(15)	0.94354(15)	0.22389(14)	0.0271(6)
O1	0.3805(5)	0.5801(5)	0.3533(4)	0.061(3)
O2	0.4403(4)	0.6583(4)	0.1086(4)	0.0326(17)
N1	0.3365(4)	0.7260(4)	0.1695(4)	0.0230(18)
N2	0.3116(5)	0.6937(5)	0.2859(5)	0.033(2)
C1	0.2920(5)	0.7425(5)	0.2270(5)	0.023(2)
C2	0.3745(6)	0.6222(6)	0.2934(6)	0.036(3)
C3	0.4196(6)	0.6082(6)	0.2312(6)	0.029(2)
C4	0.4038(5)	0.6606(5)	0.1669(5)	0.024(2)
C5	0.4862(5)	0.5389(6)	0.2344(6)	0.028(2)
C6	0.5317(6)	0.5109(6)	0.2791(6)	0.029(2)
C7	0.5958(6)	0.4459(6)	0.2797(6)	0.028(2)
C8	0.6147(5)	0.4057(6)	0.2382(6)	0.028(2)

	x/a	y/b	z/c	U(eq)
C9	0.5686(6)	0.4328(6)	0.1942(6)	0.030(2)
C10	0.5060(6)	0.4986(6)	0.1912(6)	0.031(2)
C11	0.6829(6)	0.3371(6)	0.2397(6)	0.026(2)
C12	0.6811(5)	0.2718(5)	0.2415(5)	0.024(2)
C13	0.2653(7)	0.7100(7)	0.3486(6)	0.043(3)
C14	0.2112(7)	0.6789(9)	0.3886(6)	0.056(4)
C15	0.1652(10)	0.7015(14)	0.4456(8)	0.089(7)
C16	0.1720(12)	0.7517(15)	0.4609(9)	0.100(8)
C17	0.2287(11)	0.7803(11)	0.4218(9)	0.081(6)
C18	0.2760(8)	0.7604(9)	0.3636(7)	0.060(4)
C19	0.2008(8)	0.6251(8)	0.3717(7)	0.056(4)
C20	0.1299(9)	0.6642(11)	0.3451(10)	0.081(6)
C21	0.2018(11)	0.5542(11)	0.4321(10)	0.095(7)
C22	0.3381(9)	0.7882(9)	0.3200(9)	0.062(4)
C23	0.3242(10)	0.8634(10)	0.3190(10)	0.075(5)
C24	0.4117(10)	0.7306(13)	0.3371(12)	0.097(7)
C25	0.3128(5)	0.7760(5)	0.1052(5)	0.024(2)
C26	0.3371(6)	0.8365(6)	0.0648(5)	0.028(2)
C27	0.3113(7)	0.8853(7)	0.0049(6)	0.039(3)
C28	0.2666(7)	0.8723(8)	0.9847(6)	0.046(3)
C29	0.2446(6)	0.8109(8)	0.0238(7)	0.043(3)
C30	0.2682(6)	0.7603(6)	0.0861(6)	0.032(2)
C31	0.3900(7)	0.8480(7)	0.0849(6)	0.037(3)
C32	0.3549(9)	0.9215(9)	0.0985(9)	0.061(4)
C33	0.4620(8)	0.8437(10)	0.0311(8)	0.060(4)
C34	0.2480(7)	0.6920(8)	0.1276(8)	0.046(3)
C35	0.1676(8)	0.7097(9)	0.1350(10)	0.068(5)
C36	0.2972(9)	0.6286(9)	0.0988(10)	0.066(4)
C37	0.0373(6)	0.9540(6)	0.1722(6)	0.032(2)
C38	0.0742(7)	0.9242(6)	0.1195(6)	0.037(3)
C39	0.0342(8)	0.9282(8)	0.0812(7)	0.052(3)
C40	0.9573(9)	0.9628(9)	0.0948(7)	0.059(4)
C41	0.9222(8)	0.9939(10)	0.1457(7)	0.058(4)
C42	0.9613(7)	0.9887(9)	0.1852(7)	0.052(4)
C43	0.1057(6)	0.0320(6)	0.1921(5)	0.028(2)
C44	0.1681(7)	0.0303(6)	0.2001(6)	0.035(3)
C45	0.1788(8)	0.0967(7)	0.1798(6)	0.045(3)
C46	0.1257(8)	0.1643(7)	0.1533(6)	0.044(3)
C47	0.0634(8)	0.1668(7)	0.1454(6)	0.047(3)
C48	0.0527(6)	0.1016(6)	0.1649(6)	0.037(3)
C49	0.0339(12)	0.9366(10)	0.3107(9)	0.090(3)

	x/a	y/b	z/c	U(eq)
C50	0.0140(12)	0.8764(10)	0.3462(9)	0.094(3)
C51	0.9748(12)	0.8667(11)	0.4164(9)	0.097(3)
C52	0.9526(12)	0.9149(10)	0.4455(9)	0.096(3)
C53	0.9710(12)	0.9789(11)	0.4080(9)	0.096(3)
C54	0.0134(12)	0.9872(10)	0.3388(9)	0.093(3)
Au1'	0.30333(2)	0.25614(3)	0.28889(2)	0.03092(12)
P1'	0.41792(18)	0.2363(2)	0.29388(17)	0.0451(9)
O1'	0.0518(4)	0.2147(4)	0.3872(4)	0.0315(17)
O2'	0.1133(4)	0.3424(5)	0.1461(4)	0.0346(18)
N1'	0.1832(5)	0.3063(5)	0.2210(4)	0.0247(18)
N2'	0.1592(4)	0.2362(5)	0.3340(4)	0.0225(17)
C1'	0.2038(5)	0.2679(6)	0.2799(5)	0.024(2)
C2'	0.0892(6)	0.2414(6)	0.3317(5)	0.026(2)
C3'	0.0743(5)	0.2747(5)	0.2642(5)	0.022(2)
C4'	0.1203(6)	0.3105(6)	0.2066(5)	0.026(2)
C5'	0.0094(5)	0.2726(6)	0.2567(5)	0.025(2)
C6'	0.9704(6)	0.3281(6)	0.2052(6)	0.029(2)
C7'	0.9080(6)	0.3271(6)	0.2004(6)	0.033(2)
C8'	0.8820(6)	0.2702(6)	0.2453(6)	0.027(2)
C9'	0.9237(6)	0.2109(6)	0.2943(5)	0.025(2)
C10'	0.9856(6)	0.2125(6)	0.2994(6)	0.028(2)
C11'	0.8127(6)	0.2707(6)	0.2429(5)	0.025(2)
C12'	0.7490(6)	0.3356(6)	0.2398(6)	0.032(2)
C13'	0.1831(6)	0.1903(6)	0.3986(5)	0.026(2)
C14'	0.1685(6)	0.2259(7)	0.4446(6)	0.035(3)
C15'	0.1956(7)	0.1796(9)	0.5043(6)	0.045(3)
C16'	0.2326(7)	0.1035(10)	0.5181(6)	0.054(4)
C17'	0.2440(7)	0.0698(8)	0.4729(7)	0.049(3)
C18'	0.2188(6)	0.1134(7)	0.4118(6)	0.034(3)
C19'	0.1263(7)	0.3090(7)	0.4307(6)	0.042(3)
C20'	0.0521(8)	0.3254(9)	0.4834(8)	0.056(4)
C21'	0.1702(10)	0.3489(10)	0.4298(10)	0.073(5)
C22'	0.2319(8)	0.0760(7)	0.3610(7)	0.044(3)
C23'	0.3131(8)	0.0368(8)	0.3335(9)	0.064(5)
C24'	0.1892(9)	0.0261(11)	0.3919(10)	0.075(5)
C25'	0.2306(6)	0.3469(7)	0.1637(6)	0.035(3)
C26'	0.2853(6)	0.3094(7)	0.1195(5)	0.033(3)
C27'	0.3349(8)	0.3447(9)	0.0690(6)	0.047(3)
C28'	0.3278(10)	0.4112(10)	0.0657(8)	0.066(5)
C29'	0.2710(11)	0.4491(11)	0.1094(10)	0.081(6)
C30'	0.2202(10)	0.4170(9)	0.1587(10)	0.073(5)

	x/a	y/b	z/c	U(eq)
C31'	0.2924(7)	0.2359(8)	0.1201(6)	0.043(3)
C32'	0.3654(9)	0.1732(10)	0.1345(10)	0.071(5)
C33'	0.2775(10)	0.2462(12)	0.0549(8)	0.075(5)
C34'	0.1637(12)	0.4510(12)	0.2137(16)	0.125(12)
C35'	0.1785(16)	0.4877(16)	0.2391(13)	0.134(11)
C36'	0.096(2)	0.492(2)	0.190(2)	0.195(16)
C37'	0.4201(8)	0.2985(10)	0.3248(7)	0.051(4)
C38'	0.4783(10)	0.2816(12)	0.3506(7)	0.069(5)
C39'	0.4811(12)	0.3303(13)	0.3707(8)	0.077(6)
C40'	0.4260(11)	0.3974(11)	0.3640(7)	0.062(5)
C41'	0.3640(13)	0.4204(13)	0.3383(8)	0.090(7)
C42'	0.3644(11)	0.3677(11)	0.3170(8)	0.069(5)
C43'	0.4616(7)	0.1410(11)	0.3463(7)	0.062(5)
C44'	0.5388(8)	0.1020(12)	0.3370(7)	0.072(6)
C45'	0.5682(10)	0.0268(13)	0.3753(10)	0.090(7)
C46'	0.5209(11)	0.9905(14)	0.4253(11)	0.102(8)
C47'	0.4478(10)	0.0257(13)	0.4335(11)	0.096(7)
C48'	0.4176(9)	0.0991(12)	0.3943(8)	0.071(5)
C49'	0.4780(7)	0.2478(9)	0.2083(7)	0.048(4)
C50'	0.5038(7)	0.1940(10)	0.1792(7)	0.055(4)
C51'	0.5436(8)	0.2046(11)	0.1110(7)	0.063(5)
C52'	0.5571(8)	0.2695(11)	0.0730(8)	0.065(5)
C53'	0.5316(9)	0.3244(11)	0.1013(8)	0.066(4)
C54'	0.4918(8)	0.3132(11)	0.1701(7)	0.061(4)
Au1"	0.76996(5)	0.71249(3)	0.21966(4)	0.0205(2)
Au1B	0.7316(2)	0.71185(13)	0.2592(3)	0.0669(14)
P1"	0.7980(2)	0.60685(19)	0.19845(18)	0.0458(8)
O1"	0.6873(6)	0.0006(4)	0.1456(4)	0.050(3)
O2"	0.7716(5)	0.8577(4)	0.3543(4)	0.038(2)
N1"	0.7666(5)	0.8051(5)	0.2885(4)	0.0258(19)
N2"	0.7187(5)	0.8761(5)	0.1937(4)	0.0257(18)
C1"	0.7473(6)	0.8079(6)	0.2378(5)	0.030(2)
C2"	0.7134(6)	0.9464(6)	0.1915(5)	0.030(2)
C3"	0.7372(6)	0.9396(6)	0.2461(5)	0.024(2)
C4"	0.7570(6)	0.8707(5)	0.3009(5)	0.025(2)
C5"	0.7361(6)	0.0082(5)	0.2486(5)	0.025(2)
C6"	0.7783(6)	0.0026(6)	0.2873(5)	0.026(2)
C7"	0.7796(6)	0.0659(6)	0.2868(5)	0.026(2)
C8"	0.7409(5)	0.1384(6)	0.2479(5)	0.026(2)
C9"	0.6985(5)	0.1442(5)	0.2087(5)	0.023(2)
C10"	0.6959(5)	0.0815(5)	0.2091(5)	0.023(2)

	x/a	y/b	z/c	U(eq)
C11"	0.7445(6)	0.2076(6)	0.2449(6)	0.029(2)
C12"	0.8092(6)	0.2055(6)	0.2471(6)	0.026(2)
C13"	0.6934(7)	0.8815(6)	0.1377(6)	0.037(3)
C14"	0.6203(8)	0.8946(7)	0.1488(8)	0.048(3)
C15"	0.5993(9)	0.8950(8)	0.0942(9)	0.058(4)
C16"	0.6502(11)	0.8865(9)	0.0371(9)	0.068(5)
C17"	0.7217(10)	0.8766(8)	0.0253(8)	0.057(4)
C18"	0.7460(8)	0.8746(7)	0.0758(6)	0.045(3)
C19"	0.5663(8)	0.9088(10)	0.2135(10)	0.072(5)
C20"	0.5009(13)	0.9836(13)	0.2011(13)	0.123(10)
C21"	0.5377(13)	0.8410(15)	0.2575(13)	0.127(10)
C22"	0.8247(9)	0.8674(9)	0.0620(8)	0.063(4)
C23"	0.8824(12)	0.7909(11)	0.0549(10)	0.105(8)
C24"	0.8420(10)	0.9304(10)	0.9991(9)	0.078(5)
C25"	0.8042(7)	0.7324(6)	0.3351(6)	0.034(3)
C26"	0.8819(7)	0.7020(7)	0.3162(7)	0.041(3)
C27"	0.9167(9)	0.6320(8)	0.3616(8)	0.056(4)
C28"	0.8786(11)	0.5946(8)	0.4191(8)	0.062(5)
C29"	0.8026(10)	0.6247(8)	0.4355(7)	0.057(4)
C30"	0.7634(8)	0.6951(7)	0.3942(7)	0.045(3)
C31"	0.9247(8)	0.7430(9)	0.2532(9)	0.062(4)
C32"	0.9607(11)	0.7767(11)	0.2717(13)	0.094(7)
C33"	0.9812(10)	0.6963(13)	0.2073(10)	0.088(6)
C34"	0.6815(9)	0.7315(10)	0.4132(8)	0.069(5)
C35"	0.6564(10)	0.7537(11)	0.4766(9)	0.087(6)
C36"	0.6429(14)	0.6803(16)	0.4243(11)	0.125(10)
C37"	0.8752(8)	0.5918(8)	0.1247(7)	0.049(3)
C38"	0.9458(8)	0.5352(7)	0.1300(7)	0.050(3)
C39"	0.0004(9)	0.5277(9)	0.0732(8)	0.059(4)
C40"	0.9891(9)	0.5766(9)	0.0090(8)	0.062(4)
C41"	0.9215(9)	0.6322(9)	0.0005(8)	0.060(4)
C42"	0.8642(9)	0.6434(9)	0.0583(7)	0.059(4)
C43"	0.8277(9)	0.5217(8)	0.2708(7)	0.051(3)
C44"	0.8669(9)	0.5213(8)	0.3070(7)	0.056(4)
C45"	0.9046(10)	0.4542(9)	0.3538(9)	0.069(5)
C46"	0.8993(10)	0.3871(8)	0.3652(8)	0.063(5)
C47"	0.8555(13)	0.3895(8)	0.3340(9)	0.083(6)
C48"	0.8210(12)	0.4564(8)	0.2846(11)	0.084(6)
C49"	0.7232(9)	0.6097(7)	0.1756(7)	0.051(4)
C50"	0.6524(9)	0.6631(10)	0.1869(8)	0.058(4)
C51"	0.5959(10)	0.6709(12)	0.1630(10)	0.081(6)

	x/a	y/b	z/c	U(eq)
C52"	0.6113(10)	0.6213(11)	0.1305(7)	0.061(5)
C53"	0.6797(12)	0.5692(11)	0.1214(10)	0.076(5)
C54"	0.7364(11)	0.5610(9)	0.1433(9)	0.067(5)
C55	0.7816(12)	0.3649(14)	0.0468(12)	0.098(3)
C56	0.7780(12)	0.2947(13)	0.0715(12)	0.095(3)
C57	0.8436(12)	0.2307(14)	0.0696(12)	0.094(3)
C58	0.9091(12)	0.2383(14)	0.0425(12)	0.095(3)
C59	0.9133(13)	0.3094(13)	0.0156(12)	0.098(3)
C60	0.8505(12)	0.3692(14)	0.0182(12)	0.099(3)
C61	0.5771(14)	0.5822(19)	0.3806(12)	0.153(5)
C62	0.6449(15)	0.5264(16)	0.3708(13)	0.153(5)
C63	0.6764(15)	0.4686(18)	0.4245(10)	0.153(5)
C64	0.6403(14)	0.4667(18)	0.4909(12)	0.153(5)
C65	0.5716(14)	0.5206(16)	0.5034(13)	0.153(5)
C66	0.5404(15)	0.5734(19)	0.4481(10)	0.153(5)
C67	0.6432(17)	0.146(2)	0.4461(15)	0.080(5)
C68	0.700(2)	0.1700(18)	0.4241(17)	0.080(5)
C69	0.6999(18)	0.2306(17)	0.4300(16)	0.080(5)
C70	0.6354(16)	0.260(2)	0.4733(15)	0.080(5)
C71	0.585(2)	0.2263(17)	0.5165(16)	0.080(5)
C72	0.5896(19)	0.1715(18)	0.4981(15)	0.080(5)

Table 3.2.4 Bond lengths (Å) for 12.

Au1-C1	2.050(9)	Au1-P1	2.281(3)
P1-C43	1.825(11)	P1-C37	1.828(12)
P1-C49	1.830(15)	O1-C2	1.238(14)
O2-C4	1.236(12)	N1-C1	1.346(13)
N1-C4	1.442(12)	N1-C25	1.447(13)
N2-C1	1.319(13)	N2-C13	1.447(15)
N2-C2	1.456(14)	C2-C3	1.414(16)
C3-C4	1.404(15)	C3-C5	1.470(14)
C5-C6	1.388(15)	C5-C10	1.404(16)
C6-C7	1.397(14)	C6-H6	0.95
C7-C8	1.375(15)	C7-H7	0.95
C8-C9	1.391(15)	C8-C11	1.480(14)
C9-C10	1.388(15)	C9-H9	0.95
C10-H10	0.95	C11-C12'	1.383(15)
C11-C12	1.411(13)	C12-C11"	1.378(15)
C12-H12	0.95	C13-C14	1.39(2)

C13-C18	1.41(2)	C14-C15	1.40(2)
C14-C19	1.51(2)	C15-C16	1.36(3)
C15-H15	0.95	C16-C17	1.41(3)
C16-H16	0.95	C17-C18	1.40(2)
C17-H17	0.95	C18-C22	1.50(2)
C19-C21	1.50(2)	C19-C20	1.52(2)
C19-H19	1.0	C20-H20A	0.98
C20-H20B	0.98	C20-H20C	0.98
C21-H21A	0.98	C21-H21B	0.98
C21-H21C	0.98	C22-C23	1.49(2)
C22-C24	1.50(2)	C22-H22	1.0
C23-H23A	0.98	C23-H23B	0.98
C23-H23C	0.98	C24-H24A	0.98
C24-H24B	0.98	C24-H24C	0.98
C25-C30	1.395(15)	C25-C26	1.409(14)
C26-C27	1.385(16)	C26-C31	1.511(16)
C27-C28	1.374(19)	C27-H27	0.95
C28-C29	1.40(2)	C28-H28	0.95
C29-C30	1.414(17)	C29-H29	0.95
C30-C34	1.501(17)	C31-C32	1.512(18)
C31-C33	1.516(17)	C31-H31	1.0
C32-H32A	0.98	C32-H32B	0.98
C32-H32C	0.98	C33-H33A	0.98
C33-H33B	0.98	C33-H33C	0.98
C34-C35	1.505(18)	C34-C36	1.510(19)
C34-H34	1.0	C35-H35A	0.98
C35-H35B	0.98	C35-H35C	0.98
C36-H36A	0.98	C36-H36B	0.98
C36-H36C	0.98	C37-C42	1.374(17)
C37-C38	1.380(16)	C38-C39	1.375(19)
C38-H38	0.95	C39-C40	1.39(2)
C39-H39	0.95	C40-C41	1.36(2)
C40-H40	0.95	C41-C42	1.37(2)
C41-H41	0.95	C42-H42	0.95
C43-C44	1.381(16)	C43-C48	1.392(15)
C44-C45	1.395(16)	C44-H44	0.95
C45-C46	1.369(19)	C45-H45	0.95
C46-C47	1.37(2)	C46-H46	0.95
C47-C48	1.375(18)	C47-H47	0.95
C48-H48	0.95	C49-C54	1.32(3)
C49-C50	1.34(2)	C50-C51	1.43(2)
C50-H50	0.95	C51-C52	1.28(3)

C51-H51	0.95	C52-C53	1.40(2)
C52-H52	0.95	C53-C54	1.43(2)
C53-H53	0.95	C54-H54	0.95
Au1'-C1'	2.077(10)	Au1'-P1'	2.288(3)
P1'-C43'	1.798(18)	P1'-C37'	1.798(15)
P1'-C49'	1.815(13)	O1'-C2'	1.227(12)
O2'-C4'	1.234(12)	N1'-C1'	1.305(13)
N1'-C4'	1.443(13)	N1'-C25'	1.490(12)
N2'-C1'	1.336(13)	N2'-C13'	1.447(13)
N2'-C2'	1.450(12)	C2'-C3'	1.431(14)
C3'-C4'	1.423(14)	C3'-C5'	1.473(14)
C5'-C6'	1.399(15)	C5'-C10'	1.400(14)
C6'-C7'	1.377(15)	C6'-H6'	0.95
C7'-C8'	1.379(15)	C7'-H7'	0.95
C8'-C9'	1.409(15)	C8'-C11'	1.484(14)
C9'-C10'	1.376(14)	C9'-H9'	0.95
C10'-H10'	0.95	C11'-C12'	1.390(15)
C11'-C12"	1.402(14)	C12'-H12'	0.95
C13'-C18'	1.384(16)	C13'-C14'	1.412(15)
C14'-C15'	1.388(17)	C14'-C19'	1.502(18)
C15'-C16'	1.37(2)	C15'-H15'	0.95
C16'-C17'	1.39(2)	C16'-H16'	0.95
C17'-C18'	1.392(17)	C17'-H17'	0.95
C18'-C22'	1.551(16)	C19'-C21'	1.534(18)
C19'-C20'	1.539(17)	C19'-H19'	1.0
C20'-H20D	0.98	C20'-H20E	0.98
C20'-H20F	0.98	C21'-H21D	0.98
C21'-H21E	0.98	C21'-H21F	0.98
C22'-C24'	1.49(2)	C22'-C23'	1.509(19)
C22'-H22'	1.0	C23'-H23D	0.98
C23'-H23E	0.98	C23'-H23F	0.98
C24'-H24D	0.98	C24'-H24E	0.98
C24'-H24F	0.98	C25'-C30'	1.37(2)
C25'-C26'	1.379(17)	C26'-C27'	1.417(15)
C26'-C31'	1.512(17)	C27'-C28'	1.34(2)
C27'-H27'	0.95	C28'-C29'	1.39(3)
C28'-H28'	0.95	C29'-C30'	1.39(2)
C29'-H29'	0.95	C30'-C34'	1.52(3)
C31'-C32'	1.51(2)	C31'-C33'	1.510(19)
C31'-H31'	1.0	C32'-H32D	0.98
C32'-H32E	0.98	C32'-H32F	0.98
C33'-H33D	0.98	C33'-H33E	0.98

C33'-H33F	0.98	C34'-C35'	1.36(3)
C34'-C36'	1.420(18)	C34'-H34'	1.0
C35'-H35D	0.98	C35'-H35E	0.98
C35'-H35F	0.98	C36'-H36D	0.98
C36'-H36E	0.98	C36'-H36F	0.98
C37'-C42'	1.36(2)	C37'-C38'	1.38(2)
C38'-C39'	1.36(2)	C38'-H38'	0.95
C39'-C40'	1.33(3)	C39'-H39'	0.95
C40'-C41'	1.41(3)	C40'-H40'	0.95
C41'-C42'	1.42(2)	C41'-H41'	0.95
C42'-H42'	0.95	C43'-C48'	1.40(2)
C43'-C44'	1.407(19)	C44'-C45'	1.38(3)
C44'-H44'	0.95	C45'-C46'	1.39(3)
C45'-H45'	0.95	C46'-C47'	1.33(2)
C46'-H46'	0.95	C47'-C48'	1.36(3)
C47'-H47'	0.95	C48'-H48'	0.95
C49'-C50'	1.37(2)	C49'-C54'	1.38(2)
C50'-C51'	1.394(19)	C50'-H50'	0.95
C51'-C52'	1.36(2)	C51'-H51'	0.95
C52'-C53'	1.38(2)	C52'-H52'	0.95
C53'-C54'	1.40(2)	C53'-H53'	0.95
C54'-H54'	0.95	Au1"-C1"	2.073(12)
Au1"-P1"	2.290(3)	Au1B-C1"	2.065(12)
Au1B-P1"	2.686(5)	P1"-C49"	1.815(15)
P1"-C43"	1.821(14)	P1"-C37"	1.831(15)
O1"-C2"	1.199(13)	O2"-C4"	1.225(12)
N1"-C1"	1.318(13)	N1"-C25"	1.452(13)
N1"-C4"	1.470(12)	N2"-C1"	1.329(13)
N2"-C2"	1.446(14)	N2"-C13"	1.486(14)
C2"-C3"	1.420(14)	C3"-C4"	1.414(14)
C3"-C5"	1.497(13)	C5"-C6"	1.404(14)
C5"-C10"	1.412(14)	C6"-C7"	1.375(14)
C6"-H6"	0.95	C7"-C8"	1.390(14)
C7"-H7"	0.95	C8"-C9"	1.415(15)
C8"-C11"	1.503(15)	C9"-C10"	1.378(14)
C9"-H9"	0.95	C10"-H10"	0.95
C11"-C12"	1.368(14)	C12"-H12"	0.95
C13"-C14"	1.368(18)	C13"-C18"	1.412(18)
C14"-C15"	1.45(2)	C14"-C19"	1.50(2)
C15"-C16"	1.33(2)	C15"-H15"	0.95
C16"-C17"	1.35(2)	C16"-H16"	0.95
C17"-C18"	1.391(18)	C17"-H17"	0.95

C18"-C22"	1.51(2)	C19"-C20"	1.52(2)
C19"-C21"	1.59(3)	C19"-H19"	1.0
C20"-H20G	0.98	C20"-H20H	0.98
C20"-H20I	0.98	C21"-H21G	0.98
C21"-H21H	0.98	C21"-H21I	0.98
C22"-C24"	1.51(2)	C22"-C23"	1.54(2)
C22"-H22"	1.0	C23"-H23G	0.98
C23"-H23H	0.98	C23"-H23I	0.98
C24"-H24G	0.98	C24"-H24H	0.98
C24"-H24I	0.98	C25"-C30"	1.391(17)
C25"-C26"	1.404(18)	C26"-C27"	1.394(17)
C26"-C31"	1.49(2)	C27"-C28"	1.35(2)
C27"-H27"	0.95	C28"-C29"	1.37(2)
C28"-H28"	0.95	C29"-C30"	1.389(18)
C29"-H29"	0.95	C30"-C34"	1.48(2)
C31"-C33"	1.52(2)	C31"-C32"	1.53(2)
C31"-H31"	1.0	C32"-H32G	0.98
C32"-H32H	0.98	C32"-H32I	0.98
C33"-H33G	0.98	C33"-H33H	0.98
C33"-H33I	0.98	C34"-C35"	1.52(3)
C34"-C36"	1.55(3)	C34"-H34"	1.0
C35"-H35G	0.98	C35"-H35H	0.98
C35"-H35I	0.98	C36"-H36G	0.98
C36"-H36H	0.98	C36"-H36I	0.98
C37"-C38"	1.403(19)	C37"-C42"	1.410(19)
C38"-C39"	1.35(2)	C38"-H38"	0.95
C39"-C40"	1.36(2)	C39"-H39"	0.95
C40"-C41"	1.36(2)	C40"-H40"	0.95
C41"-C42"	1.40(2)	C41"-H41"	0.95
C42"-H42"	0.95	C43"-C48"	1.36(2)
C43"-C44"	1.37(2)	C44"-C45"	1.40(2)
C44"-H44"	0.95	C45"-C46"	1.40(2)
C45"-H45"	0.95	C46"-C47"	1.33(2)
C46"-H46"	0.95	C47"-C48"	1.40(2)
C47"-H47"	0.95	C48"-H48"	0.95
C49"-C50"	1.39(2)	C49"-C54"	1.40(2)
C50"-C51"	1.40(2)	C50"-H50"	0.95
C51"-C52"	1.41(3)	C51"-H51"	0.95
C52"-C53"	1.34(3)	C52"-H52"	0.95
C53"-C54"	1.37(2)	C53"-H53"	0.95
C54"-H54"	0.95	C55-C60	1.37(3)
C55-C56	1.38(3)	C55-H55	0.95

C56-C57	1.41(3)	C56-H56	0.95
C57-C58	1.33(3)	C57-H57	0.95
C58-C59	1.40(3)	C58-H58	0.95
C59-C60	1.33(3)	C59-H59	0.95
C60-H60	0.95	C61-C66	1.369(12)
C61-C62	1.369(13)	C61-H61	0.95
C62-C63	1.371(13)	C62-H62	0.95
C63-C64	1.369(13)	C63-H63	0.95
C64-C65	1.371(13)	C64-H64	0.95
C65-C66	1.369(12)	C65-H65	0.95
C66-H66	0.95	C67-C68	1.370(10)
C67-C72	1.377(10)	C67-H67	0.95
C68-C69	1.374(10)	C68-H68	0.95
C69-C70	1.376(10)	C69-H69	0.95
C70-C71	1.379(10)	C70-H70	0.95
C71-C72	1.375(10)	C71-H71	0.95
C72-H72	0.95		

Table 3.2.5 Bond angles (°) for 12

C1-Au1-P1	177.3(3)	C43-P1-C37	107.9(5)
C43-P1-C49	104.9(7)	C37-P1-C49	105.9(9)
C43-P1-Au1	115.3(4)	C37-P1-Au1	110.2(4)
C49-P1-Au1	112.0(7)	C1-N1-C4	125.7(9)
C1-N1-C25	117.3(8)	C4-N1-C25	116.9(8)
C1-N2-C13	118.0(9)	C1-N2-C2	125.1(9)
C13-N2-C2	116.8(9)	N2-C1-N1	116.6(9)
N2-C1-Au1	121.3(7)	N1-C1-Au1	122.1(7)
O1-C2-C3	128.1(10)	O1-C2-N2	116.2(10)
C3-C2-N2	115.7(9)	C4-C3-C2	121.3(9)
C4-C3-C5	119.7(10)	C2-C3-C5	118.9(10)
O2-C4-C3	128.5(9)	O2-C4-N1	116.1(9)
C3-C4-N1	115.4(9)	C6-C5-C10	117.7(9)
C6-C5-C3	122.1(10)	C10-C5-C3	120.2(10)
C5-C6-C7	120.9(10)	C5-C6-H6	119.5
C7-C6-H6	119.5	C8-C7-C6	121.5(10)
C8-C7-H7	119.3	C6-C7-H7	119.3
C7-C8-C9	117.8(9)	C7-C8-C11	120.4(10)
C9-C8-C11	121.7(10)	C10-C9-C8	121.6(10)
C10-C9-H9	119.2	C8-C9-H9	119.2
C9-C10-C5	120.5(10)	C9-C10-H10	119.7

C5-C10-H10	119.7	C12'-C11-C12	119.0(9)
C12'-C11-C8	121.1(9)	C12-C11-C8	119.9(9)
C11"-C12-C11	119.4(9)	C11"-C12-H12	120.3
C11-C12-H12	120.3	C14-C13-C18	123.8(13)
C14-C13-N2	119.5(13)	C18-C13-N2	116.6(12)
C13-C14-C15	116.2(17)	C13-C14-C19	123.0(12)
C15-C14-C19	120.8(16)	C16-C15-C14	122.1(19)
C16-C15-H15	119.0	C14-C15-H15	119.0
C15-C16-C17	121.1(17)	C15-C16-H16	119.4
C17-C16-H16	119.4	C18-C17-C16	119.(2)
C18-C17-H17	120.3	C16-C17-H17	120.3
C17-C18-C13	117.2(16)	C17-C18-C22	122.2(18)
C13-C18-C22	120.5(13)	C21-C19-C14	111.7(15)
C21-C19-C20	112.1(14)	C14-C19-C20	109.9(14)
C21-C19-H19	107.7	C14-C19-H19	107.7
C20-C19-H19	107.7	C19-C20-H20A	109.5
C19-C20-H20B	109.5	H20A-C20-H20B	109.5
C19-C20-H20C	109.5	H20A-C20-H20C	109.5
H20B-C20-H20C	109.5	C19-C21-H21A	109.5
C19-C21-H21B	109.5	H21A-C21-H21B	109.5
C19-C21-H21C	109.5	H21A-C21-H21C	109.5
H21B-C21-H21C	109.5	C23-C22-C18	114.4(14)
C23-C22-C24	111.9(16)	C18-C22-C24	112.1(15)
C23-C22-H22	105.9	C18-C22-H22	105.9
C24-C22-H22	105.9	C22-C23-H23A	109.5
C22-C23-H23B	109.5	H23A-C23-H23B	109.5
C22-C23-H23C	109.5	H23A-C23-H23C	109.5
H23B-C23-H23C	109.5	C22-C24-H24A	109.5
C22-C24-H24B	109.5	H24A-C24-H24B	109.5
C22-C24-H24C	109.5	H24A-C24-H24C	109.5
H24B-C24-H24C	109.5	C30-C25-C26	123.9(10)
C30-C25-N1	117.9(9)	C26-C25-N1	118.3(9)
C27-C26-C25	117.2(11)	C27-C26-C31	120.8(10)
C25-C26-C31	122.0(10)	C28-C27-C26	120.6(12)
C28-C27-H27	119.7	C26-C27-H27	119.7
C27-C28-C29	121.9(12)	C27-C28-H28	119.0
C29-C28-H28	119.0	C28-C29-C30	119.6(12)
C28-C29-H29	120.2	C30-C29-H29	120.2
C25-C30-C29	116.7(11)	C25-C30-C34	122.5(11)
C29-C30-C34	120.7(11)	C26-C31-C32	111.6(11)
C26-C31-C33	111.9(10)	C32-C31-C33	110.4(11)
C26-C31-H31	107.6	C32-C31-H31	107.6

C33-C31-H31	107.6	C31-C32-H32A	109.5
C31-C32-H32B	109.5	H32A-C32-H32B	109.5
C31-C32-H32C	109.5	H32A-C32-H32C	109.5
H32B-C32-H32C	109.5	C31-C33-H33A	109.5
C31-C33-H33B	109.5	H33A-C33-H33B	109.5
C31-C33-H33C	109.5	H33A-C33-H33C	109.5
H33B-C33-H33C	109.5	C30-C34-C35	112.4(12)
C30-C34-C36	112.1(12)	C35-C34-C36	110.4(12)
C30-C34-H34	107.2	C35-C34-H34	107.2
C36-C34-H34	107.2	C34-C35-H35A	109.5
C34-C35-H35B	109.5	H35A-C35-H35B	109.5
C34-C35-H35C	109.5	H35A-C35-H35C	109.5
H35B-C35-H35C	109.5	C34-C36-H36A	109.5
C34-C36-H36B	109.5	H36A-C36-H36B	109.5
C34-C36-H36C	109.5	H36A-C36-H36C	109.5
H36B-C36-H36C	109.5	C42-C37-C38	120.1(12)
C42-C37-P1	122.3(10)	C38-C37-P1	117.6(9)
C39-C38-C37	119.3(12)	C39-C38-H38	120.3
C37-C38-H38	120.3	C38-C39-C40	120.6(13)
C38-C39-H39	119.7	C40-C39-H39	119.7
C41-C40-C39	119.1(14)	C41-C40-H40	120.5
C39-C40-H40	120.5	C40-C41-C42	120.9(14)
C40-C41-H41	119.6	C42-C41-H41	119.6
C41-C42-C37	120.0(14)	C41-C42-H42	120.0
C37-C42-H42	120.0	C44-C43-C48	118.8(11)
C44-C43-P1	118.6(8)	C48-C43-P1	122.5(9)
C43-C44-C45	120.8(11)	C43-C44-H44	119.6
C45-C44-H44	119.6	C46-C45-C44	119.2(13)
C46-C45-H45	120.4	C44-C45-H45	120.4
C45-C46-C47	120.5(12)	C45-C46-H46	119.8
C47-C46-H46	119.8	C46-C47-C48	120.7(12)
C46-C47-H47	119.6	C48-C47-H47	119.6
C47-C48-C43	120.0(12)	C47-C48-H48	120.0
C43-C48-H48	120.0	C54-C49-C50	120.6(16)
C54-C49-P1	121.6(13)	C50-C49-P1	117.8(14)
C49-C50-C51	117.8(19)	C49-C50-H50	121.1
C51-C50-H50	121.1	C52-C51-C50	123.7(17)
C52-C51-H51	118.2	C50-C51-H51	118.2
C51-C52-C53	118.6(16)	C51-C52-H52	120.7
C53-C52-H52	120.7	C52-C53-C54	118.0(18)
C52-C53-H53	121.0	C54-C53-H53	121.0
C49-C54-C53	121.1(17)	C49-C54-H54	119.4

C53-C54-H54	119.4	C1'-Au1'-P1'	175.2(3)
C43'-P1'-C37'	108.1(7)	C43'-P1'-C49'	106.0(7)
C37'-P1'-C49'	105.9(6)	C43'-P1'-Au1'	110.7(5)
C37'-P1'-Au1'	115.7(5)	C49'-P1'-Au1'	109.8(4)
C1'-N1'-C4'	125.5(9)	C1'-N1'-C25'	116.6(9)
C4'-N1'-C25'	117.9(9)	C1'-N2'-C13'	118.7(8)
C1'-N2'-C2'	124.3(8)	C13'-N2'-C2'	117.0(8)
N1'-C1'-N2'	118.2(9)	N1'-C1'-Au1'	120.8(7)
N2'-C1'-Au1'	121.0(7)	O1'-C2'-C3'	128.6(9)
O1'-C2'-N2'	116.1(9)	C3'-C2'-N2'	115.2(9)
C4'-C3'-C2'	120.5(9)	C4'-C3'-C5'	121.3(9)
C2'-C3'-C5'	118.2(9)	O2'-C4'-C3'	127.4(9)
O2'-C4'-N1'	117.2(9)	C3'-C4'-N1'	115.4(9)
C6'-C5'-C10'	116.4(9)	C6'-C5'-C3'	122.3(9)
C10'-C5'-C3'	121.2(9)	C7'-C6'-C5'	121.8(10)
C7'-C6'-H6'	119.1	C5'-C6'-H6'	119.1
C6'-C7'-C8'	121.5(10)	C6'-C7'-H7'	119.3
C8'-C7'-H7'	119.3	C7'-C8'-C9'	117.5(9)
C7'-C8'-C11'	121.9(10)	C9'-C8'-C11'	120.6(9)
C10'-C9'-C8'	120.8(10)	C10'-C9'-H9'	119.6
C8'-C9'-H9'	119.6	C9'-C10'-C5'	121.8(10)
C9'-C10'-H10'	119.1	C5'-C10'-H10'	119.1
C12'-C11'-C12"	119.0(10)	C12'-C11'-C8'	119.7(9)
C12"-C11'-C8'	121.2(9)	C11-C12'-C11'	121.1(10)
C11-C12'-H12'	119.4	C11'-C12'-H12'	119.4
C18'-C13'-C14'	123.9(10)	C18'-C13'-N2'	117.4(9)
C14'-C13'-N2'	118.7(10)	C15'-C14'-C13'	116.2(12)
C15'-C14'-C19'	121.0(11)	C13'-C14'-C19'	122.9(11)
C16'-C15'-C14'	121.3(12)	C16'-C15'-H15'	119.4
C14'-C15'-H15'	119.4	C15'-C16'-C17'	121.2(12)
C15'-C16'-H16'	119.4	C17'-C16'-H16'	119.4
C16'-C17'-C18'	120.2(13)	C16'-C17'-H17'	119.9
C18'-C17'-H17'	119.9	C13'-C18'-C17'	117.2(11)
C13'-C18'-C22'	122.4(10)	C17'-C18'-C22'	120.4(12)
C14'-C19'-C21'	113.3(12)	C14'-C19'-C20'	111.7(11)
C21'-C19'-C20'	108.9(11)	C14'-C19'-H19'	107.6
C21'-C19'-H19'	107.6	C20'-C19'-H19'	107.6
C19'-C20'-H20D	109.5	C19'-C20'-H20E	109.5
H20D-C20'-H20E	109.5	C19'-C20'-H20F	109.5
H20D-C20'-H20F	109.5	H20E-C20'-H20F	109.5
C19'-C21'-H21D	109.5	C19'-C21'-H21E	109.5
H21D-C21'-H21E	109.5	C19'-C21'-H21F	109.5

H21D-C21'-H21F	109.5	H21E-C21'-H21F	109.5
C24'-C22'-C23'	112.8(11)	C24'-C22'-C18'	111.1(11)
C23'-C22'-C18'	112.8(12)	C24'-C22'-H22'	106.5
C23'-C22'-H22'	106.5	C18'-C22'-H22'	106.5
C22'-C23'-H23D	109.5	C22'-C23'-H23E	109.5
H23D-C23'-H23E	109.5	C22'-C23'-H23F	109.5
H23D-C23'-H23F	109.5	H23E-C23'-H23F	109.5
C22'-C24'-H24D	109.5	C22'-C24'-H24E	109.5
H24D-C24'-H24E	109.5	C22'-C24'-H24F	109.5
H24D-C24'-H24F	109.5	H24E-C24'-H24F	109.5
C30'-C25'-C26'	123.5(11)	C30'-C25'-N1'	119.8(12)
C26'-C25'-N1'	116.6(10)	C25'-C26'-C27'	116.8(11)
C25'-C26'-C31'	123.9(10)	C27'-C26'-C31'	119.3(11)
C28'-C27'-C26'	120.3(14)	C28'-C27'-H27'	119.8
C26'-C27'-H27'	119.8	C27'-C28'-C29'	122.0(13)
C27'-C28'-H28'	119.0	C29'-C28'-H28'	119.0
C28'-C29'-C30'	119.4(16)	C28'-C29'-H29'	120.3
C30'-C29'-H29'	120.3	C25'-C30'-C29'	117.8(17)
C25'-C30'-C34'	120.2(14)	C29'-C30'-C34'	121.1(16)
C32'-C31'-C33'	112.4(13)	C32'-C31'-C26'	112.6(11)
C33'-C31'-C26'	111.2(12)	C32'-C31'-H31'	106.7
C33'-C31'-H31'	106.7	C26'-C31'-H31'	106.7
C31'-C32'-H32D	109.5	C31'-C32'-H32E	109.5
H32D-C32'-H32E	109.5	C31'-C32'-H32F	109.5
H32D-C32'-H32F	109.5	H32E-C32'-H32F	109.5
C31'-C33'-H33D	109.5	C31'-C33'-H33E	109.5
H33D-C33'-H33E	109.5	C31'-C33'-H33F	109.5
H33D-C33'-H33F	109.5	H33E-C33'-H33F	109.5
C35'-C34'-C36'	114.(2)	C35'-C34'-C30'	122.(2)
C36'-C34'-C30'	105.(3)	C35'-C34'-H34'	104.6
C36'-C34'-H34'	104.6	C30'-C34'-H34'	104.6
C34'-C35'-H35D	109.5	C34'-C35'-H35E	109.5
H35D-C35'-H35E	109.5	C34'-C35'-H35F	109.5
H35D-C35'-H35F	109.5	H35E-C35'-H35F	109.5
C34'-C36'-H36D	109.5	C34'-C36'-H36E	109.5
H36D-C36'-H36E	109.5	C34'-C36'-H36F	109.5
H36D-C36'-H36F	109.5	H36E-C36'-H36F	109.5
C42'-C37'-C38'	119.2(16)	C42'-C37'-P1'	117.7(12)
C38'-C37'-P1'	122.9(14)	C39'-C38'-C37'	122.(2)
C39'-C38'-H38'	118.8	C37'-C38'-H38'	118.8
C40'-C39'-C38'	118.1(18)	C40'-C39'-H39'	120.9
C38'-C39'-H39'	120.9	C39'-C40'-C41'	124.0(16)

C39'-C40'-H40'	118.0	C41'-C40'-H40'	118.0
C40'-C41'-C42'	116.(2)	C40'-C41'-H41'	122.2
C42'-C41'-H41'	122.2	C37'-C42'-C41'	120.6(18)
C37'-C42'-H42'	119.7	C41'-C42'-H42'	119.7
C48'-C43'-C44'	116.7(17)	C48'-C43'-P1'	119.2(11)
C44'-C43'-P1'	123.7(13)	C45'-C44'-C43'	120.4(17)
C45'-C44'-H44'	119.8	C43'-C44'-H44'	119.8
C44'-C45'-C46'	119.5(16)	C44'-C45'-H45'	120.2
C46'-C45'-H45'	120.2	C47'-C46'-C45'	121.(2)
C47'-C46'-H46'	119.6	C45'-C46'-H46'	119.6
C46'-C47'-C48'	121.(2)	C46'-C47'-H47'	119.7
C48'-C47'-H47'	119.7	C47'-C48'-C43'	121.8(16)
C47'-C48'-H48'	119.1	C43'-C48'-H48'	119.1
C50'-C49'-C54'	119.8(13)	C50'-C49'-P1'	119.3(12)
C54'-C49'-P1'	120.5(11)	C49'-C50'-C51'	120.9(17)
C49'-C50'-H50'	119.6	C51'-C50'-H50'	119.6
C52'-C51'-C50'	119.3(16)	C52'-C51'-H51'	120.3
C50'-C51'-H51'	120.3	C51'-C52'-C53'	120.7(14)
C51'-C52'-H52'	119.7	C53'-C52'-H52'	119.7
C52'-C53'-C54'	119.6(17)	C52'-C53'-H53'	120.2
C54'-C53'-H53'	120.2	C49'-C54'-C53'	119.6(16)
C49'-C54'-H54'	120.2	C53'-C54'-H54'	120.2
C1"-Au1"-P1"	178.5(3)	C1"-Au1B-P1"	132.9(4)
C49"-P1"-C43"	110.5(6)	C49"-P1"-C37"	102.7(7)
C43"-P1"-C37"	104.2(7)	C49"-P1"-Au1"	113.3(5)
C43"-P1"-Au1"	111.5(5)	C37"-P1"-Au1"	114.0(5)
C49"-P1"-Au1B	104.1(5)	C43"-P1"-Au1B	100.8(5)
C37"-P1"-Au1B	133.7(5)	C1"-N1"-C25"	119.3(9)
C1"-N1"-C4"	125.5(9)	C25"-N1"-C4"	115.1(8)
C1"-N2"-C2"	126.9(9)	C1"-N2"-C13"	117.6(9)
C2"-N2"-C13"	115.5(8)	N1"-C1"-N2"	116.1(10)
N1"-C1"-Au1B	112.6(7)	N2"-C1"-Au1B	127.3(8)
N1"-C1"-Au1"	123.1(7)	N2"-C1"-Au1"	120.5(7)
O1"-C2"-C3"	131.2(11)	O1"-C2"-N2"	114.6(10)
C3"-C2"-N2"	114.1(9)	C4"-C3"-C2"	121.6(9)
C4"-C3"-C5"	119.0(9)	C2"-C3"-C5"	119.2(9)
O2"-C4"-C3"	129.2(9)	O2"-C4"-N1"	116.2(8)
C3"-C4"-N1"	114.3(9)	C6"-C5"-C10"	117.0(9)
C6"-C5"-C3"	121.4(9)	C10"-C5"-C3"	121.5(9)
C7"-C6"-C5"	121.0(9)	C7"-C6"-H6"	119.5
C5"-C6"-H6"	119.5	C6"-C7"-C8"	122.9(10)
C6"-C7"-H7"	118.6	C8"-C7"-H7"	118.6

C7"-C8"-C9"	116.2(10)	C7"-C8"-C11"	123.2(10)
C9"-C8"-C11"	120.6(9)	C10"-C9"-C8"	121.7(9)
C10"-C9"-H9"	119.1	C8"-C9"-H9"	119.1
C9"-C10"-C5"	121.2(9)	C9"-C10"-H10"	119.4
C5"-C10"-H10"	119.4	C12"-C11"-C12	121.5(10)
C12"-C11"-C8"	120.0(10)	C12-C11"-C8"	118.5(9)
C11"-C12"-C11'	119.8(10)	C11"-C12"-H12"	120.1
C11'-C12"-H12"	120.1	C14"-C13"-C18"	124.2(12)
C14"-C13"-N2"	117.9(12)	C18"-C13"-N2"	117.8(11)
C13"-C14"-C15"	115.7(14)	C13"-C14"-C19"	120.9(12)
C15"-C14"-C19"	123.4(13)	C16"-C15"-C14"	118.9(15)
C16"-C15"-H15"	120.5	C14"-C15"-H15"	120.5
C15"-C16"-C17"	124.9(15)	C15"-C16"-H16"	117.5
C17"-C16"-H16"	117.5	C16"-C17"-C18"	119.3(16)
C16"-C17"-H17"	120.3	C18"-C17"-H17"	120.3
C17"-C18"-C13"	116.7(14)	C17"-C18"-C22"	119.9(13)
C13"-C18"-C22"	123.4(11)	C14"-C19"-C20"	114.4(15)
C14"-C19"-C21"	108.6(17)	C20"-C19"-C21"	110.2(17)
C14"-C19"-H19"	107.8	C20"-C19"-H19"	107.8
C21"-C19"-H19"	107.8	C19"-C20"-H20G	109.5
C19"-C20"-H20H	109.5	H20G-C20"-H20H	109.5
C19"-C20"-H20I	109.5	H20G-C20"-H20I	109.5
H20H-C20"-H20I	109.5	C19"-C21"-H21G	109.5
C19"-C21"-H21H	109.5	H21G-C21"-H21H	109.5
C19"-C21"-H21I	109.5	H21G-C21"-H21I	109.5
H21H-C21"-H21I	109.5	C24"-C22"-C18"	111.8(13)
C24"-C22"-C23"	109.8(14)	C18"-C22"-C23"	112.7(16)
C24"-C22"-H22"	107.4	C18"-C22"-H22"	107.4
C23"-C22"-H22"	107.4	C22"-C23"-H23G	109.5
C22"-C23"-H23H	109.5	H23G-C23"-H23H	109.5
C22"-C23"-H23I	109.5	H23G-C23"-H23I	109.5
H23H-C23"-H23I	109.5	C22"-C24"-H24G	109.5
C22"-C24"-H24H	109.5	H24G-C24"-H24H	109.5
C22"-C24"-H24I	109.5	H24G-C24"-H24I	109.5
H24H-C24"-H24I	109.5	C30"-C25"-C26"	122.9(11)
C30"-C25"-N1"	120.2(11)	C26"-C25"-N1"	116.8(10)
C27"-C26"-C25"	115.8(13)	C27"-C26"-C31"	122.0(13)
C25"-C26"-C31"	122.2(11)	C28"-C27"-C26"	122.6(15)
C28"-C27"-H27"	118.7	C26"-C27"-H27"	118.7
C27"-C28"-C29"	120.5(13)	C27"-C28"-H28"	119.8
C29"-C28"-H28"	119.8	C28"-C29"-C30"	120.9(14)
C28"-C29"-H29"	119.6	C30"-C29"-H29"	119.6

C29"-C30"-C25"	117.3(14)	C29"-C30"-C34"	122.1(13)
C25"-C30"-C34"	120.5(11)	C26"-C31"-C33"	113.9(15)
C26"-C31"-C32"	111.0(15)	C33"-C31"-C32"	111.4(15)
C26"-C31"-H31"	106.7	C33"-C31"-H31"	106.7
C32"-C31"-H31"	106.7	C31"-C32"-H32G	109.5
C31"-C32"-H32H	109.5	H32G-C32"-H32H	109.5
C31"-C32"-H32I	109.5	H32G-C32"-H32I	109.5
H32H-C32"-H32I	109.5	C31"-C33"-H33G	109.5
C31"-C33"-H33H	109.5	H33G-C33"-H33H	109.5
C31"-C33"-H33I	109.5	H33G-C33"-H33I	109.5
H33H-C33"-H33I	109.5	C30"-C34"-C35"	112.0(14)
C30"-C34"-C36"	111.3(17)	C35"-C34"-C36"	110.6(15)
C30"-C34"-H34"	107.6	C35"-C34"-H34"	107.6
C36"-C34"-H34"	107.6	C34"-C35"-H35G	109.5
C34"-C35"-H35H	109.5	H35G-C35"-H35H	109.5
C34"-C35"-H35I	109.5	H35G-C35"-H35I	109.5
H35H-C35"-H35I	109.5	C34"-C36"-H36G	109.5
C34"-C36"-H36H	109.5	H36G-C36"-H36H	109.5
C34"-C36"-H36I	109.5	H36G-C36"-H36I	109.5
H36H-C36"-H36I	109.5	C38"-C37"-C42"	117.8(14)
C38"-C37"-P1"	124.4(10)	C42"-C37"-P1"	117.7(11)
C39"-C38"-C37"	121.2(14)	C39"-C38"-H38"	119.4
C37"-C38"-H38"	119.4	C38"-C39"-C40"	120.9(16)
C38"-C39"-H39"	119.6	C40"-C39"-H39"	119.6
C41"-C40"-C39"	120.5(16)	C41"-C40"-H40"	119.8
C39"-C40"-H40"	119.8	C40"-C41"-C42"	120.2(14)
C40"-C41"-H41"	119.9	C42"-C41"-H41"	119.9
C41"-C42"-C37"	119.1(14)	C41"-C42"-H42"	120.4
C37"-C42"-H42"	120.4	C48"-C43"-C44"	118.9(14)
C48"-C43"-P1"	123.4(12)	C44"-C43"-P1"	117.2(11)
C43"-C44"-C45"	121.0(15)	C43"-C44"-H44"	119.5
C45"-C44"-H44"	119.5	C44"-C45"-C46"	119.0(16)
C44"-C45"-H45"	120.5	C46"-C45"-H45"	120.5
C47"-C46"-C45"	119.2(14)	C47"-C46"-H46"	120.4
C45"-C46"-H46"	120.4	C46"-C47"-C48"	121.1(16)
C46"-C47"-H47"	119.5	C48"-C47"-H47"	119.5
C43"-C48"-C47"	120.5(17)	C43"-C48"-H48"	119.8
C47"-C48"-H48"	119.8	C50"-C49"-C54"	119.1(14)
C50"-C49"-P1"	119.9(11)	C54"-C49"-P1"	120.9(13)
C49"-C50"-C51"	120.4(16)	C49"-C50"-H50"	119.8
C51"-C50"-H50"	119.8	C50"-C51"-C52"	118.8(17)
C50"-C51"-H51"	120.6	C52"-C51"-H51"	120.6

C53"-C52"-C51"	119.6(16)	C53"-C52"-H52"	120.2
C51"-C52"-H52"	120.2	C52"-C53"-C54"	122.8(19)
C52"-C53"-H53"	118.6	C54"-C53"-H53"	118.6
C53"-C54"-C49"	119.2(18)	C53"-C54"-H54"	120.4
C49"-C54"-H54"	120.4	C60-C55-C56	117.(2)
C60-C55-H55	121.3	C56-C55-H55	121.3
C55-C56-C57	120.(2)	C55-C56-H56	120.0
C57-C56-H56	120.0	C58-C57-C56	120.(2)
C58-C57-H57	120.2	C56-C57-H57	120.2
C57-C58-C59	121.(2)	C57-C58-H58	119.6
C59-C58-H58	119.6	C60-C59-C58	118.(2)
C60-C59-H59	120.8	C58-C59-H59	120.8
C59-C60-C55	124.(2)	C59-C60-H60	118.2
C55-C60-H60	118.2	C66-C61-C62	115.(3)
C66-C61-H61	122.4	C62-C61-H61	122.4
C61-C62-C63	123.(3)	C61-C62-H62	118.7
C63-C62-H62	118.7	C64-C63-C62	120.(3)
C64-C63-H63	120.2	C62-C63-H63	120.2
C63-C64-C65	120.(3)	C63-C64-H64	120.1
C65-C64-H64	120.1	C66-C65-C64	118.(3)
C66-C65-H65	121.1	C64-C65-H65	121.1
C61-C66-C65	124.(3)	C61-C66-H66	117.9
C65-C66-H66	117.9	C68-C67-C72	111.(4)
C68-C67-H67	124.4	C72-C67-H67	124.4
C67-C68-C69	129.(4)	C67-C68-H68	115.5
C69-C68-H68	115.5	C68-C69-C70	110.(4)
C68-C69-H69	124.8	C70-C69-H69	124.8
C69-C70-C71	125.(4)	C69-C70-H70	117.3
C71-C70-H70	117.3	C72-C71-C70	114.(4)
C72-C71-H71	123.0	C70-C71-H71	123.0
C71-C72-C67	125.(4)	C71-C72-H72	117.6
C67-C72-H72	117.6		

Table 3.2.6 Anisotropic atomic displacement parameters (Å^2) for 12 The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au1	0.0218(2)	0.01721(19)	0.0274(2)	-0.00635(15)	0.00103(15)	-0.00735(15)
P1	0.0227(13)	0.0208(13)	0.0287(14)	-0.0075(11)	0.0024(11)	-0.0084(11)
O1	0.047(6)	0.045(6)	0.029(5)	0.005(4)	-0.002(4)	0.005(4)
O2	0.030(4)	0.027(4)	0.033(4)	-0.012(3)	-0.002(3)	-0.008(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	0.017(4)	0.018(4)	0.029(5)	-0.010(4)	0.001(3)	-0.006(3)
N2	0.020(4)	0.029(5)	0.026(5)	-0.003(4)	0.001(4)	-0.004(4)
C1	0.017(5)	0.015(5)	0.025(5)	-0.005(4)	0.002(4)	-0.004(4)
C2	0.028(6)	0.023(5)	0.032(6)	0.001(5)	-0.002(5)	-0.005(5)
C3	0.020(5)	0.023(5)	0.035(6)	-0.006(5)	-0.002(4)	-0.008(4)
C4	0.022(5)	0.016(5)	0.029(5)	-0.009(4)	-0.001(4)	-0.005(4)
C5	0.019(5)	0.019(5)	0.039(6)	-0.007(4)	-0.002(4)	-0.007(4)
C6	0.026(5)	0.024(5)	0.038(6)	-0.012(5)	-0.003(5)	-0.011(4)
C7	0.024(5)	0.023(5)	0.037(6)	-0.007(5)	-0.009(4)	-0.011(4)
C8	0.019(5)	0.021(5)	0.043(6)	-0.014(5)	-0.003(4)	-0.008(4)
C9	0.031(6)	0.020(5)	0.039(6)	-0.010(5)	-0.007(5)	-0.010(4)
C10	0.027(5)	0.025(5)	0.042(6)	-0.009(5)	-0.011(5)	-0.011(5)
C11	0.025(5)	0.019(5)	0.035(6)	-0.012(4)	-0.005(4)	-0.008(4)
C12	0.022(5)	0.022(5)	0.031(5)	-0.011(4)	-0.005(4)	-0.009(4)
C13	0.039(7)	0.040(7)	0.027(6)	-0.010(5)	-0.004(5)	-0.003(6)
C14	0.038(7)	0.067(10)	0.022(6)	-0.005(6)	0.005(5)	-0.009(7)
C15	0.065(12)	0.14(2)	0.036(9)	-0.033(11)	0.017(8)	-0.038(12)
C16	0.084(14)	0.15(2)	0.045(10)	-0.051(13)	0.020(10)	-0.034(14)
C17	0.085(13)	0.092(14)	0.047(9)	-0.038(10)	-0.011(9)	-0.009(11)
C18	0.050(9)	0.059(9)	0.034(7)	-0.011(7)	-0.006(6)	-0.001(7)
C19	0.049(8)	0.046(8)	0.045(8)	-0.001(7)	0.003(6)	-0.021(7)
C20	0.049(9)	0.080(13)	0.075(12)	-0.002(10)	-0.005(8)	-0.026(9)
C21	0.074(12)	0.078(13)	0.075(13)	0.024(10)	-0.009(10)	-0.039(11)
C22	0.063(10)	0.057(9)	0.063(10)	-0.032(8)	-0.016(8)	-0.007(8)
C23	0.076(12)	0.081(13)	0.082(13)	-0.038(10)	-0.029(10)	-0.020(10)
C24	0.061(12)	0.102(16)	0.109(17)	-0.027(14)	-0.023(11)	-0.021(11)
C25	0.023(5)	0.018(5)	0.026(5)	-0.009(4)	-0.004(4)	-0.004(4)
C26	0.029(5)	0.023(5)	0.022(5)	-0.010(4)	0.005(4)	-0.008(4)
C27	0.040(7)	0.029(6)	0.029(6)	-0.008(5)	-0.006(5)	-0.002(5)
C28	0.035(7)	0.053(8)	0.027(6)	-0.013(6)	-0.004(5)	-0.004(6)
C29	0.027(6)	0.063(9)	0.043(7)	-0.034(7)	-0.006(5)	-0.005(6)
C30	0.025(5)	0.033(6)	0.034(6)	-0.020(5)	0.002(5)	-0.007(5)
C31	0.042(7)	0.032(6)	0.036(6)	-0.006(5)	-0.001(5)	-0.023(5)
C32	0.062(10)	0.054(9)	0.072(10)	-0.033(8)	0.002(8)	-0.026(8)
C33	0.045(8)	0.094(12)	0.062(9)	-0.048(9)	0.017(7)	-0.042(8)
C34	0.039(7)	0.050(8)	0.062(9)	-0.031(7)	-0.006(6)	-0.019(6)
C35	0.043(8)	0.050(9)	0.122(15)	-0.047(10)	0.002(9)	-0.025(7)
C36	0.058(9)	0.049(9)	0.097(13)	-0.040(9)	-0.012(9)	-0.014(7)
C37	0.032(6)	0.024(5)	0.029(6)	-0.007(5)	0.000(5)	-0.009(5)
C38	0.038(6)	0.029(6)	0.038(7)	-0.010(5)	-0.003(5)	-0.012(5)
C39	0.060(9)	0.047(8)	0.042(7)	-0.018(6)	-0.010(7)	-0.014(7)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C40	0.064(10)	0.077(11)	0.040(8)	-0.007(7)	-0.013(7)	-0.041(9)
C41	0.039(8)	0.081(11)	0.045(8)	-0.021(8)	-0.003(6)	-0.022(7)
C42	0.030(7)	0.066(9)	0.045(8)	-0.015(7)	-0.009(6)	-0.010(6)
C43	0.034(6)	0.021(5)	0.024(5)	-0.010(4)	-0.001(4)	-0.008(4)
C44	0.044(7)	0.027(6)	0.029(6)	-0.001(5)	-0.008(5)	-0.018(5)
C45	0.061(8)	0.037(7)	0.038(7)	-0.007(6)	-0.007(6)	-0.026(6)
C46	0.065(9)	0.035(7)	0.031(6)	-0.012(5)	0.002(6)	-0.027(6)
C47	0.051(8)	0.023(6)	0.034(7)	-0.005(5)	0.000(6)	-0.002(6)
C48	0.030(6)	0.029(6)	0.030(6)	-0.006(5)	0.002(5)	-0.006(5)
C49	0.115(6)	0.063(5)	0.054(4)	-0.023(4)	0.046(4)	-0.052(5)
C50	0.116(6)	0.065(5)	0.056(5)	-0.021(4)	0.047(4)	-0.051(5)
C51	0.117(6)	0.066(5)	0.057(5)	-0.019(4)	0.047(4)	-0.051(5)
C52	0.117(6)	0.067(5)	0.056(5)	-0.020(4)	0.046(4)	-0.051(5)
C53	0.118(6)	0.067(5)	0.055(5)	-0.021(4)	0.046(4)	-0.050(5)
C54	0.117(6)	0.065(5)	0.054(5)	-0.023(4)	0.046(4)	-0.051(5)
Au1'	0.0243(2)	0.0506(3)	0.0320(2)	-0.0260(2)	0.00245(16)	-0.01961(19)
P1'	0.0315(16)	0.088(3)	0.0367(17)	-0.0392(18)	0.0074(13)	-0.0320(18)
O1'	0.031(4)	0.040(4)	0.025(4)	-0.008(3)	0.001(3)	-0.023(4)
O2'	0.034(4)	0.043(5)	0.023(4)	-0.001(3)	-0.010(3)	-0.019(4)
N1'	0.026(4)	0.028(5)	0.026(5)	-0.012(4)	0.000(4)	-0.017(4)
N2'	0.024(4)	0.027(4)	0.024(4)	-0.007(4)	-0.005(3)	-0.016(4)
C1'	0.025(5)	0.030(5)	0.030(5)	-0.020(5)	-0.007(4)	-0.010(4)
C2'	0.021(5)	0.029(5)	0.031(6)	-0.011(5)	-0.004(4)	-0.011(4)
C3'	0.027(5)	0.019(5)	0.023(5)	-0.009(4)	-0.004(4)	-0.011(4)
C4'	0.028(5)	0.025(5)	0.030(6)	-0.008(4)	-0.012(4)	-0.010(4)
C5'	0.019(5)	0.023(5)	0.033(6)	-0.011(4)	-0.003(4)	-0.008(4)
C6'	0.024(5)	0.023(5)	0.039(6)	-0.006(5)	-0.010(5)	-0.009(4)
C7'	0.027(6)	0.026(6)	0.043(7)	-0.008(5)	-0.014(5)	-0.007(5)
C8'	0.027(5)	0.022(5)	0.034(6)	-0.008(4)	-0.007(4)	-0.010(4)
C9'	0.025(5)	0.024(5)	0.031(5)	-0.010(4)	-0.001(4)	-0.015(4)
C10'	0.028(5)	0.023(5)	0.034(6)	-0.005(4)	-0.011(5)	-0.011(4)
C11'	0.027(5)	0.024(5)	0.031(6)	-0.013(4)	-0.008(4)	-0.009(4)
C12'	0.031(6)	0.027(6)	0.038(6)	-0.010(5)	-0.012(5)	-0.008(5)
C13'	0.024(5)	0.035(6)	0.023(5)	-0.012(4)	-0.001(4)	-0.014(4)
C14'	0.036(6)	0.053(7)	0.028(6)	-0.019(5)	0.000(5)	-0.024(6)
C15'	0.044(7)	0.069(10)	0.029(6)	-0.018(6)	-0.007(5)	-0.026(7)
C16'	0.043(8)	0.087(12)	0.019(6)	-0.002(7)	-0.010(5)	-0.029(8)
C17'	0.036(7)	0.049(8)	0.041(7)	-0.003(6)	-0.014(6)	-0.008(6)
C18'	0.037(6)	0.036(6)	0.027(6)	-0.011(5)	-0.004(5)	-0.013(5)
C19'	0.057(8)	0.050(8)	0.031(6)	-0.027(6)	0.004(6)	-0.027(6)
C20'	0.045(8)	0.060(9)	0.060(9)	-0.030(8)	0.006(7)	-0.024(7)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C21'	0.075(11)	0.083(12)	0.087(12)	-0.055(10)	0.025(9)	-0.057(10)
C22'	0.053(8)	0.034(7)	0.045(7)	-0.021(6)	-0.010(6)	-0.009(6)
C23'	0.057(9)	0.047(8)	0.077(11)	-0.018(8)	0.019(8)	-0.040(7)
C24'	0.060(10)	0.091(13)	0.093(13)	-0.066(12)	0.015(9)	-0.034(10)
C25'	0.026(6)	0.037(6)	0.029(6)	0.005(5)	0.001(5)	-0.024(5)
C26'	0.038(6)	0.048(7)	0.019(5)	0.000(5)	-0.006(5)	-0.032(6)
C27'	0.048(8)	0.078(10)	0.024(6)	-0.009(6)	0.003(5)	-0.045(8)
C28'	0.082(12)	0.081(12)	0.052(9)	0.004(8)	-0.008(8)	-0.072(10)
C29'	0.087(13)	0.076(12)	0.088(13)	-0.024(10)	0.013(11)	-0.065(11)
C30'	0.074(11)	0.041(8)	0.091(13)	0.000(8)	-0.008(10)	-0.040(8)
C31'	0.043(7)	0.061(8)	0.028(6)	-0.024(6)	0.012(5)	-0.028(6)
C32'	0.052(9)	0.069(11)	0.092(13)	-0.046(10)	0.010(9)	-0.025(8)
C33'	0.088(12)	0.127(16)	0.051(9)	-0.049(10)	0.011(9)	-0.072(12)
C34'	0.085(15)	0.065(13)	0.20(3)	-0.069(16)	0.058(17)	-0.054(12)
C35'	0.15(2)	0.12(2)	0.095(18)	-0.042(16)	-0.057(17)	0.012(18)
C36'	0.198(19)	0.202(19)	0.197(19)	-0.079(11)	-0.047(10)	-0.071(11)
C37'	0.051(8)	0.080(11)	0.038(7)	-0.030(7)	0.012(6)	-0.042(8)
C38'	0.086(11)	0.141(16)	0.027(7)	-0.024(8)	0.006(7)	-0.094(12)
C39'	0.107(15)	0.123(18)	0.041(9)	-0.014(10)	-0.009(9)	-0.090(15)
C40'	0.108(14)	0.090(13)	0.030(7)	-0.015(8)	-0.001(8)	-0.084(12)
C41'	0.142(19)	0.111(16)	0.042(9)	-0.036(10)	0.027(11)	-0.091(15)
C42'	0.105(14)	0.087(13)	0.050(9)	-0.014(9)	-0.005(9)	-0.079(12)
C43'	0.032(7)	0.123(14)	0.028(7)	-0.041(8)	-0.002(5)	-0.016(8)
C44'	0.032(7)	0.140(17)	0.032(7)	-0.029(9)	0.006(6)	-0.033(9)
C45'	0.042(9)	0.129(18)	0.062(11)	-0.026(12)	-0.023(9)	-0.001(10)
C46'	0.060(12)	0.123(19)	0.074(13)	-0.017(13)	-0.022(10)	-0.009(12)
C47'	0.056(11)	0.100(16)	0.090(15)	-0.005(12)	-0.037(11)	-0.008(11)
C48'	0.039(8)	0.112(15)	0.054(9)	-0.021(10)	-0.005(7)	-0.033(9)
C49'	0.027(6)	0.091(11)	0.044(7)	-0.039(8)	0.000(5)	-0.026(7)
C50'	0.039(7)	0.087(11)	0.038(7)	-0.033(8)	-0.010(6)	-0.010(7)
C51'	0.044(8)	0.104(14)	0.037(8)	-0.040(9)	-0.005(6)	-0.013(9)
C52'	0.033(7)	0.109(14)	0.040(8)	-0.041(9)	0.003(6)	-0.011(8)
C53'	0.060(10)	0.092(13)	0.049(9)	-0.022(9)	0.004(7)	-0.045(9)
C54'	0.048(8)	0.107(14)	0.045(8)	-0.043(9)	0.007(7)	-0.037(9)
Au1"	0.0313(5)	0.0129(3)	0.0187(4)	-0.0028(2)	-0.0095(3)	-0.0086(2)
Au1B	0.061(2)	0.0352(12)	0.124(4)	-0.0336(15)	-0.024(3)	-0.0235(12)
P1"	0.072(2)	0.0325(17)	0.0407(18)	-0.0085(14)	-0.0237(17)	-0.0195(17)
O1"	0.105(8)	0.022(4)	0.033(5)	0.000(4)	-0.038(5)	-0.022(5)
O2"	0.071(6)	0.021(4)	0.029(4)	-0.002(3)	-0.024(4)	-0.019(4)
N1"	0.035(5)	0.015(4)	0.027(5)	-0.003(3)	-0.009(4)	-0.011(4)
N2"	0.035(5)	0.024(4)	0.025(4)	-0.011(4)	-0.007(4)	-0.013(4)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1"	0.031(6)	0.034(6)	0.013(5)	0.002(4)	-0.010(4)	-0.009(5)
C2"	0.033(6)	0.033(6)	0.019(5)	-0.004(5)	0.001(4)	-0.020(5)
C3"	0.035(6)	0.028(5)	0.017(5)	0.001(4)	-0.001(4)	-0.029(5)
C4"	0.038(6)	0.014(5)	0.027(5)	-0.002(4)	-0.010(5)	-0.014(4)
C5"	0.036(6)	0.018(5)	0.025(5)	-0.011(4)	-0.006(4)	-0.010(4)
C6"	0.033(6)	0.018(5)	0.028(5)	-0.005(4)	-0.007(4)	-0.011(4)
C7"	0.026(5)	0.027(5)	0.025(5)	-0.011(4)	-0.004(4)	-0.009(4)
C8"	0.017(5)	0.026(5)	0.020(5)	-0.005(4)	0.005(4)	-0.006(4)
C9"	0.026(5)	0.014(5)	0.027(5)	-0.006(4)	-0.003(4)	-0.010(4)
C10"	0.026(5)	0.021(5)	0.020(5)	-0.003(4)	-0.004(4)	-0.011(4)
C11"	0.025(4)	0.027(4)	0.030(4)	0.005(3)	-0.004(3)	-0.020(3)
C12"	0.028(5)	0.018(5)	0.036(6)	-0.018(4)	-0.007(4)	-0.003(4)
C13"	0.059(8)	0.015(5)	0.042(7)	-0.001(5)	-0.030(6)	-0.011(5)
C14"	0.059(9)	0.029(6)	0.063(9)	0.000(6)	-0.036(7)	-0.019(6)
C15"	0.059(9)	0.053(9)	0.069(10)	-0.009(8)	-0.030(8)	-0.024(7)
C16"	0.100(14)	0.058(10)	0.063(11)	-0.018(8)	-0.039(10)	-0.027(10)
C17"	0.096(13)	0.042(8)	0.046(8)	-0.015(6)	-0.030(8)	-0.023(8)
C18"	0.077(10)	0.032(6)	0.031(6)	-0.013(5)	-0.021(6)	-0.016(6)
C19"	0.034(8)	0.071(11)	0.085(12)	-0.001(9)	-0.030(8)	-0.012(7)
C20"	0.095(17)	0.086(16)	0.113(19)	-0.019(14)	-0.007(14)	-0.005(13)
C21"	0.094(17)	0.12(2)	0.112(19)	-0.009(16)	0.014(14)	-0.061(16)
C22"	0.073(11)	0.064(10)	0.046(8)	-0.037(8)	-0.018(8)	0.001(8)
C23"	0.113(17)	0.068(13)	0.062(12)	-0.012(10)	-0.031(12)	0.018(12)
C24"	0.065(11)	0.071(12)	0.062(11)	-0.024(9)	0.003(9)	-0.011(9)
C25"	0.051(7)	0.020(5)	0.036(6)	-0.003(5)	-0.024(6)	-0.012(5)
C26"	0.054(8)	0.030(6)	0.044(7)	-0.009(5)	-0.027(6)	-0.010(6)
C27"	0.061(9)	0.037(7)	0.060(9)	-0.017(7)	-0.034(8)	0.005(7)
C28"	0.104(14)	0.024(7)	0.059(10)	0.002(6)	-0.053(10)	-0.010(8)
C29"	0.100(13)	0.033(7)	0.043(8)	0.002(6)	-0.033(8)	-0.029(8)
C30"	0.069(9)	0.036(7)	0.037(7)	0.005(6)	-0.024(6)	-0.031(7)
C31"	0.038(8)	0.056(9)	0.071(10)	-0.013(8)	-0.021(7)	-0.004(7)
C32"	0.063(12)	0.068(12)	0.15(2)	-0.043(13)	-0.025(13)	-0.012(10)
C33"	0.060(11)	0.132(19)	0.071(12)	-0.054(13)	-0.003(9)	-0.026(12)
C34"	0.073(11)	0.068(11)	0.041(8)	0.023(8)	-0.015(8)	-0.046(9)
C35"	0.057(10)	0.072(12)	0.070(12)	0.001(10)	0.009(9)	-0.022(9)
C36"	0.13(2)	0.18(3)	0.081(15)	0.021(16)	-0.028(14)	-0.12(2)
C37"	0.064(9)	0.042(7)	0.042(7)	-0.011(6)	-0.020(7)	-0.018(7)
C38"	0.061(9)	0.035(7)	0.043(7)	-0.007(6)	-0.010(7)	-0.017(6)
C39"	0.065(10)	0.057(9)	0.052(9)	-0.017(7)	-0.010(8)	-0.022(8)
C40"	0.067(10)	0.056(9)	0.047(9)	-0.014(7)	-0.012(8)	-0.014(8)
C41"	0.074(11)	0.061(10)	0.041(8)	-0.013(7)	-0.020(7)	-0.022(8)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C42"	0.063(10)	0.064(10)	0.037(7)	-0.006(7)	-0.019(7)	-0.019(8)
C43"	0.070(10)	0.037(7)	0.046(8)	-0.007(6)	-0.018(7)	-0.022(7)
C44"	0.081(11)	0.042(8)	0.048(8)	-0.011(7)	-0.028(8)	-0.018(7)
C45"	0.089(13)	0.058(10)	0.061(10)	-0.008(8)	-0.033(9)	-0.027(9)
C46"	0.087(12)	0.034(7)	0.040(8)	-0.012(6)	-0.017(8)	0.000(7)
C47"	0.16(2)	0.029(8)	0.061(10)	-0.008(7)	-0.048(12)	-0.025(10)
C48"	0.140(18)	0.032(8)	0.106(15)	-0.012(9)	-0.069(14)	-0.028(10)
C49"	0.077(10)	0.034(7)	0.054(8)	-0.003(6)	-0.018(7)	-0.037(7)
C50"	0.070(10)	0.073(11)	0.056(9)	-0.024(8)	-0.011(8)	-0.046(9)
C51"	0.052(10)	0.104(15)	0.086(13)	-0.031(12)	-0.013(9)	-0.031(10)
C52"	0.069(11)	0.110(14)	0.034(7)	-0.020(8)	0.007(7)	-0.072(11)
C53"	0.102(15)	0.080(13)	0.073(12)	-0.004(10)	-0.031(11)	-0.065(12)
C54"	0.096(13)	0.053(9)	0.080(11)	-0.020(8)	-0.036(10)	-0.038(9)
C55	0.083(6)	0.105(7)	0.109(7)	-0.029(6)	-0.016(5)	-0.048(5)
C56	0.082(6)	0.105(7)	0.107(7)	-0.030(6)	-0.017(5)	-0.049(5)
C57	0.081(6)	0.104(7)	0.106(7)	-0.030(6)	-0.018(5)	-0.049(5)
C58	0.082(6)	0.104(7)	0.108(7)	-0.030(6)	-0.018(5)	-0.049(5)
C59	0.082(6)	0.105(7)	0.110(7)	-0.029(6)	-0.016(5)	-0.048(5)
C60	0.083(6)	0.105(7)	0.111(7)	-0.029(6)	-0.016(5)	-0.048(5)
C61	0.114(8)	0.218(13)	0.081(7)	-0.031(8)	-0.026(7)	-0.044(8)
C62	0.114(8)	0.218(13)	0.081(7)	-0.030(8)	-0.026(7)	-0.044(8)
C63	0.114(8)	0.218(13)	0.080(7)	-0.030(8)	-0.026(7)	-0.044(8)
C64	0.114(8)	0.218(13)	0.081(7)	-0.030(8)	-0.026(7)	-0.044(8)
C65	0.114(8)	0.218(13)	0.081(7)	-0.030(8)	-0.026(7)	-0.044(8)
C66	0.114(8)	0.218(13)	0.081(7)	-0.030(8)	-0.026(7)	-0.044(8)
C67	0.095(10)	0.076(9)	0.050(8)	-0.013(7)	-0.037(7)	-0.011(8)
C68	0.096(10)	0.076(9)	0.050(8)	-0.013(7)	-0.036(7)	-0.011(8)
C69	0.095(10)	0.077(9)	0.050(8)	-0.013(7)	-0.036(7)	-0.011(8)
C70	0.095(10)	0.077(10)	0.051(8)	-0.013(7)	-0.036(7)	-0.012(8)
C71	0.095(10)	0.077(10)	0.051(8)	-0.013(7)	-0.037(7)	-0.012(8)
C72	0.095(10)	0.076(9)	0.051(8)	-0.013(7)	-0.037(7)	-0.011(8)

Table 3.2.7 Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 12.

	x/a	y/b	z/c	U(eq)
H6	0.5191	0.5363	0.3096	0.035
H7	0.6270	0.4290	0.3095	0.033
H9	0.5802	0.4056	0.1655	0.036
H10	0.4764	0.5166	0.1596	0.037

	x/a	y/b	z/c	U(eq)
H12	0.6366	0.2721	0.2403	0.028
H15	0.1281	0.6812	0.4746	0.107
H16	0.1379	0.7677	0.4987	0.12
H17	0.2348	0.8128	0.4349	0.097
H19	0.2433	0.6109	0.3335	0.067
H20A	0.1315	0.7101	0.3058	0.121
H20B	0.1257	0.6303	0.3305	0.121
H20C	0.0871	0.6773	0.3820	0.121
H21A	0.1949	0.5205	0.4193	0.143
H21B	0.2495	0.5291	0.4456	0.143
H21C	0.1617	0.5665	0.4710	0.143
H22	0.3420	0.7951	0.2715	0.075
H23A	0.3670	0.8776	0.2896	0.113
H23B	0.2799	0.9011	0.3007	0.113
H23C	0.3165	0.8609	0.3661	0.113
H24A	0.4188	0.6821	0.3373	0.145
H24B	0.4515	0.7471	0.3024	0.145
H24C	0.4126	0.7249	0.3828	0.145
H27	0.3245	0.9282	-0.0225	0.047
H28	0.2503	0.9062	-0.0570	0.055
H29	0.2139	0.8030	0.0085	0.052
H31	0.4022	0.8063	0.1289	0.045
H32A	0.3905	0.9271	0.1113	0.092
H32B	0.3405	0.9634	0.0567	0.092
H32C	0.3109	0.9216	0.1362	0.092
H33A	0.4947	0.8513	0.0459	0.09
H33B	0.4862	0.7940	0.0257	0.09
H33C	0.4515	0.8828	-0.0131	0.09
H34	0.2558	0.6738	0.1751	0.055
H35A	0.1570	0.6637	0.1624	0.102
H35B	0.1363	0.7472	0.1583	0.102
H35C	0.1574	0.7299	0.0892	0.102
H36A	0.2821	0.5853	0.1273	0.098
H36B	0.2926	0.6453	0.0513	0.098
H36C	0.3488	0.6140	0.0990	0.098
H38	0.1268	0.9010	0.1098	0.045
H39	0.0592	0.9073	0.0452	0.062
H40	-0.0704	0.9647	0.0689	0.071
H41	-0.1301	1.0196	0.1538	0.069
H42	-0.0640	1.0090	0.2217	0.062
H44	0.2042	0.9833	0.2196	0.042

	x/a	y/b	z/c	U(eq)
H45	0.2224	1.0950	0.1844	0.054
H46	0.1320	1.2099	0.1402	0.052
H47	0.0273	1.2140	0.1264	0.056
H48	0.0090	1.1040	0.1597	0.044
H50	0.0255	0.8416	0.3253	0.113
H51	-0.0353	0.8220	0.4431	0.116
H52	-0.0757	0.9074	0.4916	0.115
H53	-0.0442	1.0157	0.4280	0.115
H54	0.0269	1.0300	0.3125	0.111
H6'	0.9873	0.3677	0.1727	0.035
H7'	0.8824	0.3664	0.1653	0.04
H9'	0.9089	0.1694	0.3242	0.03
H10'	1.0129	0.1717	0.3327	0.034
H12'	0.7508	0.3797	0.2377	0.038
H15'	1.1883	0.2010	0.5363	0.054
H16'	1.2509	0.0733	0.5592	0.064
H17'	1.2690	0.0168	0.4838	0.059
H19'	1.1149	0.3317	0.3840	0.051
H20D	1.0260	0.3800	0.4728	0.083
H20E	1.0215	0.3045	0.4809	0.083
H20F	1.0614	0.3021	0.5300	0.083
H21D	1.1399	0.4027	0.4206	0.109
H21E	1.1831	0.3270	0.4747	0.109
H21F	1.2156	0.3424	0.3936	0.109
H22'	1.2113	0.1177	0.3204	0.053
H23D	1.3385	0.0720	0.3139	0.096
H23E	1.3350	-0.0066	0.3712	0.096
H23F	1.3184	0.0197	0.2976	0.096
H24D	1.1370	0.0542	0.4088	0.113
H24E	1.1928	0.0088	0.3567	0.113
H24F	1.2095	-0.0175	0.4304	0.113
H27'	1.3735	0.3210	0.0373	0.057
H28'	1.3627	0.4331	0.0325	0.079
H29'	1.2669	0.4965	0.1056	0.097
H31'	1.2528	0.2207	0.1591	0.052
H32D	1.3727	0.1687	0.1772	0.107
H32E	1.3650	0.1257	0.1398	0.107
H32F	1.4058	0.1845	0.0961	0.107
H33D	1.2297	0.2874	0.0476	0.112
H33E	1.3169	0.2583	0.0155	0.112
H33F	1.2761	0.1995	0.0592	0.112

	x/a	y/b	z/c	U(eq)
H34'	1.1552	0.4071	0.2546	0.15
H35D	1.2255	0.4558	0.2541	0.201
H35E	1.1821	0.5348	0.2029	0.201
H35F	1.1385	0.4989	0.2784	0.201
H36D	1.0898	0.4620	0.1729	0.292
H36E	1.0548	0.5034	0.2286	0.292
H36F	1.0984	0.5393	0.1531	0.292
H38'	1.5179	0.2339	0.3543	0.083
H39'	1.5212	0.3170	0.3891	0.092
H40'	1.4285	0.4319	0.3772	0.074
H41'	1.3246	0.4680	0.3356	0.108
H42'	1.3255	0.3808	0.2971	0.082
H44'	1.5710	0.1275	0.3041	0.086
H45'	1.6203	0.0000	0.3675	0.108
H46'	1.5412	-0.0601	0.4541	0.122
H47'	1.4164	-0.0005	0.4668	0.116
H48'	1.3652	0.1226	0.3997	0.085
H50'	1.4945	0.1488	0.2058	0.066
H51'	1.5612	0.1671	0.0911	0.075
H52'	1.5842	0.2770	0.0265	0.078
H53'	1.5410	0.3695	0.0745	0.079
H54'	1.4744	0.3504	0.1902	0.073
H6"	0.8064	-0.0458	0.3143	0.032
H7"	0.8082	0.0598	0.3143	0.031
H9"	0.6711	0.1927	0.1813	0.027
H10"	0.6665	0.0875	0.1824	0.028
H12"	0.8516	0.1600	0.2515	0.031
H15"	0.5500	-0.0986	0.0992	0.07
H16"	0.6351	-0.1127	0.0019	0.082
H17"	0.7550	-0.1289	-0.0169	0.069
H19"	0.5937	-0.0915	0.2412	0.086
H20G	0.4684	-0.0114	0.2455	0.184
H20H	0.5190	0.0249	0.1758	0.184
H20I	0.4730	-0.0146	0.1738	0.184
H21G	0.5024	-0.1504	0.2999	0.19
H21H	0.5133	-0.1619	0.2303	0.19
H21I	0.5800	-0.2063	0.2695	0.19
H22"	0.8298	-0.1286	0.1026	0.076
H23G	0.8710	-0.2499	0.0960	0.158
H23H	0.8810	-0.2135	0.0138	0.158
H23I	0.9320	-0.2128	0.0504	0.158

	x/a	y/b	z/c	U(eq)
H24G	0.8934	-0.0761	-0.0081	0.117
H24H	0.8355	-0.0706	-0.0414	0.117
H24I	0.8084	-0.0212	0.0060	0.117
H27"	0.9693	-0.3901	0.3515	0.067
H28"	0.9046	-0.4531	0.4485	0.075
H29"	0.7765	-0.4029	0.4757	0.068
H31"	0.8881	-0.2136	0.2253	0.074
H32G	0.9885	-0.1966	0.2294	0.142
H32H	0.9221	-0.1879	0.2955	0.142
H32I	0.9945	-0.2638	0.3020	0.142
H33G	1.0072	-0.2733	0.1669	0.132
H33H	1.0170	-0.3482	0.2333	0.132
H33I	0.9557	-0.3195	0.1920	0.132
H34"	0.6655	-0.2214	0.3738	0.082
H35G	0.6022	-0.2225	0.4874	0.13
H35H	0.6729	-0.2913	0.5159	0.13
H35I	0.6780	-0.2107	0.4673	0.13
H36G	0.5891	-0.2943	0.4367	0.188
H36H	0.6562	-0.3297	0.3815	0.188
H36I	0.6592	-0.3674	0.4615	0.188
H38"	0.9554	-0.4986	0.1743	0.06
H39"	1.0472	-0.5120	0.0781	0.071
H40"	1.0287	-0.4282	-0.0302	0.075
H41"	0.9131	-0.3365	-0.0446	0.071
H42"	0.8186	-0.3149	0.0528	0.07
H44"	0.8686	-0.4327	0.3004	0.067
H45"	0.9333	-0.5459	0.3775	0.083
H46"	0.9266	-0.6594	0.3947	0.076
H47"	0.8476	-0.6547	0.3453	0.1
H48"	0.7927	-0.5439	0.2608	0.101
H50"	0.6422	-0.3055	0.2110	0.07
H51"	0.5481	-0.2909	0.1687	0.098
H52"	0.5735	-0.3753	0.1151	0.074
H53"	0.6894	-0.4635	0.0988	0.091
H54"	0.7839	-0.4772	0.1366	0.08
H55	0.7381	0.4085	0.0495	0.118
H56	0.7313	0.2898	0.0898	0.114
H57	0.8413	0.1823	0.0875	0.112
H58	0.9533	0.1950	0.0414	0.114
H59	0.9599	0.3149	-0.0040	0.117
H60	0.8535	0.4174	-0.0008	0.119

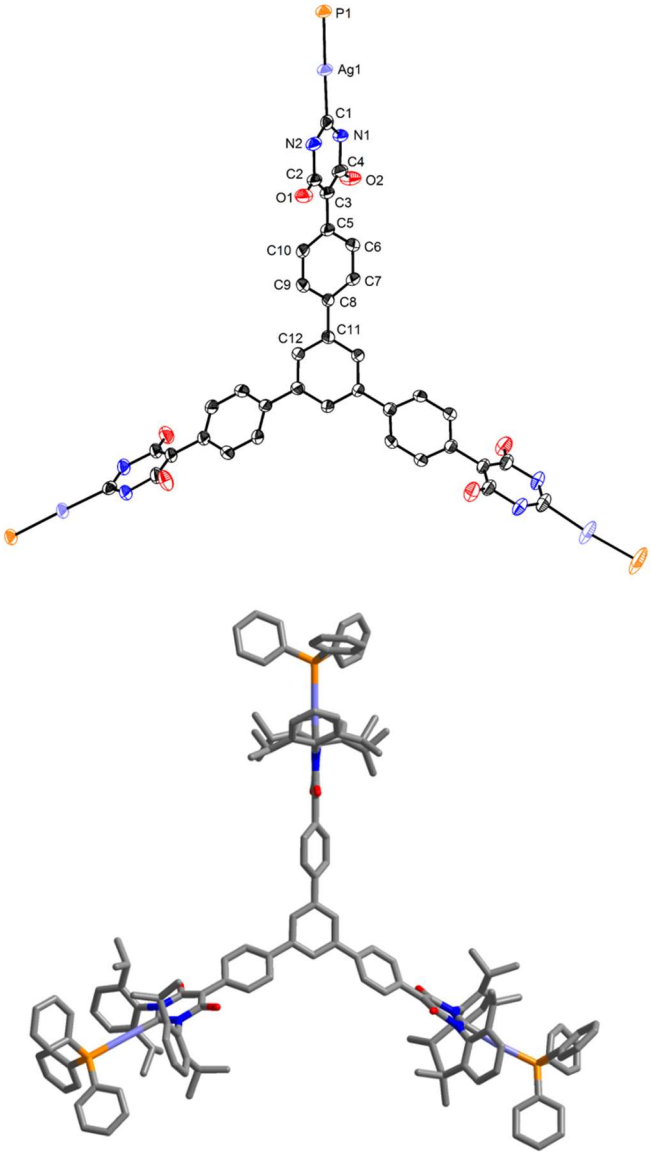
	x/a	y/b	z/c	U(eq)
H61	0.5570	0.6241	0.3433	0.183
H62	0.6712	0.5277	0.3249	0.184
H63	0.7230	0.4302	0.4157	0.184
H64	0.6627	0.4280	0.5283	0.184
H65	0.5464	0.5214	0.5490	0.183
H66	0.4901	0.6060	0.4571	0.184
H67	0.6410	0.1150	0.4279	0.096
H68	0.7459	0.1410	0.4016	0.096
H69	0.7388	0.2493	0.4075	0.096
H70	0.6246	0.3086	0.4733	0.096
H71	0.5507	0.2394	0.5556	0.096
H72	0.5528	0.1499	0.5231	0.096

3.3 X-ray crystallography data for compound 13 ($C_{162}H_{162}Ag_3N_6O_6P_3 \cdot 2\ C_6H_6$)

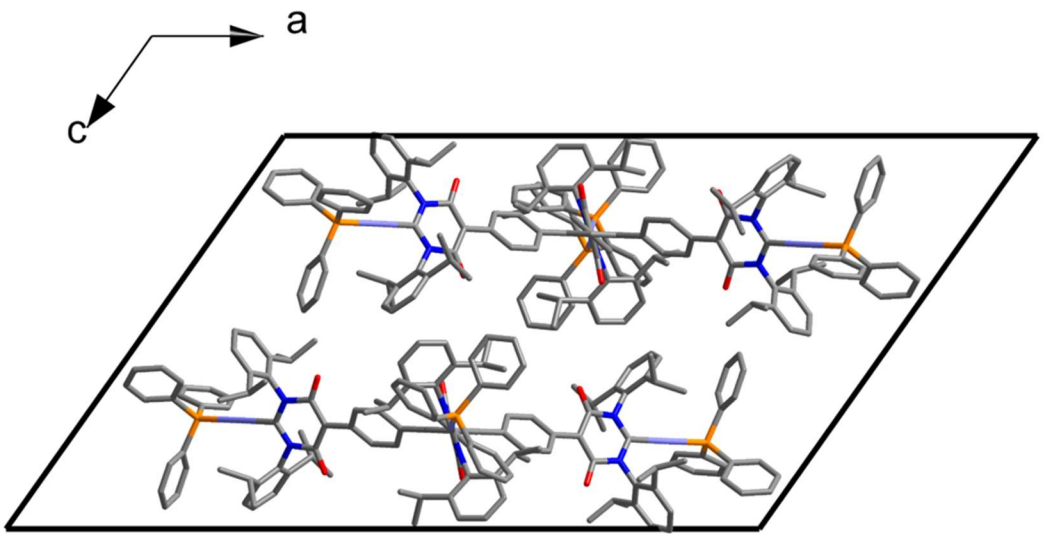
A specimen of $C_{174}H_{174}Ag_3N_6O_6P_3$, approximate dimensions 0.178 mm x 0.209 mm x 0.298 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using a monoclinic unit cell yielded a total of 223523 reflections to a maximum θ angle of 25.50° (0.83 Å resolution), of which 14232 were independent (average redundancy 15.706, completeness = 99.7%, R_{int} = 4.32%, R_{sig} = 1.82%) and 12235 (85.97%) were greater than $2\sigma(F^2)$. The final cell constants of a = 36.8106(16) Å, b = 21.7138(16) Å, c = 23.4910(16) Å, β = 125.324(3)°, volume = 15319.5(17) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9306 and 1.0000.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group C 1 2/c 1, with Z = 4 for the formula unit, $C_{174}H_{174}Ag_3N_6O_6P_3$. The final anisotropic full-matrix least-squares refinement on F^2 with 958 variables converged at R1 = 5.88%, for the observed data and wR2 = 14.70% for all data. The goodness-of-fit was 1.129. The largest peak in the final difference electron density synthesis was 1.422 $e^-/Å^3$ and the largest hole was -1.072 $e^-/Å^3$ with an RMS deviation of 0.091 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.241 g/cm^3 and F(000), 5976 e^-.



Solid state molecular structure of **13** with 50% probability ellipsoids. Hydrogen atoms and solvent molecules are omitted for clarity. Only half of the atoms are numbered, since the other half of the molecule is completed by inversion symmetry.



Partial packing diagram of the Ag complex (solvent molecules omitted for clarity).

Table 3.3.1 Sample and crystal data for 13.

Chemical formula	$C_{174}H_{174}Ag_3N_6O_6P_3$	
Formula weight	2861.70 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.178 x 0.209 x 0.298 mm	
Crystal system	monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 36.8106(16) Å	α = 90°
	b = 21.7138(16) Å	β = 125.324(3)°
	c = 23.4910(16) Å	γ = 90°
Volume	15319.5(17) $Å^3$	
Z	4	
Density (calculated)	1.241 g/cm^3	
Absorption coefficient	0.468 mm^{-1}	
F(000)	5976	

Table 3.3.2 Data collection and structure refinement for 13

Theta range for data collection	2.74 to 25.50°
Index ranges	$-44 \leq h \leq 44$, $-26 \leq k \leq 26$, $-28 \leq l \leq 28$
Reflections collected	223523

Independent reflections	14232 [R(int) = 0.0432]
Max. and min. transmission	1.0000 and 0.9306
Structure solution technique	direct methods
Structure solution program	SHELXT-2014 (Sheldrick 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014 (Sheldrick 2014)
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	14232 / 165 / 958
Goodness-of-fit on F^2	1.129
Δ/σ_{max}	0.001
Final R indices	12235 data; I>2σ(I) R1 = 0.0588, wR2 = 0.1353 all data R1 = 0.0708, wR2 = 0.1470
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0377P)^2+128.6354P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	1.422 and -1.072 eÅ^{-3}
R.M.S. deviation from mean	0.091 eÅ^{-3}

Table 3.3.3 Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 13. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Ag1	0.20730(2)	0.93821(2)	0.72344(2)	0.02468(9)
P1	0.15135(3)	0.88165(5)	0.71949(6)	0.0240(2)
O1'	0.55841(10)	0.56789(13)	0.87070(15)	0.0326(7)
O2	0.27155(9)	0.07618(14)	0.61502(15)	0.0320(7)
O1	0.36986(9)	0.02694(13)	0.85587(15)	0.0301(6)
N1	0.24990(10)	0.02256(14)	0.67371(17)	0.0227(7)
N2	0.29911(11)	0.99183(15)	0.78752(18)	0.0254(7)
C1	0.25749(13)	0.99080(17)	0.7282(2)	0.0218(8)
C2	0.33510(13)	0.02692(17)	0.7960(2)	0.0246(8)
C3	0.32629(13)	0.05688(17)	0.7361(2)	0.0231(8)
C4	0.28356(13)	0.05471(17)	0.6717(2)	0.0251(8)
C5	0.36214(13)	0.09225(17)	0.7393(2)	0.0234(8)
C6	0.35264(13)	0.14449(17)	0.6980(2)	0.0250(8)
C7	0.38582(13)	0.17722(17)	0.7009(2)	0.0236(8)
C8	0.43031(12)	0.15880(17)	0.7453(2)	0.0219(8)
C9	0.44013(13)	0.10667(18)	0.7866(2)	0.0269(8)
C10	0.40665(13)	0.07431(17)	0.7839(2)	0.0263(8)
C11	0.46613(12)	0.19341(17)	0.7476(2)	0.0219(8)
C12	0.5	0.1621(2)	0.75	0.0240(11)
C13	0.30535(13)	0.95833(18)	0.8453(2)	0.0257(8)

	x/a	y/b	z/c	U(eq)
C14	0.32206(15)	0.8975(2)	0.8575(3)	0.0369(10)
C15	0.32286(18)	0.8644(2)	0.9090(3)	0.0461(12)
C16	0.30753(18)	0.8895(2)	0.9457(3)	0.0478(13)
C17	0.29301(17)	0.9492(2)	0.9344(3)	0.0416(11)
C18	0.29219(14)	0.9855(2)	0.8846(2)	0.0307(9)
C19	0.33775(16)	0.8704(2)	0.8160(3)	0.0386(10)
C20	0.30092(17)	0.8329(2)	0.7545(3)	0.0465(12)
C21	0.3795(2)	0.8298(3)	0.8621(3)	0.0612(16)
C22	0.27711(16)	0.0524(2)	0.8740(3)	0.0363(10)
C23	0.22894(18)	0.0586(2)	0.8494(3)	0.0509(13)
C24	0.3074(2)	0.0893(3)	0.9409(3)	0.0564(15)
C25	0.20473(13)	0.02443(18)	0.6116(2)	0.0252(8)
C26	0.18926(14)	0.97578(19)	0.5639(2)	0.0298(9)
C27	0.14510(15)	0.9771(2)	0.5067(2)	0.0356(10)
C28	0.11788(15)	0.0255(2)	0.4969(2)	0.0383(11)
C29	0.13419(15)	0.0738(2)	0.5444(2)	0.0392(11)
C30	0.17784(14)	0.0743(2)	0.6032(2)	0.0319(9)
C31	0.21970(17)	0.9243(2)	0.5722(2)	0.0374(10)
C32	0.1988(2)	0.8606(2)	0.5612(3)	0.0587(15)
C33	0.2333(2)	0.9336(3)	0.5220(3)	0.0550(14)
C34	0.19546(17)	0.1272(2)	0.6546(3)	0.0405(11)
C35	0.2056(2)	0.1827(2)	0.6259(3)	0.0522(13)
C36	0.1633(2)	0.1454(3)	0.6731(3)	0.0579(15)
C37	0.14436(13)	0.80343(17)	0.6869(2)	0.0252(8)
C38	0.18022(15)	0.7769(2)	0.6910(2)	0.0343(10)
C39	0.17803(16)	0.7162(2)	0.6702(3)	0.0396(11)
C40	0.14000(17)	0.6821(2)	0.6451(2)	0.0391(11)
C41	0.10404(16)	0.70812(19)	0.6403(2)	0.0369(10)
C42	0.10599(15)	0.76869(19)	0.6612(2)	0.0308(9)
C43	0.16282(14)	0.8735(2)	0.8058(2)	0.0306(9)
C44	0.18214(17)	0.8207(2)	0.8446(2)	0.0437(12)
C45	0.1953(2)	0.8187(3)	0.9134(3)	0.0656(17)
C46	0.1900(2)	0.8692(4)	0.9434(3)	0.0664(19)
C47	0.16990(19)	0.9211(3)	0.9040(3)	0.0561(16)
C48	0.15683(16)	0.9242(2)	0.8359(3)	0.0425(11)
C49	0.09877(14)	0.92238(19)	0.6677(2)	0.0276(9)
C50	0.09462(15)	0.9714(2)	0.6264(2)	0.0341(10)
C51	0.05643(16)	0.0063(2)	0.5907(3)	0.0432(11)
C52	0.02118(16)	0.9921(2)	0.5949(3)	0.0417(11)
C53	0.02435(15)	0.9427(2)	0.6341(2)	0.0342(10)
C54	0.06288(14)	0.9081(2)	0.6711(2)	0.0320(9)

	x/a	y/b	z/c	U(eq)
Ag1'	0.50664(4)	0.78492(3)	0.76710(3)	0.0440(3)
P1'	0.50963(11)	0.89133(12)	0.78998(19)	0.0742(12)
N2'	0.53028(12)	0.65546(14)	0.80593(17)	0.0265(7)
C1'	0.5	0.6871(3)	0.75	0.0305(13)
C2'	0.53134(13)	0.58900(17)	0.8126(2)	0.0248(8)
C3'	0.5	0.5580(2)	0.75	0.0211(11)
C5'	0.5	0.4887(2)	0.75	0.0210(11)
C6'	0.53978(12)	0.45564(17)	0.7919(2)	0.0218(8)
C7'	0.53973(12)	0.39198(17)	0.7920(2)	0.0218(8)
C8'	0.5	0.3583(2)	0.75	0.0201(10)
C11'	0.5	0.2903(2)	0.75	0.0209(11)
C12'	0.46629(12)	0.25741(16)	0.7471(2)	0.0211(8)
C13'	0.56502(16)	0.69039(19)	0.8660(2)	0.0362(10)
C14'	0.55936(17)	0.7043(2)	0.9188(3)	0.0408(11)
C15'	0.5913(2)	0.7418(2)	0.9728(3)	0.0551(14)
C16'	0.6263(2)	0.7639(2)	0.9727(3)	0.0574(15)
C17'	0.6318(2)	0.7497(2)	0.9213(3)	0.0564(15)
C18'	0.60048(18)	0.7111(2)	0.8652(3)	0.0452(12)
C19'	0.52066(19)	0.6805(2)	0.9182(3)	0.0481(13)
C20'	0.5371(2)	0.6453(3)	0.9853(3)	0.0600(16)
C21'	0.4889(3)	0.7330(3)	0.9058(4)	0.0732(19)
C22'	0.60646(18)	0.6913(2)	0.8096(3)	0.0488(13)
C23'	0.6275(2)	0.6278(3)	0.8242(4)	0.0657(17)
C24'	0.6326(3)	0.7371(4)	0.7963(5)	0.098(3)
C37'	0.5047(3)	0.9075(5)	0.8665(7)	0.068(3)
C38'	0.5419(4)	0.9000(5)	0.9320(5)	0.068(3)
C39'	0.5409(4)	0.9103(6)	0.9882(7)	0.073(3)
C40'	0.5030(3)	0.9278(5)	0.9813(7)	0.072(3)
C41'	0.4664(4)	0.9382(5)	0.9162(6)	0.073(3)
C42'	0.4674(4)	0.9260(5)	0.8611(8)	0.076(3)
C43'	0.5605(5)	0.9317(5)	0.8160(8)	0.069(3)
C44'	0.5927(4)	0.8990(6)	0.8131(9)	0.071(3)
C45'	0.6330(5)	0.9273(5)	0.8328(7)	0.071(3)
C46'	0.6437(5)	0.9850(5)	0.8663(7)	0.068(2)
C47'	0.6122(4)	0.0166(6)	0.8718(9)	0.073(3)
C48'	0.5713(4)	0.9888(5)	0.8498(7)	0.070(3)
C49'	0.4651(6)	0.9299(6)	0.7198(11)	0.137(5)
C50'	0.4601(6)	0.9922(5)	0.7054(9)	0.123(5)
C51'	0.4247(5)	0.0224(7)	0.6481(9)	0.132(5)
C52'	0.3834(6)	0.9966(7)	0.6233(13)	0.148(6)
C54'	0.4214(5)	0.9109(9)	0.6897(14)	0.148(6)

	x/a	y/b	z/c	U(eq)
C53'	0.3804(7)	0.9347(7)	0.6359(11)	0.154(6)
C55	0.4146(3)	0.2031(5)	0.5648(4)	0.100(3)
C56	0.4145(3)	0.2663(5)	0.5668(4)	0.105(3)
C57	0.4461(3)	0.2972(4)	0.5629(4)	0.099(3)
C58	0.4739(3)	0.2662(5)	0.5536(4)	0.084(2)
C59	0.4733(3)	0.2048(6)	0.5502(4)	0.103(3)
C60	0.4439(3)	0.1738(5)	0.5561(4)	0.101(3)

Table 3.3.4 Bond lengths (Å) for 13.

Ag1-C1	2.119(4)	Ag1-P1	2.3531(10)
P1-C49	1.813(4)	P1-C37	1.819(4)
P1-C43	1.825(4)	O1'-C2'	1.223(5)
O2-C4	1.226(5)	O1-C2	1.238(5)
N1-C1	1.335(5)	N1-C25	1.446(5)
N1-C4	1.447(5)	N2-C1	1.349(5)
N2-C13	1.437(5)	N2-C2	1.438(5)
C2-C3	1.408(5)	C3-C4	1.420(6)
C3-C5	1.491(5)	C5-C10	1.396(6)
C5-C6	1.399(5)	C6-C7	1.381(5)
C6-H6	0.95	C7-C8	1.398(5)
C7-H7	0.95	C8-C9	1.396(5)
C8-C11	1.491(5)	C9-C10	1.388(5)
C9-H9	0.95	C10-H10	0.95
C11-C12'	1.390(5)	C11-C12	1.392(4)
C12-C11	1.392(4)	C12-H12	0.95
C13-C18	1.396(6)	C13-C14	1.415(6)
C14-C15	1.392(7)	C14-C19	1.511(6)
C15-C16	1.387(7)	C15-H15	0.95
C16-C17	1.368(7)	C16-H16	0.95
C17-C18	1.397(6)	C17-H17	0.95
C18-C22	1.522(6)	C19-C20	1.523(7)
C19-C21	1.545(7)	C19-H19	1.0
C20-H20A	0.98	C20-H20B	0.98
C20-H20C	0.98	C21-H21A	0.98
C21-H21B	0.98	C21-H21C	0.98
C22-C23	1.520(7)	C22-C24	1.526(7)
C22-H22	1.0	C23-H23A	0.98
C23-H23B	0.98	C23-H23C	0.98
C24-H24A	0.98	C24-H24B	0.98
C24-H24C	0.98	C25-C26	1.399(6)
C25-C30	1.401(6)	C26-C27	1.386(6)

C26-C31	1.513(6)	C27-C28	1.377(7)
C27-H27	0.95	C28-C29	1.388(7)
C28-H28	0.95	C29-C30	1.387(6)
C29-H29	0.95	C30-C34	1.516(6)
C31-C32	1.531(7)	C31-C33	1.536(7)
C31-H31	1.0	C32-H32A	0.98
C32-H32B	0.98	C32-H32C	0.98
C33-H33A	0.98	C33-H33B	0.98
C33-H33C	0.98	C34-C35	1.528(7)
C34-C36	1.531(7)	C34-H34	1.0
C35-H35A	0.98	C35-H35B	0.98
C35-H35C	0.98	C36-H36A	0.98
C36-H36B	0.98	C36-H36C	0.98
C37-C38	1.392(6)	C37-C42	1.394(5)
C38-C39	1.391(6)	C38-H38	0.95
C39-C40	1.379(6)	C39-H39	0.95
C40-C41	1.383(6)	C40-H40	0.95
C41-C42	1.391(6)	C41-H41	0.95
C42-H42	0.95	C43-C44	1.378(7)
C43-C48	1.393(6)	C44-C45	1.396(7)
C44-H44	0.95	C45-C46	1.376(10)
C45-H45	0.95	C46-C47	1.372(9)
C46-H46	0.95	C47-C48	1.379(7)
C47-H47	0.95	C48-H48	0.95
C49-C50	1.388(6)	C49-C54	1.403(5)
C50-C51	1.376(7)	C50-H50	0.95
C51-C52	1.391(7)	C51-H51	0.95
C52-C53	1.374(7)	C52-H52	0.95
C53-C54	1.382(6)	C53-H53	0.95
C54-H54	0.95	Ag1'-C1'	2.149(5)
Ag1'-P1'	2.360(3)	P1'-C49'	1.727(15)
P1'-C43'	1.824(15)	P1'-C37'	1.939(15)
N2'-C1'	1.322(4)	N2'-C2'	1.450(5)
N2'-C13'	1.454(5)	C1'-N2'	1.322(4)
C2'-C3'	1.408(5)	C3'-C2'	1.409(5)
C3'-C5'	1.505(7)	C5'-C6'	1.400(4)
C5'-C6'	1.400(4)	C6'-C7'	1.382(5)
C6'-H6'	0.95	C7'-C8'	1.407(5)
C7'-H7'	0.95	C8'-C7'	1.407(5)
C8'-C11'	1.476(7)	C11'-C12'	1.398(4)
C11'-C12'	1.398(4)	C12'-H12'	0.95
C13'-C18'	1.391(7)	C13'-C14'	1.405(7)

C14'-C15'	1.388(7)	C14'-C19'	1.507(7)
C15'-C16'	1.376(8)	C15'-H15'	0.95
C16'-C17'	1.369(8)	C16'-H16'	0.95
C17'-C18'	1.419(7)	C17'-H17'	0.95
C18'-C22'	1.507(8)	C19'-C20'	1.528(8)
C19'-C21'	1.535(8)	C19'-H19'	1.0
C20'-H20D	0.98	C20'-H20E	0.98
C20'-H20F	0.98	C21'-H21D	0.98
C21'-H21E	0.98	C21'-H21F	0.98
C22'-C23'	1.521(8)	C22'-C24'	1.537(8)
C22'-H22'	1.0	C23'-H23D	0.98
C23'-H23E	0.98	C23'-H23F	0.98
C24'-H24D	0.98	C24'-H24E	0.98
C24'-H24F	0.98	C37'-C38'	1.354(8)
C37'-C42'	1.366(8)	C38'-C39'	1.359(8)
C38'-H38'	0.95	C39'-C40'	1.362(8)
C39'-H39'	0.95	C40'-C41'	1.352(8)
C40'-H40'	0.95	C41'-C42'	1.344(8)
C41'-H41'	0.95	C42'-H42'	0.95
C43'-C48'	1.400(9)	C43'-C44'	1.418(9)
C44'-C45'	1.413(9)	C44'-H44'	0.95
C45'-C46'	1.410(9)	C45'-H45'	0.95
C46'-C47'	1.417(9)	C46'-H46'	0.95
C47'-C48'	1.413(9)	C47'-H47'	0.95
C48'-H48'	0.95	C49'-C50'	1.379(10)
C49'-C54'	1.394(10)	C50'-C51'	1.383(10)
C50'-H50'	0.95	C51'-C52'	1.392(10)
C51'-H51'	0.95	C52'-C53'	1.393(10)
C52'-H52'	0.95	C54'-C53'	1.392(10)
C54'-H54'	0.95	C53'-H53'	0.95
C55-C60	1.364(11)	C55-C56	1.373(11)
C55-H55	0.95	C56-C57	1.393(11)
C56-H56	0.95	C57-C58	1.342(11)
C57-H57	0.95	C58-C59	1.336(11)
C58-H58	0.95	C59-C60	1.348(11)
C59-H59	0.95	C60-H60	0.95

Table 3.3.5 Bond angles (°) for 13.

C1-Ag1-P1	178.66(10)	C49-P1-C37	109.69(19)
C49-P1-C43	105.30(19)	C37-P1-C43	105.22(19)
C49-P1-Ag1	110.03(13)	C37-P1-Ag1	114.30(13)
C43-P1-Ag1	111.84(13)	C1-N1-C25	117.6(3)

C1-N1-C4	125.0(3)	C25-N1-C4	117.4(3)
C1-N2-C13	115.6(3)	C1-N2-C2	123.9(3)
C13-N2-C2	120.4(3)	N1-C1-N2	117.7(3)
N1-C1-Ag1	122.4(3)	N2-C1-Ag1	119.9(3)
O1-C2-C3	128.6(3)	O1-C2-N2	115.0(3)
C3-C2-N2	116.4(3)	C2-C3-C4	121.6(3)
C2-C3-C5	120.2(4)	C4-C3-C5	118.2(3)
O2-C4-C3	128.8(3)	O2-C4-N1	116.2(3)
C3-C4-N1	115.0(3)	C10-C5-C6	117.5(3)
C10-C5-C3	120.9(3)	C6-C5-C3	121.6(3)
C7-C6-C5	121.6(4)	C7-C6-H6	119.2
C5-C6-H6	119.2	C6-C7-C8	120.7(4)
C6-C7-H7	119.6	C8-C7-H7	119.6
C9-C8-C7	118.1(3)	C9-C8-C11	121.0(3)
C7-C8-C11	120.8(3)	C10-C9-C8	120.9(4)
C10-C9-H9	119.6	C8-C9-H9	119.6
C9-C10-C5	121.2(4)	C9-C10-H10	119.4
C5-C10-H10	119.4	C12'-C11-C12	118.7(4)
C12'-C11-C8	120.8(3)	C12-C11-C8	120.5(3)
C11-C12-C11	121.5(5)	C11-C12-H12	119.2
C11-C12-H12	119.2	C18-C13-C14	122.5(4)
C18-C13-N2	118.9(4)	C14-C13-N2	118.5(4)
C15-C14-C13	116.5(4)	C15-C14-C19	122.4(4)
C13-C14-C19	121.1(4)	C16-C15-C14	121.7(5)
C16-C15-H15	119.1	C14-C15-H15	119.1
C17-C16-C15	120.3(4)	C17-C16-H16	119.9
C15-C16-H16	119.9	C16-C17-C18	121.0(4)
C16-C17-H17	119.5	C18-C17-H17	119.5
C13-C18-C17	117.8(4)	C13-C18-C22	122.0(4)
C17-C18-C22	120.2(4)	C14-C19-C20	110.9(4)
C14-C19-C21	111.4(4)	C20-C19-C21	109.8(4)
C14-C19-H19	108.2	C20-C19-H19	108.2
C21-C19-H19	108.2	C19-C20-H20A	109.5
C19-C20-H20B	109.5	H20A-C20-H20B	109.5
C19-C20-H20C	109.5	H20A-C20-H20C	109.5
H20B-C20-H20C	109.5	C19-C21-H21A	109.5
C19-C21-H21B	109.5	H21A-C21-H21B	109.5
C19-C21-H21C	109.5	H21A-C21-H21C	109.5
H21B-C21-H21C	109.5	C23-C22-C18	112.5(4)
C23-C22-C24	110.0(4)	C18-C22-C24	110.7(4)
C23-C22-H22	107.8	C18-C22-H22	107.8
C24-C22-H22	107.8	C22-C23-H23A	109.5

C22-C23-H23B	109.5	H23A-C23-H23B	109.5
C22-C23-H23C	109.5	H23A-C23-H23C	109.5
H23B-C23-H23C	109.5	C22-C24-H24A	109.5
C22-C24-H24B	109.5	H24A-C24-H24B	109.5
C22-C24-H24C	109.5	H24A-C24-H24C	109.5
H24B-C24-H24C	109.5	C26-C25-C30	122.9(4)
C26-C25-N1	119.0(4)	C30-C25-N1	118.1(4)
C27-C26-C25	117.8(4)	C27-C26-C31	120.4(4)
C25-C26-C31	121.7(4)	C28-C27-C26	120.7(4)
C28-C27-H27	119.7	C26-C27-H27	119.7
C27-C28-C29	120.5(4)	C27-C28-H28	119.8
C29-C28-H28	119.8	C30-C29-C28	121.3(4)
C30-C29-H29	119.4	C28-C29-H29	119.4
C29-C30-C25	116.9(4)	C29-C30-C34	121.0(4)
C25-C30-C34	122.1(4)	C26-C31-C32	112.5(4)
C26-C31-C33	110.4(4)	C32-C31-C33	110.2(4)
C26-C31-H31	107.9	C32-C31-H31	107.9
C33-C31-H31	107.9	C31-C32-H32A	109.5
C31-C32-H32B	109.5	H32A-C32-H32B	109.5
C31-C32-H32C	109.5	H32A-C32-H32C	109.5
H32B-C32-H32C	109.5	C31-C33-H33A	109.5
C31-C33-H33B	109.5	H33A-C33-H33B	109.5
C31-C33-H33C	109.5	H33A-C33-H33C	109.5
H33B-C33-H33C	109.5	C30-C34-C35	110.4(4)
C30-C34-C36	112.1(4)	C35-C34-C36	110.4(4)
C30-C34-H34	107.9	C35-C34-H34	107.9
C36-C34-H34	107.9	C34-C35-H35A	109.5
C34-C35-H35B	109.5	H35A-C35-H35B	109.5
C34-C35-H35C	109.5	H35A-C35-H35C	109.5
H35B-C35-H35C	109.5	C34-C36-H36A	109.5
C34-C36-H36B	109.5	H36A-C36-H36B	109.5
C34-C36-H36C	109.5	H36A-C36-H36C	109.5
H36B-C36-H36C	109.5	C38-C37-C42	119.3(4)
C38-C37-P1	117.4(3)	C42-C37-P1	123.3(3)
C39-C38-C37	120.5(4)	C39-C38-H38	119.7
C37-C38-H38	119.7	C40-C39-C38	119.8(4)
C40-C39-H39	120.1	C38-C39-H39	120.1
C39-C40-C41	120.1(4)	C39-C40-H40	119.9
C41-C40-H40	119.9	C40-C41-C42	120.4(4)
C40-C41-H41	119.8	C42-C41-H41	119.8
C41-C42-C37	119.8(4)	C41-C42-H42	120.1
C37-C42-H42	120.1	C44-C43-C48	119.6(4)

C44-C43-P1	120.9(3)	C48-C43-P1	119.0(4)
C43-C44-C45	119.5(5)	C43-C44-H44	120.2
C45-C44-H44	120.2	C46-C45-C44	120.7(6)
C46-C45-H45	119.7	C44-C45-H45	119.7
C47-C46-C45	119.4(5)	C47-C46-H46	120.3
C45-C46-H46	120.3	C46-C47-C48	120.8(6)
C46-C47-H47	119.6	C48-C47-H47	119.6
C47-C48-C43	120.0(5)	C47-C48-H48	120.0
C43-C48-H48	120.0	C50-C49-C54	118.9(4)
C50-C49-P1	119.1(3)	C54-C49-P1	121.9(3)
C51-C50-C49	120.7(4)	C51-C50-H50	119.7
C49-C50-H50	119.7	C50-C51-C52	120.0(4)
C50-C51-H51	120.0	C52-C51-H51	120.0
C53-C52-C51	119.9(4)	C53-C52-H52	120.0
C51-C52-H52	120.0	C52-C53-C54	120.4(4)
C52-C53-H53	119.8	C54-C53-H53	119.8
C53-C54-C49	120.1(4)	C53-C54-H54	120.0
C49-C54-H54	120.0	C1'-Ag1'-P1'	174.43(14)
C49'-P1'-C43'	108.1(9)	C49'-P1'-C37'	104.6(10)
C43'-P1'-C37'	103.3(5)	C49'-P1'-Ag1'	111.4(5)
C43'-P1'-Ag1'	116.8(4)	C37'-P1'-Ag1'	111.8(4)
C1'-N2'-C2'	125.4(4)	C1'-N2'-C13'	117.2(3)
C2'-N2'-C13'	117.5(3)	N2'-C1'-N2'	117.4(5)
N2'-C1'-Ag1'	112.9(2)	N2'-C1'-Ag1'	129.7(3)
O1'-C2'-C3'	129.3(4)	O1'-C2'-N2'	116.6(3)
C3'-C2'-N2'	114.2(4)	C2'-C3'-C2'	122.8(5)
C2'-C3'-C5'	118.6(2)	C2'-C3'-C5'	118.6(2)
C6'-C5'-C6'	118.4(5)	C6'-C5'-C3'	120.8(2)
C6'-C5'-C3'	120.8(2)	C7'-C6'-C5'	120.8(4)
C7'-C6'-H6'	119.6	C5'-C6'-H6'	119.6
C6'-C7'-C8'	121.4(4)	C6'-C7'-H7'	119.3
C8'-C7'-H7'	119.3	C7'-C8'-C7'	117.3(5)
C7'-C8'-C11'	121.4(2)	C7'-C8'-C11'	121.4(2)
C12'-C11'-C12'	118.6(5)	C12'-C11'-C8'	120.7(2)
C12'-C11'-C8'	120.7(2)	C11-C12'-C11'	121.2(3)
C11-C12'-H12'	119.4	C11'-C12'-H12'	119.4
C18'-C13'-C14'	124.2(4)	C18'-C13'-N2'	117.5(4)
C14'-C13'-N2'	118.2(4)	C15'-C14'-C13'	116.9(5)
C15'-C14'-C19'	120.5(5)	C13'-C14'-C19'	122.6(4)
C16'-C15'-C14'	120.2(5)	C16'-C15'-H15'	119.9
C14'-C15'-H15'	119.9	C17'-C16'-C15'	122.6(5)
C17'-C16'-H16'	118.7	C15'-C16'-H16'	118.7

C16'-C17'-C18'	119.8(5)	C16'-C17'-H17'	120.1
C18'-C17'-H17'	120.1	C13'-C18'-C17'	116.3(5)
C13'-C18'-C22'	121.9(5)	C17'-C18'-C22'	121.8(5)
C14'-C19'-C20'	110.7(5)	C14'-C19'-C21'	111.1(5)
C20'-C19'-C21'	111.7(5)	C14'-C19'-H19'	107.7
C20'-C19'-H19'	107.7	C21'-C19'-H19'	107.7
C19'-C20'-H20D	109.5	C19'-C20'-H20E	109.5
H20D-C20'-H20E	109.5	C19'-C20'-H20F	109.5
H20D-C20'-H20F	109.5	H20E-C20'-H20F	109.5
C19'-C21'-H21D	109.5	C19'-C21'-H21E	109.5
H21D-C21'-H21E	109.5	C19'-C21'-H21F	109.5
H21D-C21'-H21F	109.5	H21E-C21'-H21F	109.5
C18'-C22'-C23'	112.0(5)	C18'-C22'-C24'	114.5(5)
C23'-C22'-C24'	109.6(5)	C18'-C22'-H22'	106.8
C23'-C22'-H22'	106.8	C24'-C22'-H22'	106.8
C22'-C23'-H23D	109.5	C22'-C23'-H23E	109.5
H23D-C23'-H23E	109.5	C22'-C23'-H23F	109.5
H23D-C23'-H23F	109.5	H23E-C23'-H23F	109.5
C22'-C24'-H24D	109.5	C22'-C24'-H24E	109.5
H24D-C24'-H24E	109.5	C22'-C24'-H24F	109.5
H24D-C24'-H24F	109.5	H24E-C24'-H24F	109.5
C38'-C37'-C42'	116.3(12)	C38'-C37'-P1'	117.2(8)
C42'-C37'-P1'	126.5(9)	C37'-C38'-C39'	120.5(12)
C37'-C38'-H38'	119.8	C39'-C38'-H38'	119.8
C38'-C39'-C40'	122.1(12)	C38'-C39'-H39'	119.0
C40'-C39'-H39'	119.0	C41'-C40'-C39'	117.7(12)
C41'-C40'-H40'	121.2	C39'-C40'-H40'	121.2
C42'-C41'-C40'	119.5(13)	C42'-C41'-H41'	120.3
C40'-C41'-H41'	120.3	C41'-C42'-C37'	123.8(13)
C41'-C42'-H42'	118.1	C37'-C42'-H42'	118.1
C48'-C43'-C44'	120.0(13)	C48'-C43'-P1'	121.1(9)
C44'-C43'-P1'	118.0(8)	C45'-C44'-C43'	121.0(12)
C45'-C44'-H44'	119.5	C43'-C44'-H44'	119.5
C46'-C45'-C44'	118.0(12)	C46'-C45'-H45'	121.0
C44'-C45'-H45'	121.0	C45'-C46'-C47'	120.3(12)
C45'-C46'-H46'	119.9	C47'-C46'-H46'	119.9
C48'-C47'-C46'	120.9(12)	C48'-C47'-H47'	119.5
C46'-C47'-H47'	119.5	C43'-C48'-C47'	118.7(12)
C43'-C48'-H48'	120.7	C47'-C48'-H48'	120.7
C50'-C49'-C54'	102.3(16)	C50'-C49'-P1'	128.9(12)
C54'-C49'-P1'	121.3(12)	C49'-C50'-C51'	128.4(14)
C49'-C50'-H50'	115.8	C51'-C50'-H50'	115.8

C50'-C51'-C52'	113.7(16)	C50'-C51'-H51'	123.1
C52'-C51'-H51'	123.1	C51'-C52'-C53'	120.1(17)
C51'-C52'-H52'	120.0	C53'-C52'-H52'	120.0
C53'-C54'-C49'	133.(2)	C53'-C54'-H54'	113.7
C49'-C54'-H54'	113.7	C54'-C53'-C52'	111.9(17)
C54'-C53'-H53'	124.0	C52'-C53'-H53'	124.0
C60-C55-C56	119.4(8)	C60-C55-H55	120.3
C56-C55-H55	120.3	C55-C56-C57	117.3(8)
C55-C56-H56	121.3	C57-C56-H56	121.3
C58-C57-C56	120.9(9)	C58-C57-H57	119.6
C56-C57-H57	119.6	C59-C58-C57	121.6(8)
C59-C58-H58	119.2	C57-C58-H58	119.2
C58-C59-C60	118.5(9)	C58-C59-H59	120.7
C60-C59-H59	120.7	C59-C60-C55	122.2(10)
C59-C60-H60	118.9	C55-C60-H60	118.9

Table 3.3.6 Anisotropic atomic displacement parameters (Å^2) for 13.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[\, h^2\, a^{*2}\, U_{11} + ... + 2\, h\, k\, a^*\, b^*\, U_{12}\,]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ag1	0.02832(16)	0.01976(15)	0.03803(18)	-0.00223(12)	0.02612(14)	-0.00548(12)
P1	0.0281(5)	0.0214(5)	0.0333(5)	-0.0020(4)	0.0240(5)	-0.0056(4)
O1'	0.0361(16)	0.0218(14)	0.0278(15)	0.0004(12)	0.0115(14)	0.0018(12)
O2	0.0308(15)	0.0382(17)	0.0308(16)	0.0007(13)	0.0199(13)	-0.0112(13)
O1	0.0259(15)	0.0297(15)	0.0366(17)	0.0041(12)	0.0193(14)	-0.0040(12)
N1	0.0229(16)	0.0211(16)	0.0301(17)	-0.0006(13)	0.0189(15)	-0.0036(13)
N2	0.0310(18)	0.0201(16)	0.0359(19)	-0.0016(14)	0.0257(17)	-0.0051(14)
C1	0.028(2)	0.0172(17)	0.029(2)	-0.0009(15)	0.0216(18)	0.0017(15)
C2	0.026(2)	0.0191(18)	0.039(2)	-0.0038(16)	0.024(2)	-0.0049(15)
C3	0.0250(19)	0.0178(18)	0.035(2)	-0.0017(16)	0.0221(18)	-0.0039(15)
C4	0.029(2)	0.0197(18)	0.035(2)	-0.0040(16)	0.0233(18)	-0.0066(16)
C5	0.0259(19)	0.0179(18)	0.036(2)	-0.0017(16)	0.0232(18)	-0.0030(15)
C6	0.0212(19)	0.0221(19)	0.036(2)	0.0041(16)	0.0190(18)	0.0009(15)
C7	0.026(2)	0.0163(18)	0.035(2)	0.0014(15)	0.0209(18)	-0.0020(15)
C8	0.0244(19)	0.0161(17)	0.035(2)	0.0018(15)	0.0232(18)	0.0014(15)
C9	0.025(2)	0.0215(19)	0.043(2)	0.0051(17)	0.0246(19)	0.0039(16)
C10	0.029(2)	0.0163(18)	0.042(2)	0.0065(16)	0.0260(19)	0.0023(15)
C11	0.0231(19)	0.0195(18)	0.031(2)	0.0048(15)	0.0203(17)	0.0025(15)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C12	0.024(3)	0.017(3)	0.040(3)	0	0.024(3)	0
C13	0.025(2)	0.0229(19)	0.032(2)	0.0002(16)	0.0183(18)	-0.0068(16)
C14	0.037(2)	0.025(2)	0.058(3)	0.006(2)	0.032(2)	0.0014(18)
C15	0.058(3)	0.028(2)	0.058(3)	0.012(2)	0.037(3)	0.003(2)
C16	0.056(3)	0.048(3)	0.048(3)	0.010(2)	0.035(3)	-0.010(2)
C17	0.048(3)	0.048(3)	0.046(3)	0.000(2)	0.037(2)	-0.010(2)
C18	0.030(2)	0.030(2)	0.038(2)	-0.0029(18)	0.023(2)	-0.0086(17)
C19	0.040(3)	0.028(2)	0.053(3)	0.004(2)	0.031(2)	0.0052(19)
C20	0.049(3)	0.042(3)	0.052(3)	0.001(2)	0.032(3)	0.008(2)
C21	0.055(3)	0.057(4)	0.065(4)	-0.006(3)	0.031(3)	0.012(3)
C22	0.046(3)	0.030(2)	0.045(3)	-0.005(2)	0.034(2)	-0.004(2)
C23	0.058(3)	0.044(3)	0.070(4)	-0.010(3)	0.048(3)	0.003(2)
C24	0.072(4)	0.042(3)	0.070(4)	-0.021(3)	0.050(3)	-0.022(3)
C25	0.026(2)	0.027(2)	0.028(2)	0.0017(16)	0.0190(18)	-0.0059(16)
C26	0.037(2)	0.030(2)	0.033(2)	-0.0018(17)	0.027(2)	-0.0106(18)
C27	0.037(2)	0.040(2)	0.032(2)	-0.0052(19)	0.021(2)	-0.016(2)
C28	0.027(2)	0.053(3)	0.033(2)	0.003(2)	0.017(2)	-0.009(2)
C29	0.034(2)	0.045(3)	0.045(3)	0.009(2)	0.026(2)	0.008(2)
C30	0.034(2)	0.033(2)	0.035(2)	0.0027(18)	0.024(2)	-0.0006(18)
C31	0.049(3)	0.033(2)	0.034(2)	-0.0068(19)	0.027(2)	-0.004(2)
C32	0.092(5)	0.033(3)	0.067(4)	-0.004(3)	0.055(4)	-0.006(3)
C33	0.075(4)	0.051(3)	0.065(4)	-0.002(3)	0.056(3)	0.004(3)
C34	0.047(3)	0.032(2)	0.044(3)	0.001(2)	0.028(2)	0.009(2)
C35	0.063(3)	0.037(3)	0.066(4)	-0.011(3)	0.043(3)	-0.009(2)
C36	0.087(4)	0.041(3)	0.073(4)	-0.003(3)	0.062(4)	0.008(3)
C37	0.032(2)	0.0203(19)	0.027(2)	0.0022(15)	0.0194(18)	-0.0029(16)
C38	0.036(2)	0.029(2)	0.044(3)	-0.0007(19)	0.026(2)	-0.0013(18)
C39	0.046(3)	0.031(2)	0.046(3)	-0.001(2)	0.030(2)	0.002(2)
C40	0.061(3)	0.020(2)	0.042(3)	0.0049(18)	0.032(2)	0.002(2)
C41	0.049(3)	0.025(2)	0.039(2)	0.0001(18)	0.026(2)	-0.012(2)
C42	0.038(2)	0.028(2)	0.035(2)	-0.0011(17)	0.026(2)	-0.0075(18)
C43	0.028(2)	0.039(2)	0.033(2)	-0.0096(18)	0.0228(19)	-0.0167(18)
C44	0.054(3)	0.041(3)	0.037(3)	-0.002(2)	0.027(2)	-0.013(2)
C45	0.078(4)	0.073(4)	0.040(3)	0.004(3)	0.030(3)	-0.017(3)
C46	0.064(4)	0.111(6)	0.034(3)	-0.017(3)	0.034(3)	-0.034(4)
C47	0.052(3)	0.084(4)	0.050(3)	-0.028(3)	0.040(3)	-0.026(3)
C48	0.041(3)	0.053(3)	0.047(3)	-0.013(2)	0.033(2)	-0.011(2)
C49	0.031(2)	0.026(2)	0.036(2)	-0.0049(17)	0.0251(19)	-0.0054(17)
C50	0.035(2)	0.032(2)	0.046(3)	0.0001(19)	0.030(2)	-0.0029(19)
C51	0.042(3)	0.038(3)	0.051(3)	0.013(2)	0.027(2)	0.003(2)
C52	0.036(2)	0.041(3)	0.053(3)	0.003(2)	0.028(2)	0.007(2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C53	0.032(2)	0.040(2)	0.041(2)	-0.003(2)	0.027(2)	-0.0011(19)
C54	0.035(2)	0.033(2)	0.040(2)	-0.0018(19)	0.028(2)	-0.0046(18)
Ag1'	0.0552(8)	0.0124(3)	0.0385(7)	0.0011(2)	0.0121(7)	-0.0012(3)
P1'	0.0566(19)	0.0124(11)	0.079(2)	-0.0018(12)	-0.0035(16)	-0.0017(12)
N2'	0.0389(19)	0.0145(15)	0.0279(18)	-0.0027(13)	0.0204(16)	-0.0029(14)
C1'	0.045(4)	0.015(3)	0.037(3)	0	0.027(3)	0
C2'	0.033(2)	0.0159(18)	0.032(2)	-0.0014(16)	0.022(2)	-0.0012(16)
C3'	0.028(3)	0.014(2)	0.027(3)	0	0.018(2)	0
C5'	0.026(3)	0.015(2)	0.029(3)	0	0.020(2)	0
C6'	0.0189(18)	0.0202(18)	0.029(2)	-0.0015(15)	0.0154(17)	-0.0008(14)
C7'	0.0180(18)	0.0203(18)	0.031(2)	0.0029(15)	0.0163(17)	0.0031(14)
C8'	0.023(3)	0.017(3)	0.023(3)	0	0.015(2)	0
C11'	0.023(3)	0.014(2)	0.031(3)	0	0.018(2)	0
C12'	0.0220(19)	0.0168(17)	0.031(2)	-0.0006(15)	0.0187(17)	0.0001(14)
C13'	0.047(3)	0.019(2)	0.043(3)	-0.0050(18)	0.026(2)	-0.0078(19)
C14'	0.055(3)	0.025(2)	0.041(3)	-0.0088(19)	0.027(2)	-0.007(2)
C15'	0.076(4)	0.037(3)	0.052(3)	-0.017(2)	0.037(3)	-0.011(3)
C16'	0.069(4)	0.032(3)	0.058(3)	-0.015(2)	0.029(3)	-0.023(3)
C17'	0.056(3)	0.039(3)	0.065(4)	0.001(3)	0.030(3)	-0.018(3)
C18'	0.056(3)	0.027(2)	0.055(3)	0.005(2)	0.033(3)	-0.006(2)
C19'	0.068(4)	0.040(3)	0.049(3)	-0.014(2)	0.041(3)	-0.005(2)
C20'	0.088(4)	0.046(3)	0.050(3)	-0.013(3)	0.043(3)	-0.019(3)
C21'	0.104(5)	0.063(4)	0.093(5)	-0.001(4)	0.080(5)	0.012(4)
C22'	0.047(3)	0.047(3)	0.058(3)	0.010(2)	0.033(3)	-0.005(2)
C23'	0.059(4)	0.075(4)	0.083(4)	0.012(4)	0.053(4)	0.009(3)
C24'	0.134(7)	0.091(6)	0.123(7)	-0.004(5)	0.105(6)	-0.039(5)
C37'	0.041(4)	0.023(3)	0.112(6)	0.004(4)	0.030(4)	0.011(3)
C38'	0.044(4)	0.043(4)	0.108(6)	-0.001(4)	0.039(4)	0.013(3)
C39'	0.047(4)	0.051(4)	0.112(6)	0.007(4)	0.042(4)	0.010(3)
C40'	0.051(4)	0.047(4)	0.116(6)	0.018(4)	0.047(4)	0.005(3)
C41'	0.046(4)	0.040(4)	0.121(6)	0.026(4)	0.041(4)	0.005(3)
C42'	0.046(4)	0.028(4)	0.120(6)	0.017(4)	0.027(4)	0.009(3)
C43'	0.093(6)	0.029(4)	0.075(5)	-0.003(4)	0.043(5)	-0.010(4)
C44'	0.099(6)	0.042(4)	0.072(5)	-0.006(4)	0.051(5)	-0.010(4)
C45'	0.101(6)	0.052(4)	0.075(5)	-0.004(4)	0.059(4)	-0.012(4)
C46'	0.095(6)	0.047(4)	0.073(5)	0.004(4)	0.055(4)	-0.017(4)
C47'	0.094(6)	0.037(4)	0.078(5)	0.001(4)	0.044(5)	-0.013(4)
C48'	0.089(6)	0.031(4)	0.077(5)	-0.002(4)	0.041(5)	-0.012(4)
C49'	0.110(7)	0.040(5)	0.108(7)	0.014(5)	-0.025(6)	0.000(5)
C50'	0.105(7)	0.029(4)	0.102(7)	0.015(5)	-0.017(6)	0.001(5)
C51'	0.108(7)	0.040(5)	0.108(7)	0.016(5)	-0.018(6)	0.000(5)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C52'	0.117(7)	0.054(5)	0.115(7)	0.018(5)	-0.024(6)	0.001(5)
C54'	0.116(7)	0.055(5)	0.113(7)	0.018(5)	-0.026(6)	0.001(5)
C53'	0.120(7)	0.063(5)	0.118(7)	0.022(5)	-0.024(6)	-0.001(5)
C55	0.088(6)	0.164(10)	0.048(4)	-0.019(5)	0.040(4)	-0.057(6)
C56	0.081(6)	0.159(10)	0.058(5)	-0.042(6)	0.030(4)	0.001(6)
C57	0.079(6)	0.087(6)	0.076(5)	-0.004(4)	0.014(5)	-0.008(5)
C58	0.063(5)	0.129(8)	0.058(4)	0.010(5)	0.033(4)	-0.025(5)
C59	0.069(5)	0.156(10)	0.072(5)	-0.013(6)	0.033(4)	0.004(6)
C60	0.113(7)	0.105(7)	0.068(5)	0.011(5)	0.042(5)	0.013(6)

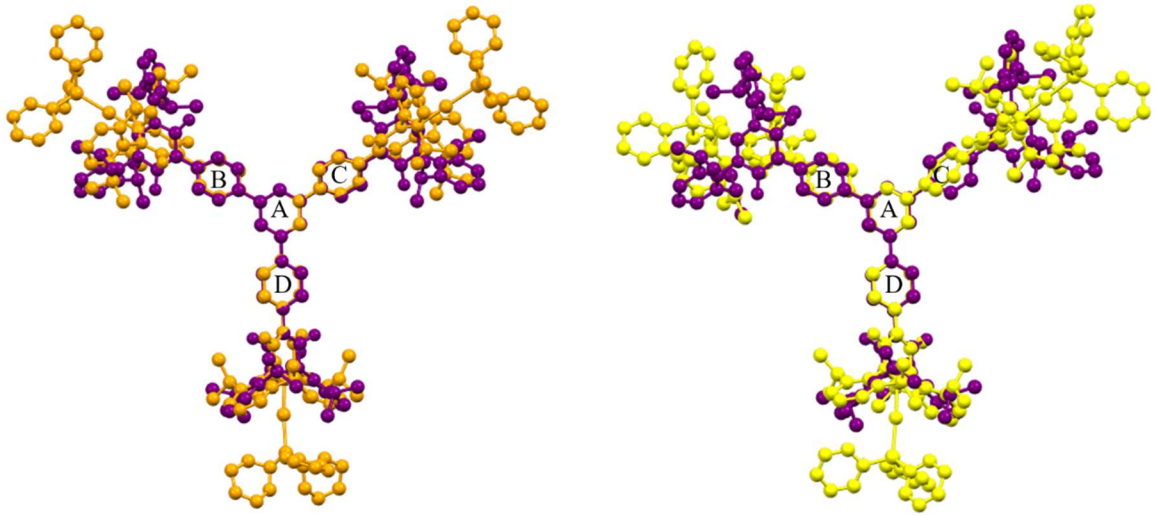
Table 3.3.7 Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 13.

	x/a	y/b	z/c	U(eq)
H6	0.3226	0.1578	0.6673	0.03
H7	0.3783	0.2126	0.6724	0.028
H9	0.4701	0.0932	0.8170	0.032
H10	0.4142	0.0393	0.8130	0.032
H12	0.5000	0.1183	0.7500	0.029
H15	0.3342	-0.1765	0.9192	0.055
H16	0.3071	-0.1349	0.9790	0.057
H17	0.2833	-0.0338	0.9608	0.05
H19	0.3458	-0.0949	0.7972	0.046
H20A	0.3118	-0.1841	0.7283	0.07
H20B	0.2920	-0.2007	0.7717	0.07
H20C	0.2752	-0.1404	0.7238	0.07
H21A	0.3888	-0.1870	0.8337	0.092
H21B	0.4036	-0.1452	0.8999	0.092
H21C	0.3725	-0.2040	0.8818	0.092
H22	0.2796	0.0704	0.8373	0.044
H23A	0.2208	0.1023	0.8434	0.076
H23B	0.2095	0.0371	0.8048	0.076
H23C	0.2255	0.0404	0.8842	0.076
H24A	0.3384	0.0850	0.9564	0.085
H24B	0.2988	0.1328	0.9320	0.085
H24C	0.3045	0.0737	0.9773	0.085
H27	0.1335	-0.0557	0.4740	0.043
H28	0.0877	0.0259	0.4574	0.046
H29	0.1151	0.1071	0.5364	0.047
H31	0.2473	-0.0740	0.6209	0.045
H32A	0.2196	-0.1711	0.5671	0.088
H32B	0.1920	-0.1459	0.5955	0.088

	x/a	y/b	z/c	U(eq)
H32C	0.1712	-0.1420	0.5140	0.088
H33A	0.2529	-0.1000	0.5280	0.083
H33B	0.2066	-0.0661	0.4738	0.083
H33C	0.2489	-0.0270	0.5322	0.083
H34	0.2240	0.1137	0.6984	0.049
H35A	0.2169	0.2166	0.6596	0.078
H35B	0.2280	0.1713	0.6178	0.078
H35C	0.1783	0.1959	0.5818	0.078
H36A	0.1759	0.1796	0.7063	0.087
H36B	0.1347	0.1580	0.6307	0.087
H36C	0.1586	0.1101	0.6941	0.087
H38	0.2064	-0.1996	0.7082	0.041
H39	0.2027	-0.3017	0.6732	0.048
H40	0.1385	-0.3595	0.6312	0.047
H41	0.0778	-0.3155	0.6227	0.044
H42	0.0812	-0.2137	0.6579	0.037
H44	0.1865	-0.2140	0.8246	0.052
H45	0.2080	-0.2180	0.9399	0.079
H46	0.2003	-0.1318	0.9909	0.08
H47	0.1649	-0.0447	0.9238	0.067
H48	0.1438	-0.0392	0.8096	0.051
H50	0.1184	-0.0191	0.6227	0.041
H51	0.0541	0.0402	0.5632	0.052
H52	-0.0051	0.0165	0.5706	0.05
H53	-0.0001	-0.0676	0.6357	0.041
H54	0.0651	-0.1255	0.6989	0.038
H6'	0.5671	0.4772	0.8205	0.026
H7'	0.5671	0.3705	0.8211	0.026
H12'	0.4431	0.2792	0.7446	0.025
H15'	0.5890	0.7522	1.0098	0.066
H16'	0.6475	0.7900	1.0098	0.069
H17'	0.6565	0.7657	0.9232	0.068
H19'	0.5037	0.6510	0.8784	0.058
H20D	0.5114	0.6302	0.9838	0.09
H20E	0.5553	0.6103	0.9896	0.09
H20F	0.5549	0.6728	1.0254	0.09
H21D	0.4641	0.7163	0.9056	0.11
H21E	0.5050	0.7635	0.9432	0.11
H21F	0.4773	0.7525	0.8608	0.11
H22'	0.5760	0.6880	0.7651	0.059
H23D	0.6308	0.6166	0.7870	0.099

	x/a	y/b	z/c	U(eq)
H23E	0.6568	0.6283	0.8691	0.099
H23F	0.6084	0.5975	0.8259	0.099
H24D	0.6350	0.7209	0.7596	0.148
H24E	0.6170	0.7767	0.7814	0.148
H24F	0.6625	0.7428	0.8393	0.148
H38'	0.5689	0.8875	0.9388	0.081
H39'	0.5675	0.9051	1.0337	0.087
H40'	0.5024	0.9325	1.0210	0.086
H41'	0.4401	0.9540	0.9094	0.088
H42'	0.4406	0.9306	0.8157	0.092
H44'	0.5872	0.8574	0.7978	0.085
H45'	0.6523	0.9079	0.8237	0.086
H46'	0.6721	1.0028	0.8852	0.081
H47'	0.6186	1.0571	0.8905	0.087
H48'	0.5516	1.0084	0.8578	0.084
H50'	0.4840	1.0176	0.7392	0.147
H51'	0.4282	1.0575	0.6276	0.158
H52'	0.3573	1.0211	0.5978	0.178
H54'	0.4192	0.8745	0.7098	0.177
H53'	0.3536	0.9116	0.6107	0.185
H55	0.3946	0.1800	0.5695	0.12
H56	0.3936	0.2881	0.5706	0.126
H57	0.4481	0.3408	0.5669	0.119
H58	0.4944	0.2885	0.5494	0.101
H59	0.4932	0.1834	0.5438	0.124
H60	0.4435	0.1301	0.5541	0.122

3.4 X-Ray structures overlays of compounds 11-13



The structure of zwitterion **11** (purple) was compared using overlays with the Ag complex (left, orange) and the Au complex (right, yellow). Upon overlaying the C11-C12 (A) rings of the molecules' cores there was very close agreement in the orientation of the C5-C10 (B, C, and D) rings of the Ag complex. Extending further, one of the N/C1-C4 rings of **11** exhibited good overlap with the same ring in the Ag complex, while the other two N/C1-C4 rings were approximately normal to their counterparts. The Au complex showed greater deviation from the ZI, even in the core region of the molecule. Again, there was good overlap for ring D, but the other two C5-C10 rings were inclined at 13.18° (ring B) and 85.18° (ring C) for the Au complex compared to **11**.