Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

for

A stable Janus bis(*malo*NHC) and its zwitterionic coinage metal complexes

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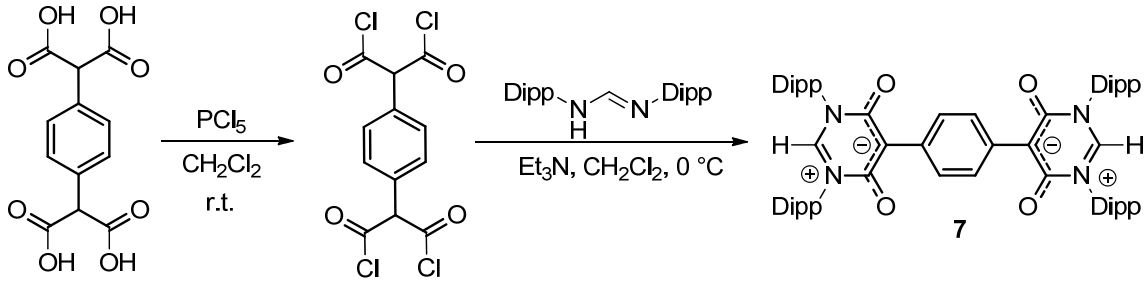
General Considerations: All reactions, unless otherwise noted, were performed using standard Schlenk techniques under an atmosphere of argon or in a nitrogen-filled gloxebox. Glassware wad dried at 100 °C in an oven for at least 12 hours. THF was distilled from sodium/benzophenone. Dry dichloromethane was purchased from Aldrich and used as received. *N,N'*-bis(2,6-di-*iso*-propylphenyl)formamidine[1] and 2.2'-(1,4-phenylene)dimalonic acid[2] were prepared following known methods. Column chromatography was performed using the solvent systems indicated on silica gel (63-200 μm) or basic alumina (Act.1 50-200 μm). ^{1}H, ^{13}C NMR, and ^{31}P spectra were recorded using a Bruker DPX 300 MHz spectrometer. Chemical shifts were reported in ppm and are referenced to internal $SiMe_4$ (^{1}H and ^{13}C) or external H_3PO_4 (^{31}P). Solid state infrared spectra of **7**, **8**, and **10**-**13** were recorded on a Perkin Elmer Frontier 100 spectrometer. FT-IR spectra of the carbenes **5** and **9** were recorded using a Thermo Scientific Nicolet iS 5 FT-IR system and analyzed in the solid state (KBr matrix). Elemental analyses were performed at Atlantic Microlab (Norcross, GA).

1. Synthesis and characterization of compounds

1.1 Synthesis of 7

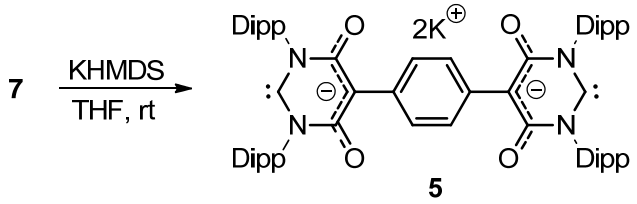


A mixture of 2.2'-(1,4-phenylene)dimalonic acid (2.14 g, 7.5 mmol) and PCl_5 (7.1 g g, 34 mmol) in anhydrous dichloromethane (50 mL) was stirred at room temperature for 2 h under inert atmosphere. The reaction mixture was then concentrated to dryness under reduced pressure. To the resulting crude 2.2'-(1,4-phenylenedimalonyl chloride) were added *N,N'*-bis(2,6-di-*iso*-propylphenyl)formamidine (6.87 g, 18.9 mmol) and 50 mL anhydrous dichloromethane. The reaction mixture was stirred at 0 °C for 25 min under argon. Et_3N (4.73 mL, 33.8 mmol) was gradually added over the course of 10 min. The reaction mixture was stirred for 3 h and the volatiles were evaporated. The brown/yellow residue was triturated with water (75 mL), filtered, dried and purified by column chromatography (Al_2O_3 basic, CH_2Cl_2) to afford the title compound as an orange solid (5.3 g, 74% yield); m.p. > 400 °C. Crystals suitable for X-ray analysis were obtained via slow evaporation of a saturated dichloromethane solution of **7** at room temperature. ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 8.11 (s, 2H, NC*H*N), 8.06 (s, 4H, Ar-C*H*), 7.43 (t, ^{3}J =7.8 Hz, 4H, Ar-C*H)*, 7.26 (d, ^{3}J = 7.8 Hz, 8H, Ar-C*H*), 2.89 (sept. ^{3}J = 6.6 Hz, 8H, C*H*$(CH_3)_2$), 1.29 (d, ^{3}J = 6.4 Hz, 24H, CH_3), 1.20 (d, ^{3}J = 6.6 Hz, 24H, CH_3). ^{13}C NMR ($CDCl_3$, 75.5 MHz, ppm): δ 158.48 (*C*-O), 147.09 (NCHN), 145.99, 132.39, 131.66, 130.93, 129.10, 124.47, 99.09 (*C*-CO),

[1] K. M. Kuhn and R. H. Grubbs, *Org. Lett.* 2008, ***10***, 2075-2077.
[2] T. Metz, C. Plueg 2,4-dioxopyrimidine-based mezoionic pigments, *US Pat.*, 8,133,997, 2012.

29.31 (*C*H(CH$_3$)$_2$), 24.29 (*C*H$_3$). FT-IR (solid ATR): 3660, 3515, 2962, 2929, 2870, 1667 (CO), 1599, 1578, 1513, 1463, 1321, 1256, 1217, 1149, 1060, 933, 847, 788, 768 cm^{-1}. Anal. Calcd for $C_{62}H_{74}O_4N_4$: C, 79.28; H, 7.94; N, 5.96. Found: C, 78.90; H, 7.83; N, 5.86.

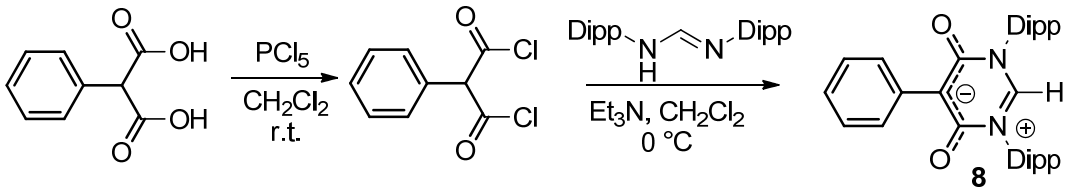
1.2 Synthesis of 5



5

To a vial containing potassium bis(trimethylsilyl)amide (KHMDS) (79 mg, 2.2 equiv.) and **7** (150 mg, 0.16 mmol), THF was added and the resulting solution was left stirring for 30 min at room temperature. The volatiles were removed *in vacuo* and the resultant solid was washed with hexanes and dried to afford the title compound as an off-white solid (quantitative yield). ^{1}H NMR (d_8-THF, 300 MHz, ppm): δ 7.38 (s, 4H, Ar-C*H*), 7.07-7.18 (m, 12H Ar-C*H*), 3.18 (sept, ^3J =6.8 Hz, 8H, C*H*(CH$_3$)$_2$), 1.18 (d, ^3J = 6.8 Hz, 24H, C*H*$_3$), 1.14 (d, ^3J=6.8 Hz, 24H, C*H*$_3$). ^{13}C NMR (d_8-THF, 75.5 MHz, ppm): δ 249.88 (N*C*N), 163.31 (*C*-CO), 146.29, 142.81, 137.05, 132.25, 127.33, 123.19, 97.37 (*C*-CO), 29.13 (*C*H(CH$_3$)$_2$), 24.36 (*C*H$_3$), 24.22 (*C*H$_3$). FT-IR (KBr pellet): 2962, 2868, 1576 (CO), 1468, 1405, 1384, 1361, 1338, 1254, 1100, 1100, 1057, 935, 824, 771 cm^{-1}.

1.3 Synthesis of 8

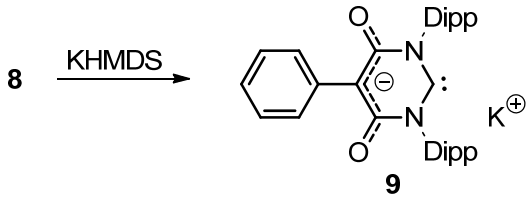


8

A mixture of phenylmalonic acid (1.5 g, 8.3 mmol) and PCl_5 (4.3 g, 20.6 mmol) in anhydrous dichloromethane (20 mL) was stirred at room temperature for 2 h under inert atmosphere. The reaction mixture was then concentrated to dryness under reduced pressure. To the resulting crude phenylenedimalonyl chloride were added *N,N'*-bis(2,6-di-*iso*-propylphenyl)formamidine (4.55 g, 12.4 mmol) and 25 mL anhydrous dichloromethane. The reaction mixture was stirred at 0 °C for 25 min under argon. Et_3N (2.32 mL, 16.6 equiv.) was gradually added over the course of 10 min. The resultant mixture was stirred at 0 °C for 3 h, followed by removal of the volatiles *in vacuo.* The residue was triturated with 25 mL of H_2O, filtered, washed with an additional 50 mL H_2O and dried under vacuum. The crude solid was purified by column chromatography (SiO_2, MeOH/CH_2Cl_2: 0.25/30) to afford the pure **8** as a yellow solid (3.5 g, 83.1 % yield); m.p. > 381-

383 °C. ^{1}H NMR (d_8-THF, 300 MHz, ppm) δ 9.33 (s, 1H, NC*H*N), 8.09 (dd, ^{3}J = 8.4 Hz, ^{3}J= 1.3 Hz, 2H, Ar-C*H*), 7.46 (t, ^{3}J = 8.4 Hz, 2H, Ar-C*H*), 7.34 (d, ^{3}J = 8.1 Hz, 4H, Ar-C*H*), 7.18 (t, ^{3}J = 7.5 Hz, 2H, Ar-C*H*), 7.02 (t, ^{3}J = 7.5 Hz, 1H, Ar-C*H*), 2.95 (sept, ^{3}J = 6.9 Hz, 4H, C*H*(CH_3)$_2$),), 1.28 (d, ^{3}J = 6.9 Hz, 12H, C*H*$_3$), 1.24 (d, ^{3}J = 6.9 Hz, 12H, C*H*$_3$). ^{13}C NMR (d_8-THF, 75.5 MHz, ppm): δ 159.29 (NCHN), 151.72, 147.18, 136.53, 134.25, 131.30, 131.20, 127.35, 125.61, 124.98, 97.52 (C-CO), 30.23 (*C*H(CH_3)$_2$), 24.57 (*C*H$_3$), 24.40 (*C*H$_3$). FT-IR (solid ATR): 3039, 2951, 2931, 2871, 1667, 1595, 1443, 1326, 1250, 1218, 1138, 1057, 802, 778 cm^{-1}. Anal. Calcd for $C_{34}H_{40}N_2O_2$ (508.69): C, 80.27; H, 7.92; N, 5.50. Found: C, 80.33; H, 7.81; N, 5.56.

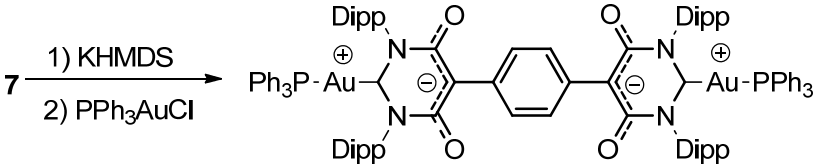
1.4 NMR tube reaction for the generation of 9



9

In a dried NMR tube, zwitterion **8** (35 mg, 0.06 mmol) and KHMDS (35 mg, 0.18 mmol) were suspended in d_8-THF under nitrogen. The NMR tube was sealed. The resulting solution was subjected to ^{1}H NMR and ^{13}C NMR measurements, which indicated the formation of the carbene **9** within 5 min. This solution did not show major decomposition overnight. ^{1}H NMR (d_8-THF, 300 MHz, ppm): δ 7.55 (d, ^{3}J = 7.5 Hz, 2H, Ar-C*H*), 7.18-7.11 (m, 8H), 6.96 (t, ^{3}J = 6.7 Hz, 1H) 3.16 (sept, ^{3}J = 6.5 Hz, 4H, C*H*(CH_3)$_2$), 1.17 (d, ^{3}J = 6.8 Hz, 12H, C*H*$_3$), 1.15 (d, ^{3}J = 6.8 Hz, 12H, C*H*$_3$). ^{13}C (d_8-THF, 75.5 MHz, ppm): δ 249.37 (N*C*N), 163.12, 146.50, 142.92, 139.73, 131.99, 128.02, 127.82, 125.07, 123.64, 96.94 (*C*-CO), 29.29 (*C*H(CH_3)$_2$), 24.51 (*C*H$_3$), 24.47 (*C*H$_3$). FT-IR (KBr pellet): 2938, 2870, 1580 (CO), 1500, 1468, 1441, 1411, 1384, 1362 1235, 1095, 882, 818, 788, 752, 652, 566 cm^{-1}.

1.5 Synthesis of 10

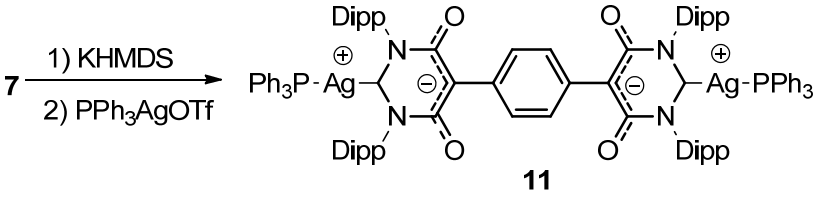


10

A mixture of **7** (200 mg, 0.21 mmol) and KHMDS (127 mg, 3 equiv) was stirred in THF (12 mL) at ambient temperature for 30 min. AuCl(SMe_2) (207 mg, 0.7 mmol) and PPh_3 (185 mg, 0.7 mmol) were placed in a separate flask and stirred in THF (5 mL) to ensure a precoordination of PPh_3 on the gold center. The last solution was added slowly to the first one. The reaction mixture became dark orange within 30 minutes and it was stirred for 12 hours. THF was removed *in vacuo* and the residue was dissolved in chloroform and precipitated with diethyl ether. After filtration, the

resulting solid was purified by column chromatography (SiO_2, CH_2Cl_2/MeOH: 30/1) to afford the title compound as an orange solid (0.302 g, 76.5 % yield); m.p. > 400 °C. Crystals of **10** were obtained via slow evaporation of a chloroform solution of **10** at room temperature under ambient conditions. ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 8.15 (s, 4H, Ar-C*H*), 7.48-7.43 (m, 6H, C*H*$_{PPh3}$), 7.29-7.50 (m, 16H, C*H*$_{PPh3}$ & Ar-C*H*), 7.18 (d, ^3J = 7.5 Hz, 8H, Ar-C*H*), 6.83-6.90 (m, 12H, C*H*$_{PPh3}$), 3.04 (sept. ^3J = 6.9 Hz, 8H, C*H*$(CH_3)_2$), 1.24 (d, ^3J = 6.9 Hz, 24H, C*H*$_3$), 1.07 (d, ^3J = 6.9 Hz, 24H, C*H*$_3$). ^{13}C NMR ($C_2D_2Cl_4$, 75.5 MHz): δ 199.8 (d, J =120.1 Hz, N*C*N), 159.82 (d, J_{CP} = 3.76 Hz), 145.22, 132.72 (d, J_{CP} =13.7), 131.21, 130.84, 128.1 (d, J_{CP} = 10.6 Hz), 128.09, 127.91, 127.48, 126.71, 122.79, 96.86 (*C*-CO), 27.75 (*C*H$(CH_3)_2$), 23.24 (*C*H$_3$), 23.04 (*C*H$_3$). ^{31}P NMR ($CDCl_3$, 121.49 MHz, ppm): 39.39. FT-IR (solid ATR): 3068, 2958, 2929, 2865, 1611 (C=O), 1434, 1385, 1327, 1272, 1098, 1054, 993, 848, 802 cm^{-1}. Anal. Calcd for $C_{99}H_{104}N_4O_4Au_2P_2Cl_2$ ($C_{98}H_{102}N_4O_4Au_2P_2$ + 1 CH_2Cl_2): C, 61.26; H, 5.40; N, 2.88. Found: C, 61.40; H, 5.60; N, 2.87.

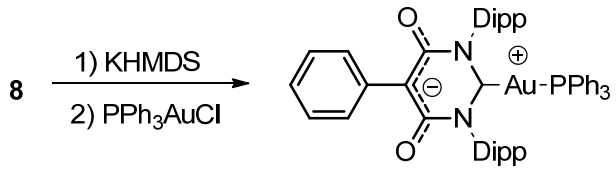
1.6 Synthesis of 11



A mixture of **7** (151 mg, 0.16 mmol) and KHMDS (96 mg, 3 equiv) was stirred in THF (12 mL) at ambient temperature for 30 min. AgOTf (103 mg, 0.40 mmol) and PPh_3 (105 mg, 0.40 mmol) were placed in a separate flask and stirred in THF (5 mL) for 30 min to ensure a precoordination of PPh_3 on the silver center. After 30 min, this solution was added slowly to the first solution. The resultant suspension was stirred overnight. THF was removed *in vacuo* and the residue was dissolved in chloroform (40 mL) and filtered through Celite. A portion of hot chloroform (20 mL) was used to elute any residual product. The combined chloroform solutions were concentrated to approximately 10 mL. The product was precipitated with diethyl ether (75 mL). The fine yellow solid was collected by filtration and washed with an additional portion of diethyl ether (5 mL) to afford the pure product as a bright yellow microcrystalline solid (247 mg, 91.6 % yield); m.p. > 400 °C. Crystals of **11** were obtained via slow evaporation of a 1:1 chloroform/dichloromethane solution of **11** at room temperature under ambient conditions. ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 8.06 (s, 4H, Ar-C*H*), 7.43-7.47 (m, 6H, C*H*$_{PPh3}$), 7.29-7.35 (m, 16H, C*H*$_{PPh3}$ & Ar-C*H*), 7.18 (d, ^3J = 7.7, 8H, Ar-C*H*), 6.77-6.84 (m, 12H, C*H*$_{PPh3}$), 3.09 (sept, ^3J = 6.8 Hz, 8H, C*H*$(CH_3)_2$), 1.25 (d, ^3J = 6.7 Hz, 24H, C*H*$_3$), 1.05 (d, ^3J = 6.8 Hz, 24H, C*H*$_3$). ^{13}C NMR ($C_2D_2Cl_4$, 75.5 MHz, ppm): δ C2 not detected, 159.97 (d, J = 5.7 Hz), 145.02, 138.99, 132.46 (d, J = 15.5 Hz), 131.21, 130.57, 128.28 (d, J = 11.0 Hz), 127.99, 127.62, 127.06, 122.97, 96.85 (d, J = 4.2 Hz, *C*-CO), 27.65 (*C*H$(CH_3)_2$), 23.45 (*C*H$_3$), 23.17 (*C*H$_3$). ^{31}P NMR ($CDCl_3$, 121.49 MHz, ppm): δ 18.1 (d + d, J(^{31}P - ^{109}Ag) = 534.7 Hz, J(^{31}P - ^{107}Ag) = 463.3 Hz). FT-IR (solid ATR): 3065, 2961, 2923, 2865, 1603 (CO), 1434, 1379, 1324, 1278, 1098, 1057, 997, 837, 799 cm^{-1}. Anal. Calcd for

$C_{100}H_{104}N_4O_4Ag_2P_2$ Cl_6 ($C_{98}H_{102}N_4O_4Ag_2P_2$ + 2 $CHCl_3$): C, 62.47; H, 5.47; N, 2.92. Found: C, 62.07; H, 5.46; N, 2.97.

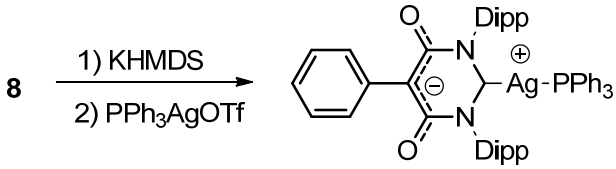
1.7 Synthesis of 12



12

A mixture of **8** (60 mg, 0.11 mmol) and KHMDS (70 mg, 0.35 mmol) was stirred in THF (6 mL) at ambient temperature for 30 min. $AuCl(SMe_2)$ (76 mg, 0.25 mmol) and PPh_3 (68 mg, 0.25 mmol) were placed in a separate flask and stirred in THF (5 mL) to ensure a precoordination of PPh_3 on the gold center. The last solution was added slowly to the first one. The reaction mixture was stirred for 12 hours. The reaction mixture was filtered through Celite. The yellow solution was concentrated to dryness. The residue was taken up in chloroform and precipitated with diethyl ether. After filtration, the resulting solid was purified by column chromatography (SiO_2, CH_2Cl_2/MeOH: 30/0.25) to afford the title compound as an yellow solid (60 mg, 52.6 % yield); m.p. = 355-357 °C. ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 8.15 (dd, 2H, J = 1.3, J = 8.3 Hz, Ar-C*H*), 7.45-7.52 (m, 3H, CH_{PPh3}), 7.31-7.42 (m, 8H, CH_{PPh3} & Ar-C*H*), 7.23 (d, ^3J = 7.5 Hz, 4H, Ar-C*H*), 7.21-7.25 (m, 2H, CH_{PPh3}), 7.08 (t, ^3J = 7.26, 1H, Ar-C*H*), 6.84-6.91 (m, 6H, CH_{PPh3}), 3.05 (sept. ^3J = 6.7 Hz, 4H, C*H*(CH_3)$_2$), 1.28 (d, ^3J = 6.7 Hz, 12 H, CH_3), 1.1 (d, ^3J = 6.7 Hz, 12 H, CH_3). ^{13}C NMR ($CDCl_3$, 75.47 MHz, ppm): δ 201.11 (d, J =119.4 Hz, N*C*N), 160.9 (d, J_{CP} = 3.87 Hz), 146.69, 138.33, 136.05, 134.00 (d, J_{CP} = 13.88 Hz), 131.96 (d, J_{CP} = 2.25 Hz), 130.40, 129.24 (d, J_{CP} = 11.48 Hz), 129.21, 128.40 (d, J_{CP} = 56.93 Hz), 127.18, 124.83, 123.86, 97.19 (*C*-CO), 28.97 (*C*H(CH_3)$_2$), 24.56 (*C*H_3), 24.25 (*C*H_3). ^{31}P NMR ($CDCl_3$, 121.49 MHz, ppm): δ 39.24. FT-IR (solid ATR): 3048, 2964, 2866, 1619 (C=O), 1439, 1360, 1329, 1227, 1102, 1056, 850, 777 cm^{-1}. Anal. Calcd for $C_{52}H_{54}N_2O_2AuP$ (966.94): C, 64.59; H, 5.62; N, 2.89. Found: C, 64.56; H, 5.70; N, 3.04.

1.8 Synthesis of 13



13

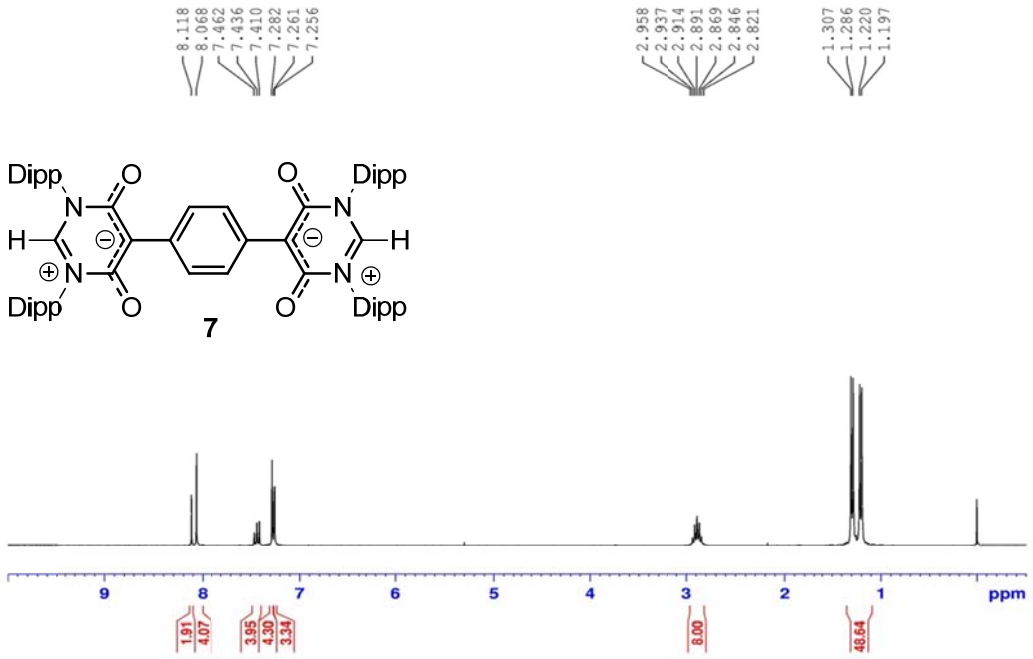
A mixture of **8** (60 mg, 0.11 mmol) and KHMDS (70 mg, 0.35 mmol) was stirred in THF (6 mL) at ambient temperature for 30 min. AgOTf (33 mg, 0.13 mmol) and PPh_3 (34 mg, 0.13 mmol) were placed in a separate flask and stirred in THF (3 mL) for 30 min to ensure a precoordination of PPh_3 on the silver center. After 30 min, this solution was added slowly to the first solution. Upon

addition, a black precipitate began to form immediately. The resultant suspension was stirred for 3 hours. THF was removed *in vacuo* and the residue was taken up in chloroform (15 mL) and filtered through Celite. The filtrate was concentrated to about 5 mL and precipitated with diethyl ether (25 mL). After filtration, the solid was further purified by column chromatography (SiO_2, CH_2Cl_2/MeOH: 30/0.25) to afford the title compound as a pale yellow solid (0.075 g, 72.4 % yield); m.p. > 296-297 °C. ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 8.17 (dd, 2H, J = 1.2, J = 8.4 Hz, Ar-C*H*), 7.46-7.51 (m, 3H, CH_{PPh3}), 7.30-7.40 (m, 8H, CH_{PPh3} & Ar-C*H*), 7.23 (d, ^3J = 7.7 Hz, 4H, Ar-C*H*), 7.21-7.23 (m, 2H, CH_{PPh3}), 7.06 (t, ^3J = 7.31, 1H, Ar-C*H*), 6.80-6.86 (m, 6H, CH_{PPh3}), 3.11 (sept. ^3J = 6.8 Hz, 4H, C*H*$(CH_3)_2$), 1.3 (d, ^3J = 6.8 Hz, 12 H, CH_3), 1.09 (d, ^3J = 6.8 Hz, 12 H, CH_3). ^{13}C NMR ($CDCl_3$, 75.5 MHz, ppm): δ 200.5 (dd + dd, J(^{13}C - ^{109}Ag) = 233.24 Hz, J(^{13}C - ^{107}Ag) = 199.56 Hz), J_{C-P} = 64.6 Hz, N*C*N), 161.07 (d, J = 6.64 Hz), 146.47, 140.34, 136.18, 133.73 (dd, J_{C-Ag} = 2.43 Hz, J_{C-P} = 16.11 Hz), 131.7 (d, J = 1.72 Hz) , 130.52, 129.43 (d, J = 10.95 Hz), 129.06, 128.58 (dd, J_{C-Ag} = 3.3 Hz, J_{C-P} = 42.0 Hz), 127.17, 124.68, 124.03, 97.17 (*C*-CO), 28.88 (*C*H$(CH_3)_2$), 24.64 (*C*H_3), 24.50 (*C*H_3). ^{31}P{^{1}H} NMR ($CDCl_3$, 121.49 MHz, ppm): δ 18.17 (d + d, J(^{31}P - ^{109}Ag) = 537.2 Hz, J(^{31}P - ^{107}Ag) = 465.4 Hz). FT-IR (solid ATR): 2954, 2925, 2858, 1611, 1479, 1434, 1380, 1329, 1278, 1155, 1099, 844 cm^{-1}. Anal. Calcd for $C_{52}H_{54}N_2O_2AgP$ (877.84): C, 71.14; H, 6.20; N, 3.19. Found: C, 70.97; H, 6.20; N, 3.38.

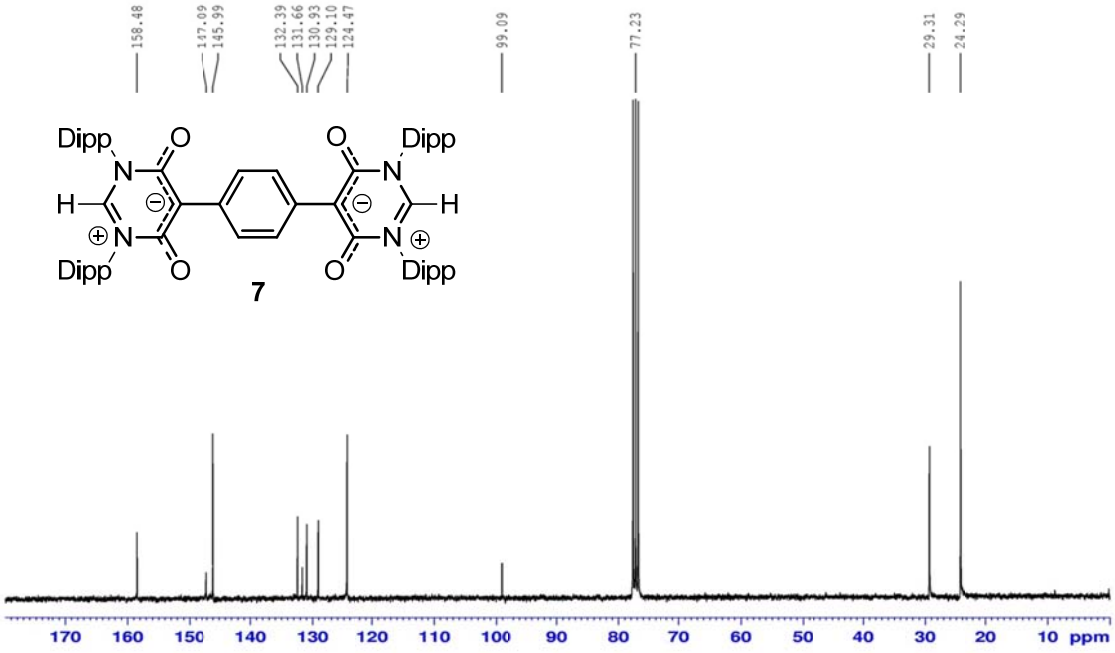
2. NMR Spectra

2.1 ^{1}H and ^{13}C NMR spectra of **7**

^{1}H NMR of **7** in $CDCl_3$

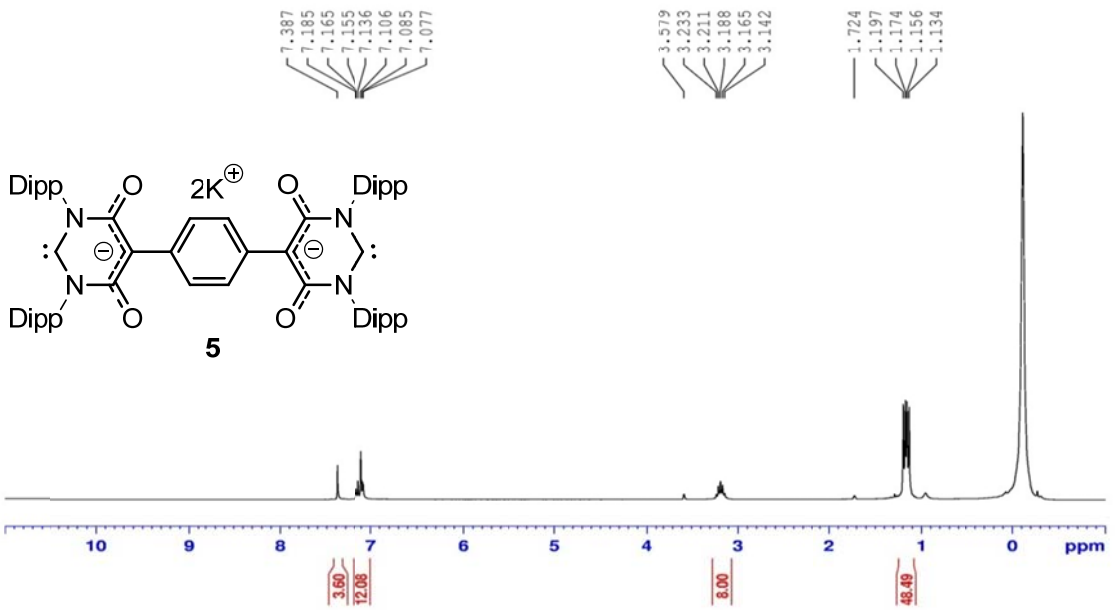


^{13}C NMR of **7** in $CDCl_3$

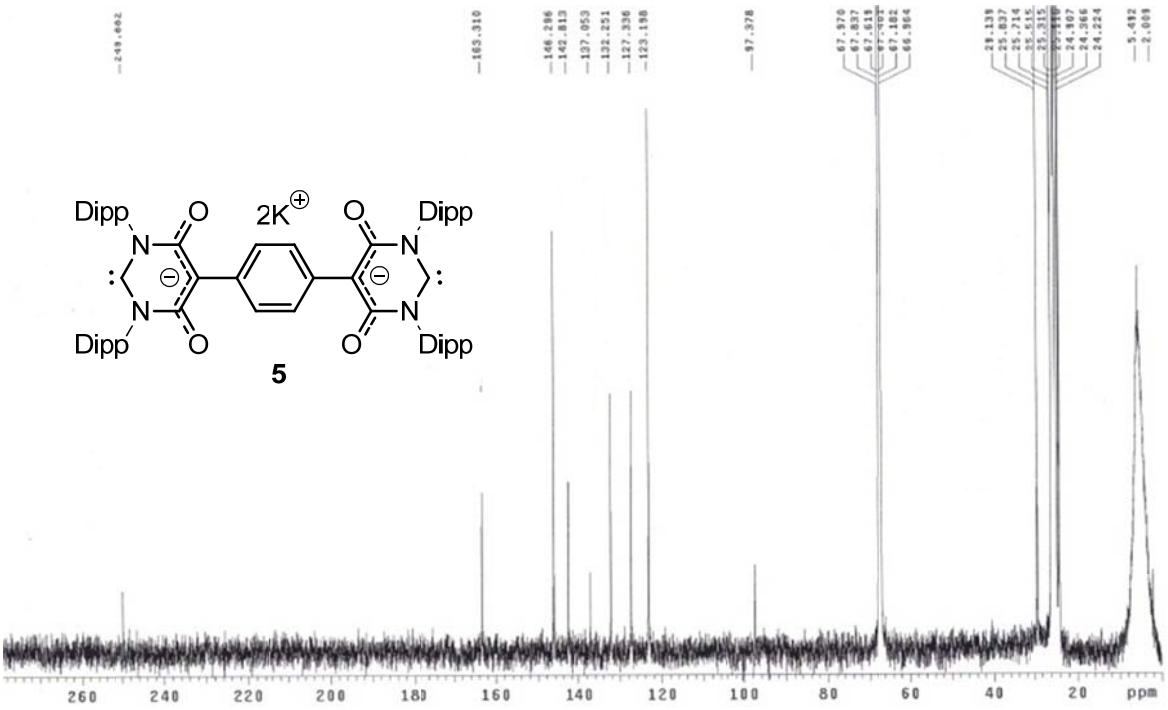


2.2 ^{1}H and ^{13}C NMR spectra of **5**

^{1}H NMR of **5** in d_8-THF

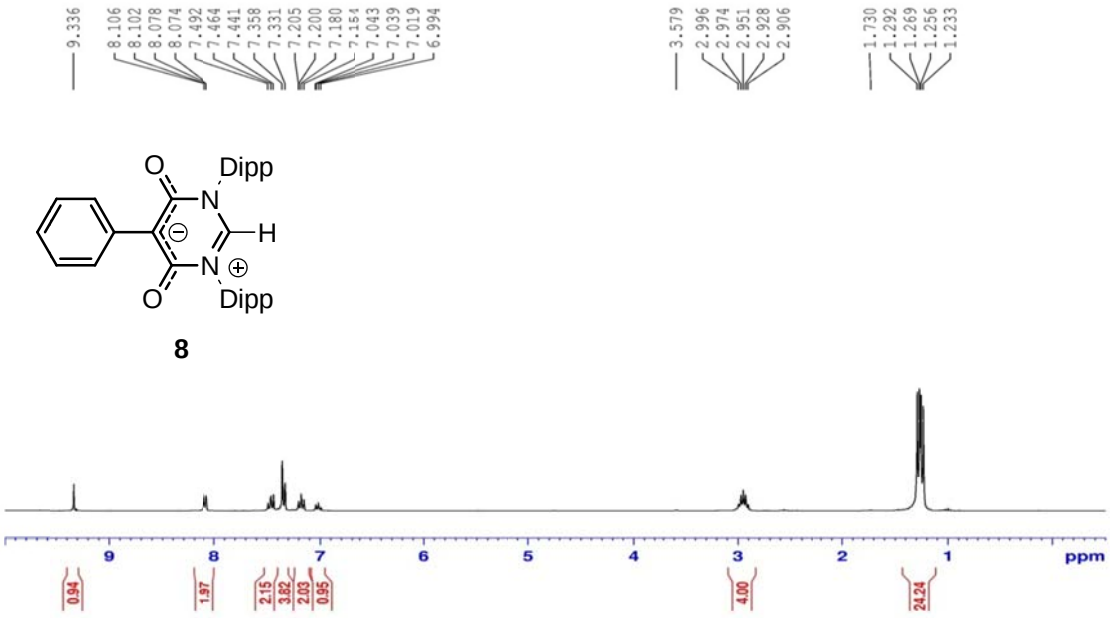


^{13}C NMR of **5** in d_8-THF

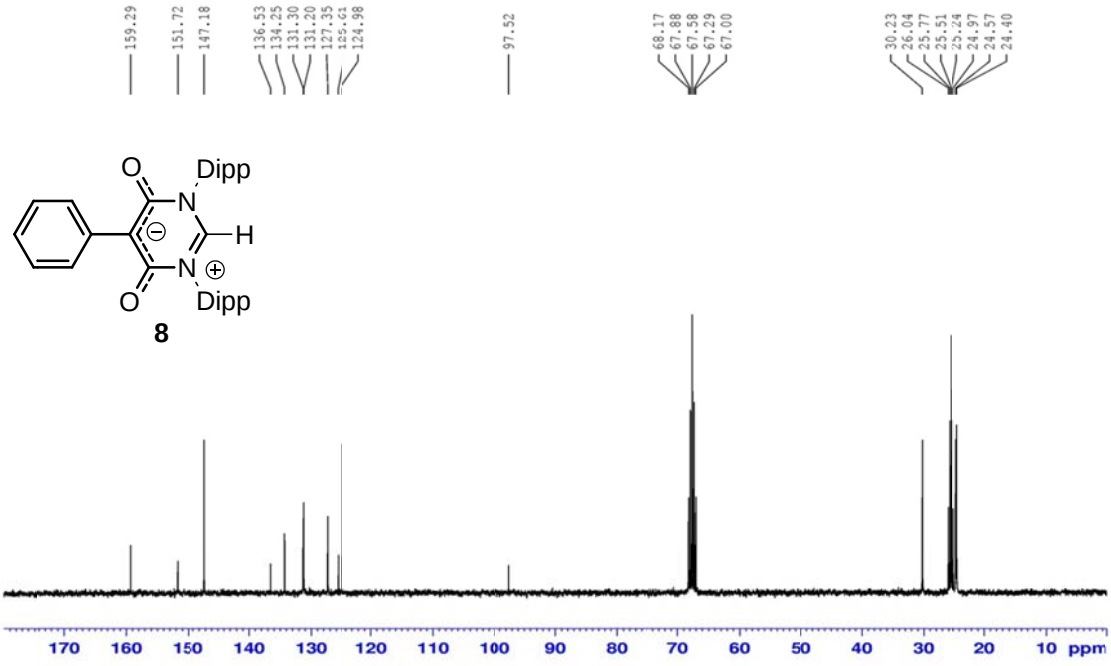


2.3 ^{1}H and ^{13}C NMR spectra of **8**

^{1}H NMR of **8** in d_8-THF

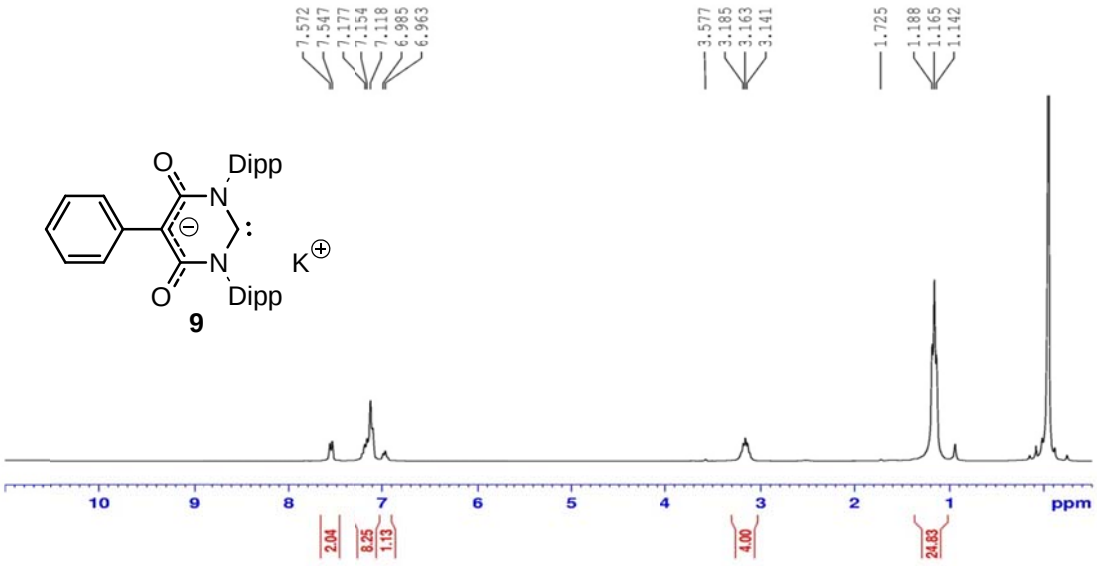


^{13}C NMR of **8** in d_8-THF

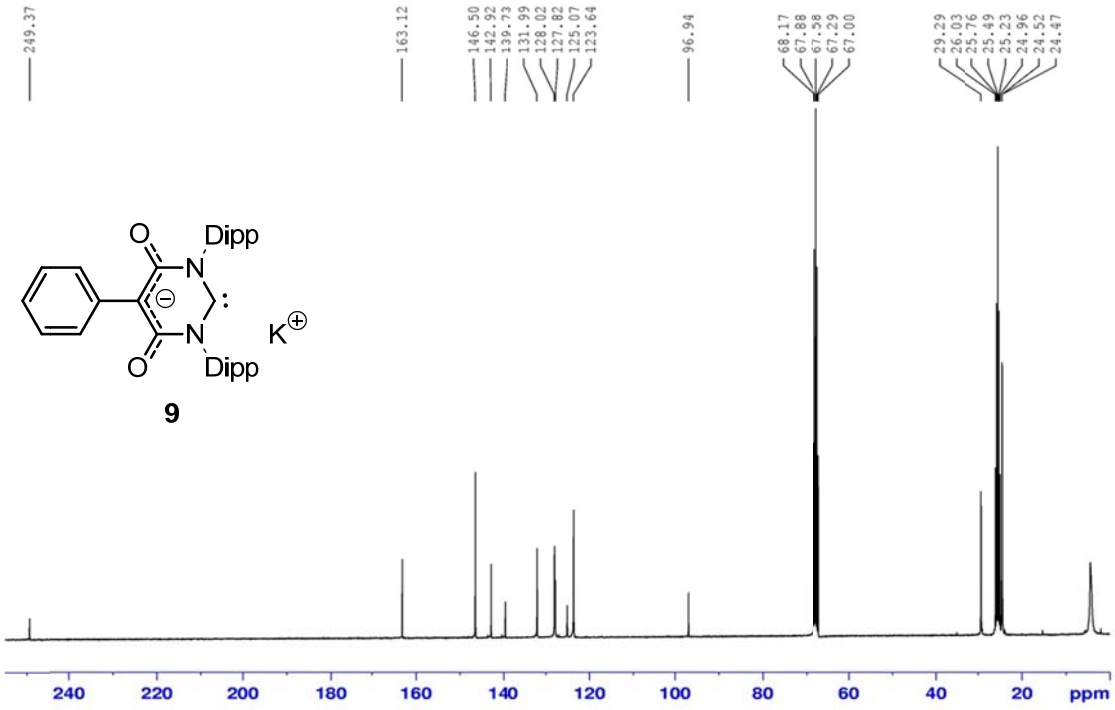


2.4 ^{1}H and ^{13}C NMR spectra of **9**

^{1}H NMR of **9** in d_8-THF

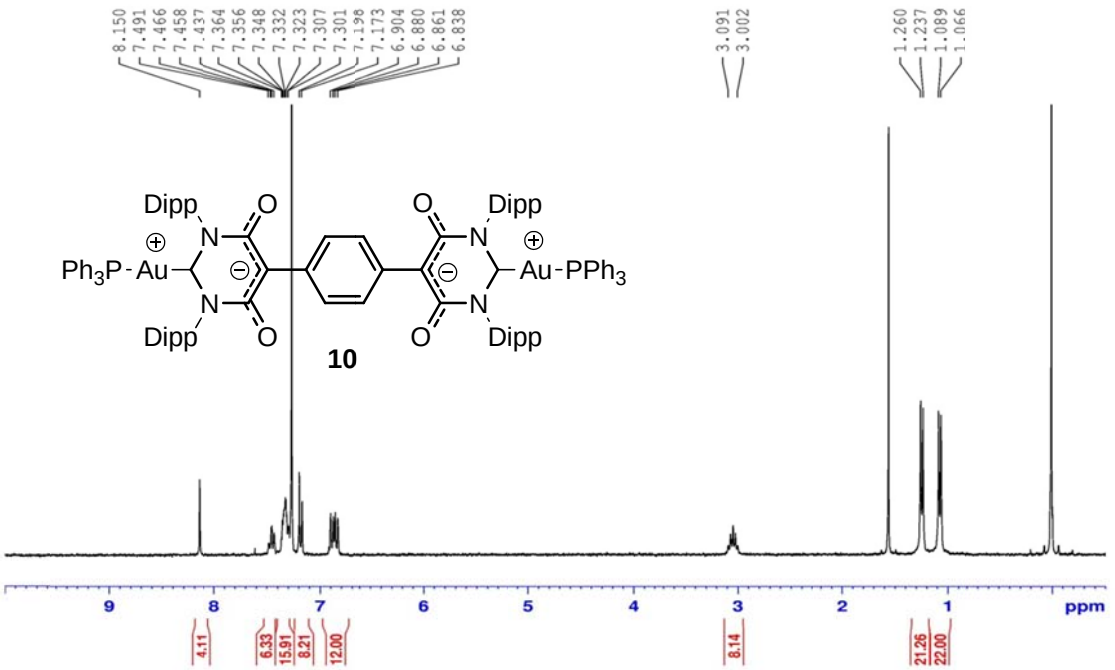


^{13}C NMR of **9** in d_8-THF

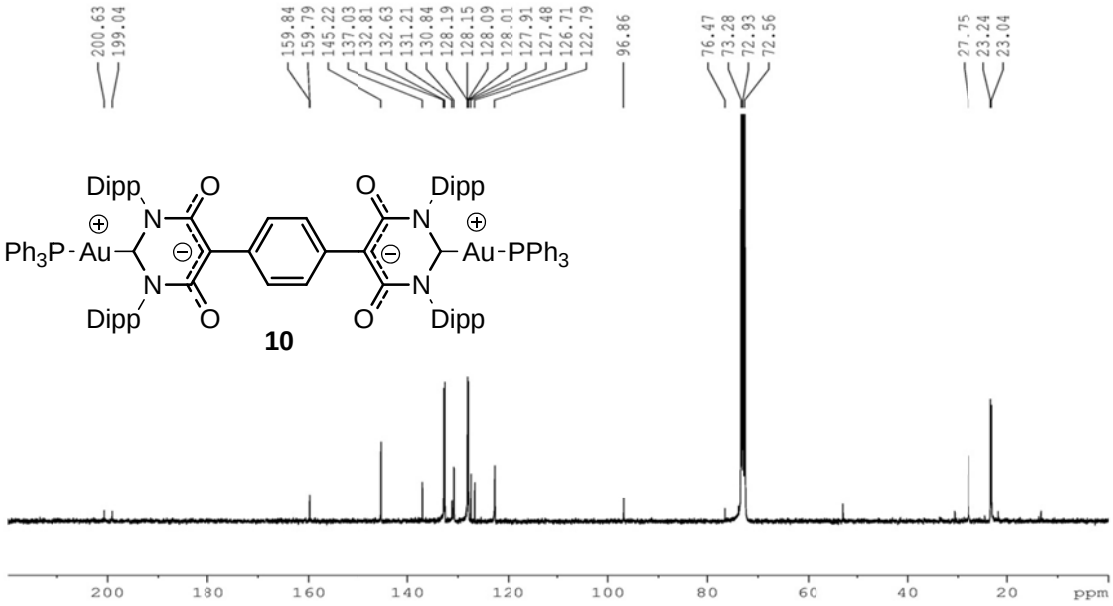


2.5 ^{1}H, ^{13}C NMR and ^{31}P spectra of **10**

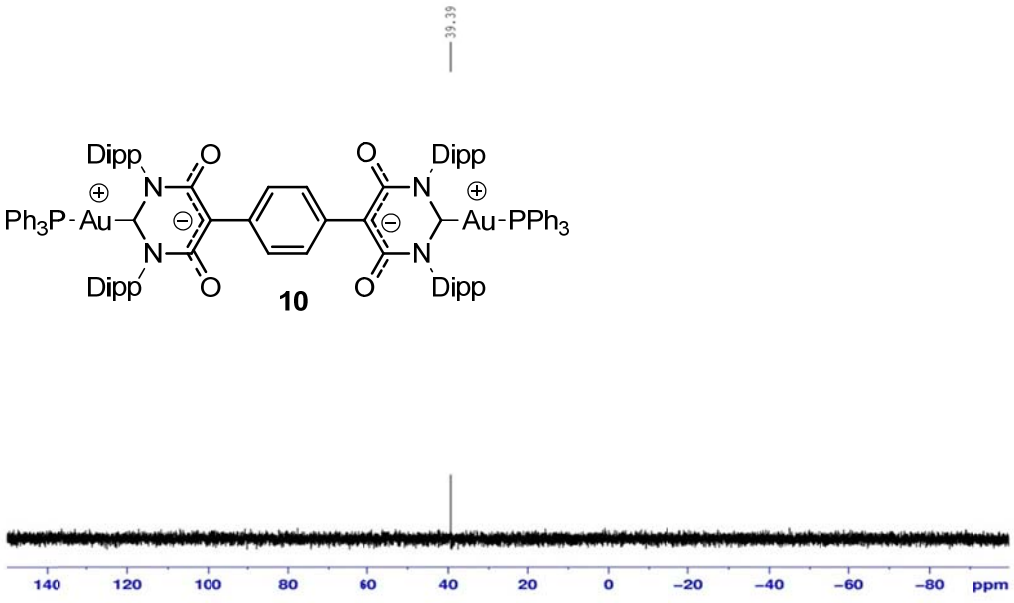
^{1}H NMR of **10** in $CDCl_3$



^{13}C NMR of **10** in $C_2D_2Cl_4$

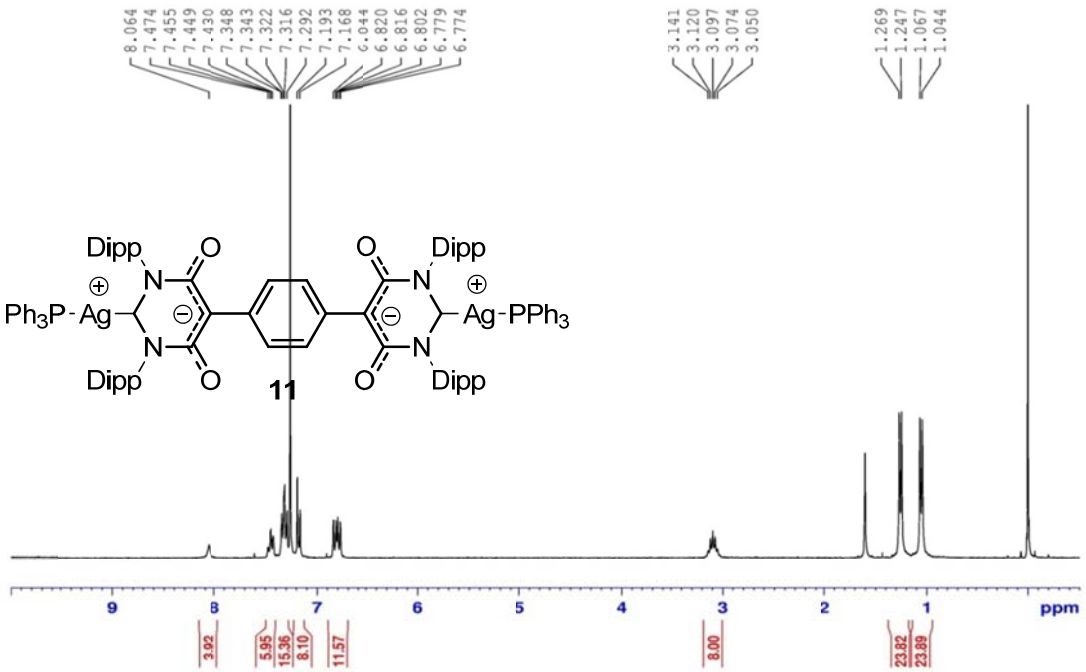


^{31}P NMR of **10** in $CDCl_3$

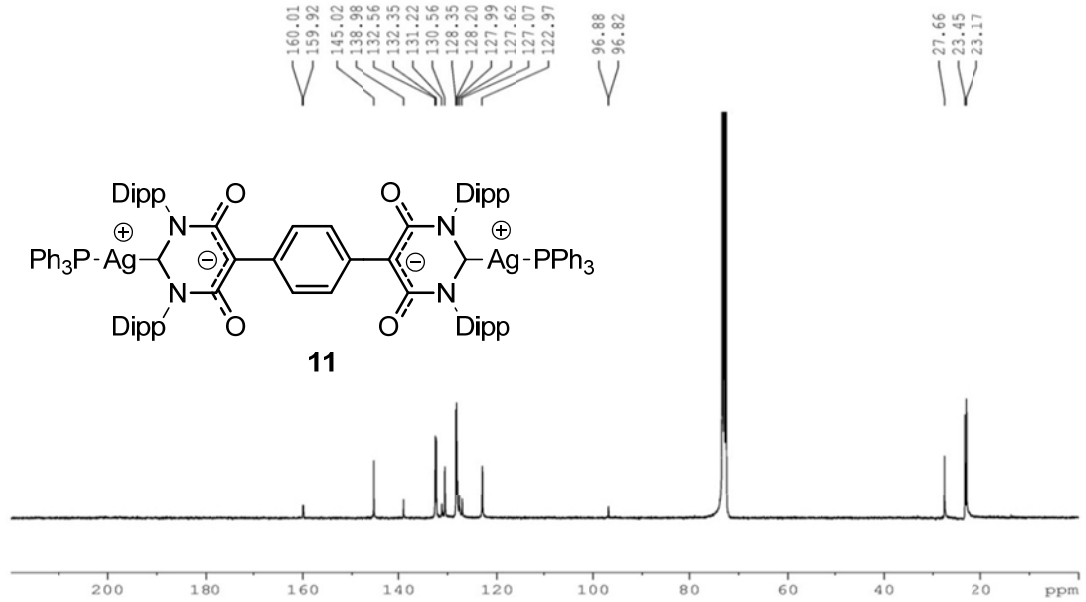


2.6 ^{1}H, ^{13}C NMR and ^{31}P spectra of **11**

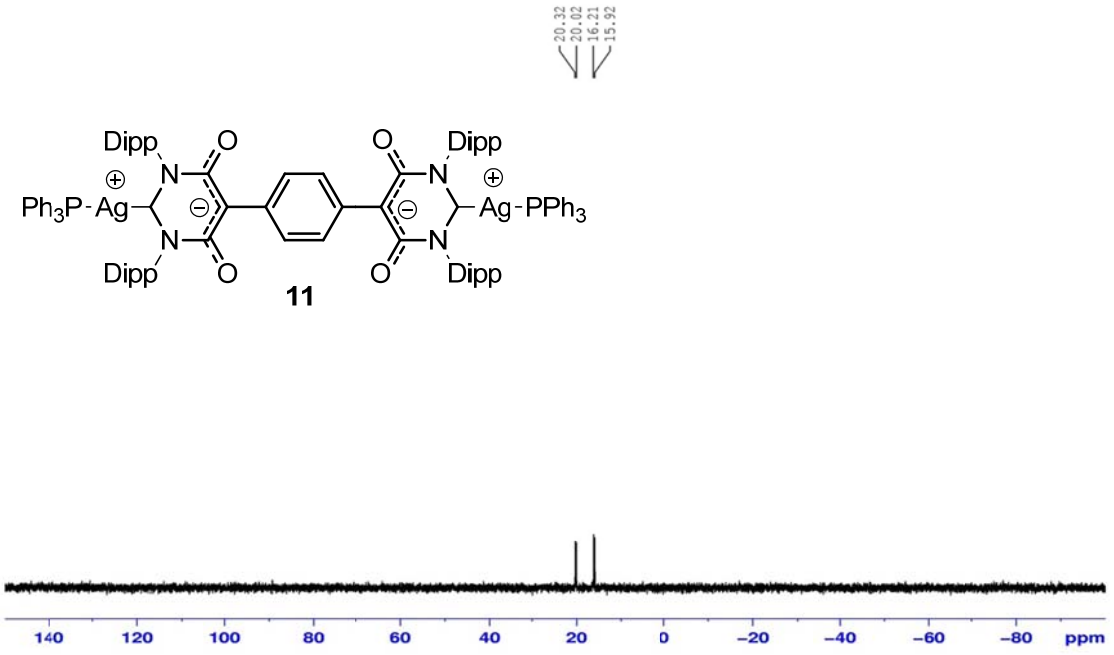
^{1}H NMR of **11** in $CDCl_3$



^{13}C NMR of **11** in $C_2D_2Cl_4$

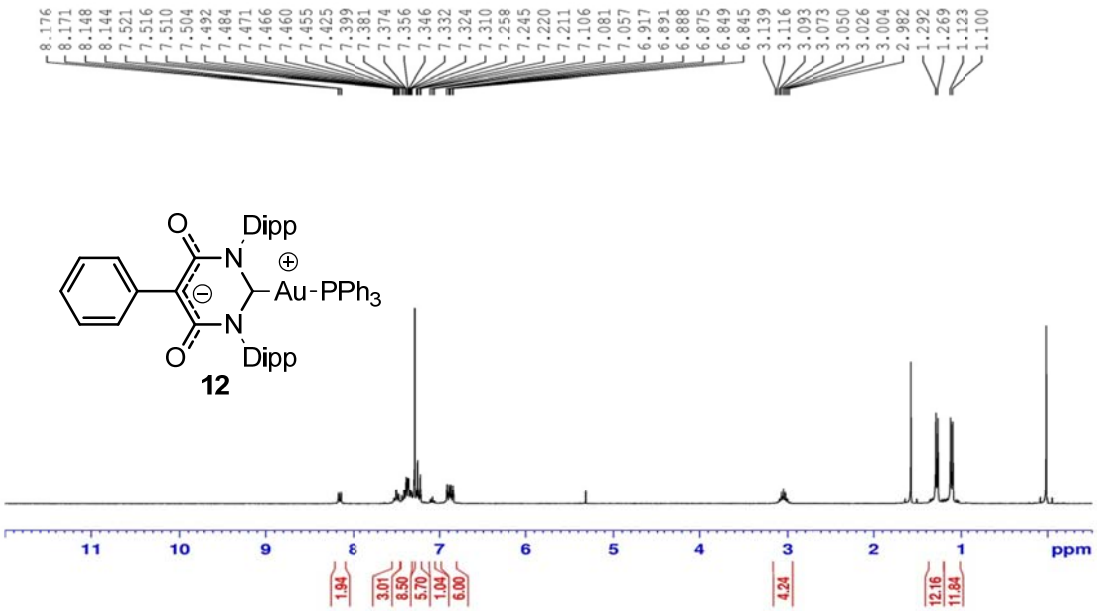


^{31}P NMR of **11** in $CDCl_3$

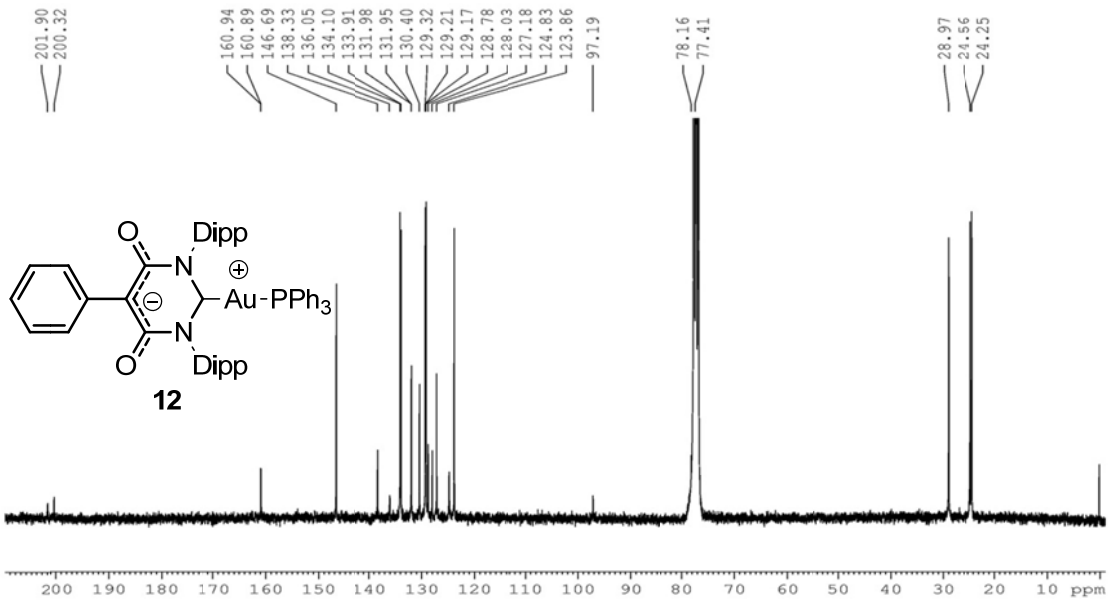


2.7 ^{1}H, ^{13}C NMR and ^{31}P spectra of **12**

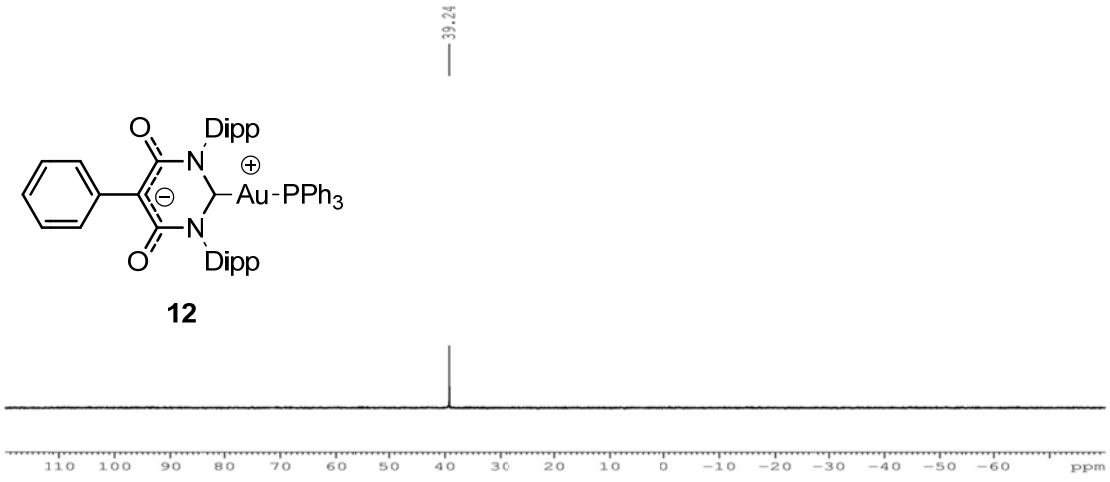
^{1}H NMR of **12** in $CDCl_3$



^{13}C NMR of **12** in $CDCl_3$

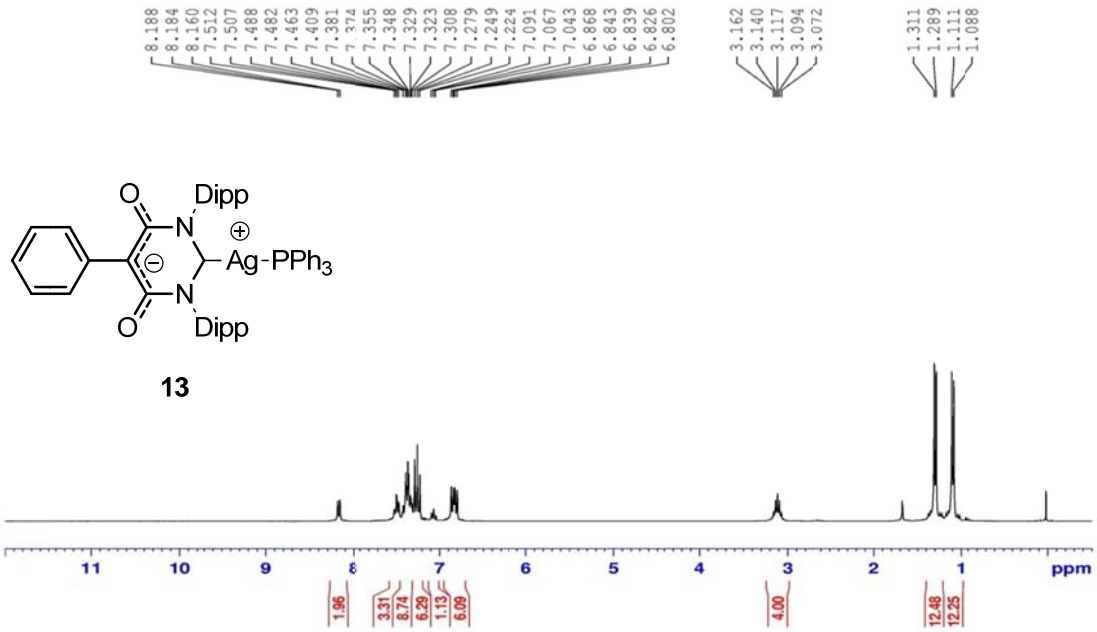


^{31}P NMR of **12** in $CDCl_3$

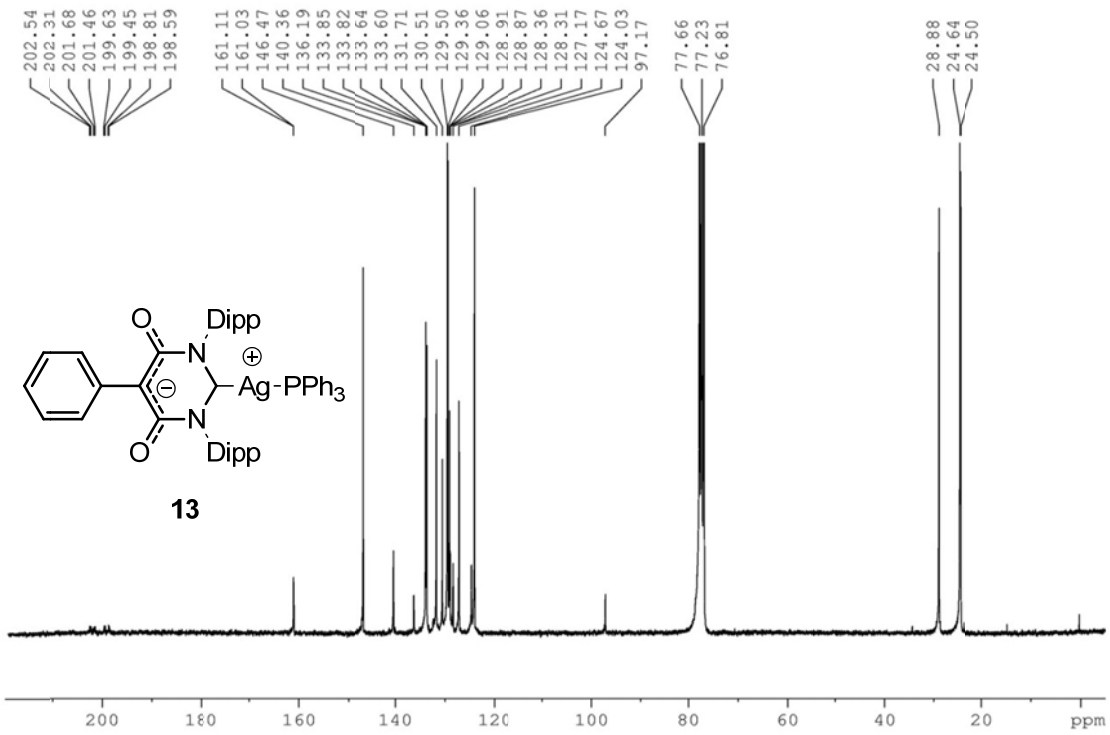


2.8 ^{1}H, ^{13}C NMR and ^{31}P spectra of **13**

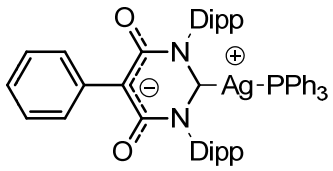
^{1}H NMR of **13** in $CDCl_3$



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



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



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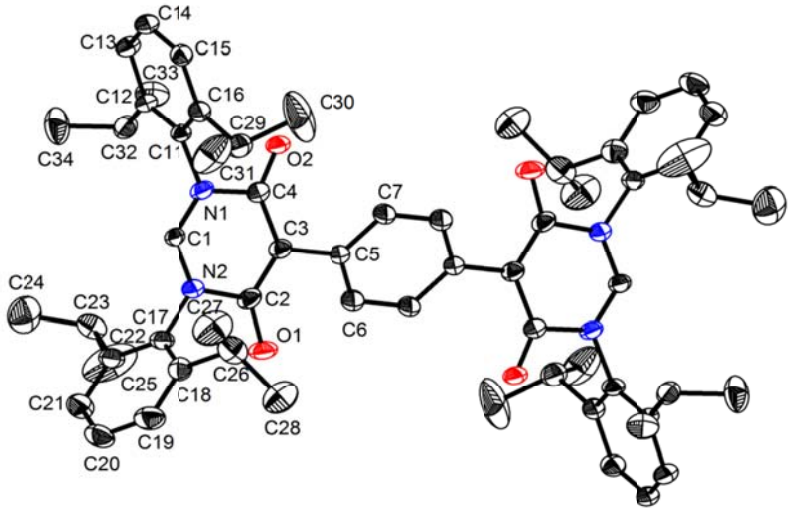
3. X-Ray Crystallography

Name	**10**	**11**	**7**
Empirical formula	$C_{98}H_{102}Au_2N_4O_4P_2 \cdot 5CHCl_3 \cdot H_2O$	$C_{98}H_{102}Ag_2N_4O_4P_2 \cdot 5CHCl_3 \cdot CH_2Cl_2$	$C_{62}H_{74}N_4O_4 \cdot 2CH_2Cl_2$
Formula sum	$C_{103}H_{109}Au_2Cl_{15}N_4O_5P_2$	$C_{104}H_{109}Ag_2Cl_{17}N_4O_4P_2$	$C_{64}H_{78}Cl_4N_4O_4$
Formula weight	2470.56	2359.28	1109.10
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	11.131(2)	11.194(2)	15.968(3)
b (Å)	24.888(5)	24.889(5)	9.4610(19)
c (Å)	21.128(4)	21.474(4)	21.052(4)
β (deg.)	93.78(3)	92.25(3)	97.31(3)
V (Å^3)	5841(2)	5978(2)	3154.6(11)
Z	2	2	2
D_{calc} (Mg/m^3)	1.405	1.311	1.168
Parameters	639	638	351
μ (mm^{-1})	2.927	0.781	0.235
Θ range (deg.)	2.18-25.15	2.24-25.15	2.36-25.15
Reflections			
Collected	40994	40841	23716
Independent	10333	10575	5647
Observed (I≥2σ(I)	8022	7885	2812
R_{int}	0.0582	0.0832	0.1578
Final *R* (obs. data)[a]			
R_1	0.0606	0.0979	0.1226
wR_2	0.1547	0.1956	0.2285
Final *R* (all data)			
R_1	0.0815	0.1250	0.2052
wR_2	0.1847	0.2167	0.2829
Goodness of fit on F^2	1.113	1.221	1.228
Largest diff. peak (e/Å^3)	3.332	0.086	0.387
Largest diff. hole (e/Å^3)	-2.114	-0.061	-0.561

[a] $R_1 = [\Sigma||F_O|-|F_c||]/\Sigma|F_O|$; $wR_2 = \{[\Sigma w[(F_O)^2-(F_c)^2]^2]\}^{1/2}$

3.1 Structural data for 7



Solid state molecular structure of **7** 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.

Table 1A. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(2)	4478(3)	2243(5)	1482(2)	52(1)
N(1)	3309(3)	3591(6)	1194(2)	41(1)
N(2)	2699(3)	3814(6)	153(2)	41(1)
O(1)	3154(3)	2582(6)	-668(2)	62(2)
C(2)	3277(4)	2802(8)	-89(3)	46(2)
C(11)	3296(4)	3925(7)	1870(3)	41(1)
C(3)	3885(4)	2216(7)	379(3)	40(1)
C(5)	4475(4)	1093(7)	181(3)	40(1)
C(1)	2733(4)	4123(7)	767(3)	39(1)
C(4)	3958(4)	2593(7)	1034(3)	43(1)
C(16)	2794(4)	3073(7)	2219(3)	45(1)
C(15)	2836(4)	3368(8)	2880(3)	48(2)
C(14)	3345(4)	4429(8)	3154(3)	48(2)
C(17)	2051(4)	4448(8)	-314(3)	45(2)
C(7)	4742(4)	-8(7)	600(3)	47(2)
C(12)	3821(4)	5000(7)	2138(3)	43(1)
C(22)	2178(4)	5815(8)	-535(3)	50(2)
C(6)	4733(4)	1081(8)	-414(3)	48(2)
C(13)	3830(4)	5246(8)	2805(3)	51(2)
C(18)	1341(4)	3667(8)	-522(3)	53(2)
C(21)	1558(5)	6400(9)	-980(4)	63(2)

C(29)	2221(5)	1895(8)	1910(3)	57(2)
C(20)	854(5)	5630(10)	-1203(4)	67(2)
C(19)	744(5)	4278(10)	-985(4)	68(2)
C(26)	1185(5)	2194(10)	-284(4)	69(2)
C(23)	2990(5)	6655(9)	-315(4)	62(2)
C(31)	1338(6)	2077(16)	1985(7)	118(5)
C(90)	1703(5)	6641(11)	2290(4)	73(2)
C(28)	1014(7)	1097(13)	-823(6)	96(3)
C(25)	3553(9)	6670(20)	-851(7)	152(7)
C(24)	2805(8)	8158(13)	-126(7)	111(4)
C(27)	440(8)	2173(15)	117(6)	108(4)
Cl(1)	1543(2)	7001(3)	1465(1)	83(1)
Cl(2)	782(2)	6183(4)	2597(1)	107(1)
C(32)	4364(4)	5909(8)	1754(3)	51(2)
C(34)	4150(7)	7453(10)	1825(6)	90(3)
C(33)	5299(5)	5674(11)	1960(4)	69(2)
C(30)	2511(13)	488(12)	2185(13)	211(13)

Table 2A. Bond lengths [Å] and angles [deg] for **7**.

O(2)-C(4)	1.220(7)
N(1)-C(1)	1.302(8)
N(1)-C(11)	1.460(7)
N(1)-C(4)	1.473(8)
N(2)-C(1)	1.321(7)
N(2)-C(17)	1.461(7)
N(2)-C(2)	1.465(8)
O(1)-C(2)	1.229(7)
C(2)-C(3)	1.406(9)
C(11)-C(12)	1.391(9)
C(11)-C(16)	1.409(9)
C(3)-C(4)	1.414(8)
C(3)-C(5)	1.515(9)
C(5)-C(6)	1.366(9)
C(5)-C(7)	1.396(9)
C(16)-C(15)	1.412(9)
C(16)-C(29)	1.533(10)
C(15)-C(14)	1.372(10)
C(14)-C(13)	1.372(10)
C(17)-C(18)	1.378(10)
C(17)-C(22)	1.397(10)
C(7)-C(6)#1	1.403(9)
C(12)-C(13)	1.422(8)
C(12)-C(32)	1.524(10)
C(22)-C(21)	1.389(10)

C(22)-C(23)	1.541(10)
C(6)-C(7)#1	1.403(9)
C(18)-C(19)	1.399(10)
C(18)-C(26)	1.511(12)
C(21)-C(20)	1.371(12)
C(29)-C(31)	1.450(13)
C(29)-C(30)	1.502(15)
C(20)-C(19)	1.378(13)
C(26)-C(28)	1.536(14)
C(26)-C(27)	1.545(14)
C(23)-C(24)	1.515(15)
C(23)-C(25)	1.529(14)
C(90)-Cl(2)	1.735(9)
C(90)-Cl(1)	1.756(9)
C(32)-C(34)	1.512(12)
C(32)-C(33)	1.517(10)
C(1)-N(1)-C(11)	119.6(5)
C(1)-N(1)-C(4)	123.0(5)
C(11)-N(1)-C(4)	117.3(4)
C(1)-N(2)-C(17)	120.4(5)
C(1)-N(2)-C(2)	122.3(5)
C(17)-N(2)-C(2)	117.3(5)
O(1)-C(2)-C(3)	129.6(6)
O(1)-C(2)-N(2)	115.3(5)
C(3)-C(2)-N(2)	115.1(5)
C(12)-C(11)-C(16)	124.1(5)
C(12)-C(11)-N(1)	118.1(5)
C(16)-C(11)-N(1)	117.6(5)
C(2)-C(3)-C(4)	123.2(6)
C(2)-C(3)-C(5)	118.8(5)
C(4)-C(3)-C(5)	118.0(5)
C(6)-C(5)-C(7)	118.0(6)
C(6)-C(5)-C(3)	122.0(5)
C(7)-C(5)-C(3)	120.0(5)
N(1)-C(1)-N(2)	122.0(6)
O(2)-C(4)-C(3)	130.4(6)
O(2)-C(4)-N(1)	115.3(5)
C(3)-C(4)-N(1)	114.3(5)
C(11)-C(16)-C(15)	116.2(6)
C(11)-C(16)-C(29)	122.8(5)
C(15)-C(16)-C(29)	120.9(6)
C(14)-C(15)-C(16)	120.7(6)
C(13)-C(14)-C(15)	122.1(6)
C(18)-C(17)-C(22)	122.6(6)
C(18)-C(17)-N(2)	118.5(6)
C(22)-C(17)-N(2)	118.9(6)

C(5)-C(7)-C(6)#1	120.6(6)
C(11)-C(12)-C(13)	116.7(6)
C(11)-C(12)-C(32)	123.5(5)
C(13)-C(12)-C(32)	119.8(6)
C(21)-C(22)-C(17)	118.2(6)
C(21)-C(22)-C(23)	119.8(7)
C(17)-C(22)-C(23)	122.0(6)
C(5)-C(6)-C(7)#1	121.4(6)
C(14)-C(13)-C(12)	120.1(6)
C(17)-C(18)-C(19)	117.4(7)
C(17)-C(18)-C(26)	123.5(6)
C(19)-C(18)-C(26)	119.1(7)
C(20)-C(21)-C(22)	120.1(8)
C(31)-C(29)-C(30)	108.6(13)
C(31)-C(29)-C(16)	113.8(7)
C(30)-C(29)-C(16)	110.0(7)
C(21)-C(20)-C(19)	120.9(7)
C(20)-C(19)-C(18)	120.8(7)
C(18)-C(26)-C(28)	113.6(8)
C(18)-C(26)-C(27)	111.3(8)
C(28)-C(26)-C(27)	108.5(8)
C(24)-C(23)-C(25)	109.7(11)
C(24)-C(23)-C(22)	112.2(7)
C(25)-C(23)-C(22)	109.6(8)
Cl(2)-C(90)-Cl(1)	113.1(5)
C(34)-C(32)-C(33)	109.8(7)
C(34)-C(32)-C(12)	110.0(6)
C(33)-C(32)-C(12)	111.8(6)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z

Table 3A. Anisotropic displacement parameters (A^2 x 10^3) for **7**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2[h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U11	U22	U33	U23	U13	U12
O(2)	63(3)	64(3)	28(2)	-8(2)	-1(2)	21(2)
N(1)	46(3)	48(3)	28(2)	-8(2)	4(2)	1(2)
N(2)	49(3)	45(3)	29(2)	-2(2)	6(2)	6(2)
O(1)	68(3)	90(4)	27(2)	-9(2)	1(2)	24(3)
C(2)	48(3)	56(4)	35(3)	-11(3)	10(2)	6(3)
C(11)	45(3)	51(4)	26(3)	-1(2)	6(2)	8(3)
C(3)	44(3)	46(4)	31(3)	-3(2)	8(2)	1(3)
C(5)	51(3)	38(3)	32(3)	0(2)	4(2)	5(3)
C(1)	46(3)	42(3)	30(3)	-3(2)	3(2)	-3(3)
C(4)	52(3)	46(4)	32(3)	-2(3)	8(3)	4(3)
C(16)	51(3)	45(4)	38(3)	1(3)	8(3)	7(3)

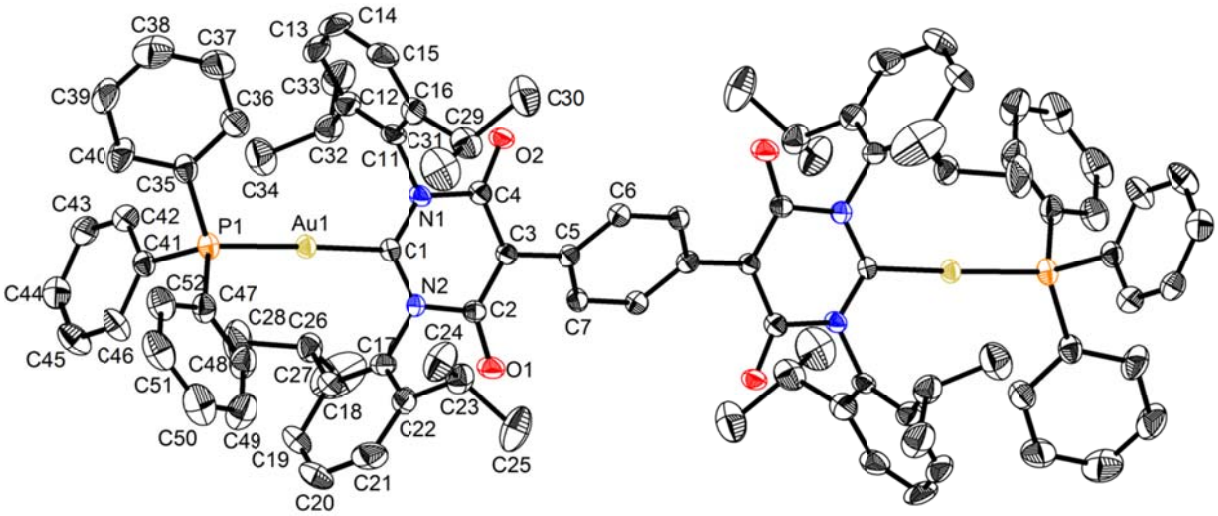
C(15)	52(3)	55(4)	38(3)	3(3)	13(3)	5(3)
C(14)	61(4)	53(4)	30(3)	-1(3)	9(3)	7(3)
C(17)	44(3)	59(4)	30(3)	0(3)	1(2)	12(3)
C(7)	64(4)	46(4)	32(3)	6(3)	10(3)	10(3)
C(12)	54(3)	44(4)	29(3)	-6(2)	0(2)	2(3)
C(22)	55(4)	55(4)	37(3)	4(3)	-2(3)	-1(3)
C(6)	60(4)	47(4)	37(3)	3(3)	10(3)	7(3)
C(13)	61(4)	57(4)	35(3)	-9(3)	5(3)	5(3)
C(18)	50(4)	61(5)	48(4)	0(3)	11(3)	0(3)
C(21)	62(4)	67(5)	59(4)	6(4)	0(3)	11(4)
C(29)	72(4)	51(4)	48(4)	-1(3)	9(3)	-10(3)
C(20)	56(4)	79(6)	60(4)	9(4)	-16(3)	9(4)
C(19)	58(4)	84(6)	56(4)	-3(4)	-11(3)	-1(4)
C(26)	59(4)	67(5)	78(5)	11(4)	-4(4)	-11(4)
C(23)	58(4)	70(5)	58(4)	16(4)	3(3)	-2(4)
C(31)	65(6)	141(12)	146(11)	-70(9)	9(6)	-24(6)
C(90)	70(5)	89(7)	56(5)	-4(4)	-5(4)	-13(4)
C(28)	98(7)	98(8)	93(7)	-24(6)	13(5)	-19(6)
C(25)	116(9)	230(20)	115(10)	-56(11)	60(8)	-84(11)
C(24)	99(8)	82(8)	145(11)	-18(7)	-10(7)	-23(6)
C(27)	129(9)	115(10)	90(7)	-2(6)	48(7)	-37(8)
Cl(1)	79(1)	91(2)	77(1)	-6(1)	5(1)	7(1)
Cl(2)	95(2)	142(3)	84(2)	-23(2)	20(1)	-10(2)
C(32)	66(4)	44(4)	45(3)	-4(3)	11(3)	-5(3)
C(34)	121(8)	45(5)	112(8)	18(5)	51(6)	6(5)
C(33)	60(4)	91(6)	57(4)	10(4)	15(3)	-13(4)
C(30)	198(15)	42(6)	340(30)	6(10)	-157(18)	-19(8)

Table 4A. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **7**.

	x	y	z	U(eq)
H(1)	2331	4745	900	47
H(15)	2512	2832	3135	57
H(14)	3362	4602	3595	57
H(7)	4569	-30	1010	57
H(6)	4555	1807	-705	57
H(13)	4168	5970	3007	61
H(21)	1622	7325	-1130	76
H(29)	2270	1883	1446	68
H(20)	441	6031	-1508	80
H(19)	263	3760	-1150	81
H(26)	1698	1894	-2	83
H(23)	3298	6173	62	75
H(31A)	1064	1161	1974	176
H(31B)	1066	2661	1640	176

H(31C)	1292	2531	2393	176
H(90A)	2111	5867	2370	88
H(90B)	1948	7478	2517	88
H(28A)	458	1254	-1055	144
H(28B)	1042	155	-640	144
H(28C)	1436	1189	-1114	144
H(25A)	3267	7163	-1220	227
H(25B)	3671	5706	-969	227
H(25C)	4079	7148	-702	227
H(24A)	3328	8692	-61	166
H(24B)	2549	8148	267	166
H(24C)	2421	8594	-464	166
H(27A)	551	2830	471	163
H(27B)	374	1228	282	163
H(27C)	-74	2449	-151	163
H(32)	4236	5649	1296	61
H(34A)	3542	7566	1786	135
H(34B)	4372	7997	1493	135
H(34C)	4400	7788	2242	135
H(33A)	5437	5938	2406	103
H(33B)	5624	6250	1699	103
H(33C)	5434	4685	1907	103
H(30A)	2509	502	2645	317
H(30B)	3079	300	2089	317
H(30C)	2134	-246	1998	317

3.2 Structural data for 10:



Solid state molecular structure of **10** 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.

Table 1B. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($A^2 \times 10^3$) for **10**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Au(1)	390(1)	6852(1)	8131(1)	36(1)
P(1)	-861(2)	7420(1)	7555(1)	43(1)
C(6)	3864(7)	5086(3)	10207(4)	35(2)
O(2)	2563(5)	6120(3)	10219(2)	44(1)
N(1)	1734(6)	6376(3)	9254(3)	34(1)
C(1)	1610(7)	6377(3)	8616(4)	34(2)
N(2)	2362(6)	6050(3)	8328(3)	35(1)
O(1)	3854(6)	5432(3)	8289(3)	51(2)
C(3)	3325(7)	5712(3)	9305(3)	33(2)
C(4)	2574(7)	6056(3)	9642(4)	37(2)
C(5)	4177(7)	5347(3)	9667(4)	35(2)
C(47)	-1622(9)	7084(4)	6874(5)	52(2)
C(2)	3253(7)	5703(3)	8641(4)	36(2)
C(17)	2299(8)	6053(4)	7647(4)	42(2)
C(11)	906(9)	6729(4)	9571(4)	45(2)
C(26)	3657(10)	6871(4)	7674(5)	56(2)
C(41)	17(8)	7957(4)	7243(4)	44(2)
C(16)	-175(8)	6512(4)	9727(5)	53(2)
C(15)	-970(11)	6872(5)	9984(5)	66(3)
C(12)	1289(10)	7262(4)	9704(4)	55(2)
C(35)	-2002(8)	7750(4)	7998(4)	49(2)
C(14)	-676(12)	7394(5)	10101(6)	78(4)
C(32)	2515(11)	7475(4)	9571(5)	62(3)
C(13)	436(12)	7596(5)	9956(5)	70(3)
C(36)	-2310(10)	7527(5)	8576(5)	64(3)
C(23)	992(11)	5208(4)	7676(5)	60(3)
C(44)	1566(10)	8732(4)	6810(5)	61(3)
C(22)	1631(9)	5637(4)	7325(4)	52(2)
C(31)	-1593(14)	5856(7)	9132(8)	103(5)
C(42)	510(10)	8356(4)	7642(5)	56(2)
C(33)	3167(16)	7707(6)	10152(7)	94(5)
C(40)	-2564(11)	8211(5)	7773(7)	72(3)
C(43)	1258(11)	8735(4)	7439(5)	60(3)
C(28)	3510(20)	7429(5)	7397(9)	113(6)
C(45)	1102(12)	8340(6)	6405(6)	74(3)
C(18)	2862(9)	6456(4)	7328(4)	50(2)
C(19)	2751(15)	6453(5)	6669(5)	82(4)
C(21)	1525(12)	5664(5)	6666(5)	73(3)

C(24)	-352(13)	5232(5)	7567(8)	89(4)
C(29)	-506(10)	5925(5)	9618(5)	66(3)
C(20)	2101(15)	6066(6)	6345(5)	86(4)
C(30)	-776(15)	5643(6)	10252(8)	95(4)
C(52)	-2708(10)	7268(5)	6589(5)	64(3)
C(7)	5335(7)	5262(3)	9462(4)	38(2)
Cl(2)	5579(3)	6660(1)	10170(2)	79(1)
C(90)	5237(10)	6279(5)	10842(5)	63(3)
C(51)	-3271(13)	7012(6)	6086(6)	82(4)
C(38)	-3738(13)	8228(7)	8679(8)	95(5)
C(37)	-3173(13)	7774(6)	8908(6)	82(4)
C(39)	-3445(13)	8455(6)	8118(8)	92(4)
Cl(1)	4641(3)	6703(2)	11411(2)	81(1)
Cl(3)	6485(4)	5948(2)	11165(2)	109(1)
C(48)	-1078(12)	6645(4)	6623(6)	68(3)
C(46)	328(11)	7958(5)	6617(5)	63(3)
C(50)	-2725(15)	6559(6)	5840(7)	90(5)
C(49)	-1623(14)	6372(5)	6102(7)	87(4)
Cl(5)	5868(7)	4521(3)	7527(4)	131(2)
Cl(6)	4470(7)	4934(4)	6528(3)	109(2)
Cl(66)	4820(30)	5335(15)	6522(14)	67(7)
Cl(7)	-2563(13)	5220(3)	4867(4)	178(4)
C(34)	2461(15)	7866(6)	9023(7)	89(4)
C(25)	1467(13)	4647(5)	7520(9)	94(5)
C(91)	5338(12)	5119(6)	7210(8)	67(4)
C(27)	4947(16)	6726(9)	7717(14)	149(10)
C(92)	-2890(40)	4777(15)	5502(15)	162(15)
Cl(4)	6290(30)	5571(12)	6909(11)	97(10)
Cl(44)	6605(17)	5546(9)	7132(11)	156(9)
Cl(9)	-1525(18)	4524(7)	5799(8)	262(8)
Cl(8)	-3798(12)	4277(4)	5183(6)	193(5)
O(3W)	-400(8)	4443(4)	6872(4)	28(2)

Table 2B . Bond lengths [Å] and angles [deg] for **10**.

Au(1)-C(1)	2.027(7)
Au(1)-P(1)	2.280(2)
P(1)-C(41)	1.805(9)
P(1)-C(35)	1.822(10)
P(1)-C(47)	1.825(9)
C(6)-C(5)	1.378(11)
C(6)-C(7)#1	1.396(11)
O(2)-C(4)	1.230(10)
N(1)-C(1)	1.346(10)
N(1)-C(4)	1.441(10)
N(1)-C(11)	1.468(11)

C(1)-N(2)	1.342(10)
N(2)-C(17)	1.435(10)
N(2)-C(2)	1.443(10)
O(1)-C(2)	1.233(10)
C(3)-C(2)	1.399(11)
C(3)-C(4)	1.422(11)
C(3)-C(5)	1.487(10)
C(5)-C(7)	1.402(11)
C(47)-C(48)	1.371(16)
C(47)-C(52)	1.391(14)
C(17)-C(18)	1.382(13)
C(17)-C(22)	1.421(13)
C(11)-C(16)	1.379(14)
C(11)-C(12)	1.417(14)
C(26)-C(27)	1.48(2)
C(26)-C(28)	1.513(16)
C(26)-C(18)	1.516(15)
C(41)-C(46)	1.389(14)
C(41)-C(42)	1.394(14)
C(16)-C(15)	1.395(14)
C(16)-C(29)	1.519(16)
C(15)-C(14)	1.359(19)
C(12)-C(13)	1.394(15)
C(12)-C(32)	1.508(17)
C(35)-C(40)	1.376(13)
C(35)-C(36)	1.404(14)
C(14)-C(13)	1.39(2)
C(32)-C(33)	1.500(15)
C(32)-C(34)	1.511(17)
C(36)-C(37)	1.372(17)
C(23)-C(24)	1.500(18)
C(23)-C(22)	1.505(15)
C(23)-C(25)	1.535(17)
C(44)-C(45)	1.377(17)
C(44)-C(43)	1.394(16)
C(22)-C(21)	1.391(15)
C(31)-C(29)	1.545(19)
C(42)-C(43)	1.347(15)
C(40)-C(39)	1.398(18)
C(45)-C(46)	1.377(16)
C(18)-C(19)	1.389(14)
C(19)-C(20)	1.36(2)
C(21)-C(20)	1.39(2)
C(29)-C(30)	1.558(17)
C(52)-C(51)	1.357(17)
C(7)-C(6)#1	1.396(11)

Cl(2)-C(90)	1.770(13)
C(90)-Cl(3)	1.718(12)
C(90)-Cl(1)	1.761(11)
C(51)-C(50)	1.40(2)
C(38)-C(37)	1.37(2)
C(38)-C(39)	1.37(2)
C(48)-C(49)	1.398(16)
C(50)-C(49)	1.39(2)
Cl(5)-C(91)	1.720(16)
Cl(6)-Cl(66)	1.07(4)
Cl(6)-C(91)	1.743(19)
Cl(66)-Cl(4)	1.87(4)
Cl(66)-Cl(44)	2.35(4)
Cl(7)-C(92)	1.79(4)
C(91)-Cl(4)	1.70(3)
C(92)-Cl(8)	1.71(3)
C(92)-Cl(9)	1.72(4)
Cl(4)-Cl(44)	0.57(5)
C(1)-Au(1)-P(1)	175.6(2)
C(41)-P(1)-C(35)	105.5(4)
C(41)-P(1)-C(47)	106.6(4)
C(35)-P(1)-C(47)	108.0(5)
C(41)-P(1)-Au(1)	109.1(3)
C(35)-P(1)-Au(1)	115.3(3)
C(47)-P(1)-Au(1)	111.9(3)
C(5)-C(6)-C(7)#1	121.3(7)
C(1)-N(1)-C(4)	126.2(7)
C(1)-N(1)-C(11)	115.5(6)
C(4)-N(1)-C(11)	118.3(6)
N(2)-C(1)-N(1)	115.3(6)
N(2)-C(1)-Au(1)	122.8(5)
N(1)-C(1)-Au(1)	121.9(6)
C(1)-N(2)-C(17)	117.4(6)
C(1)-N(2)-C(2)	125.8(6)
C(17)-N(2)-C(2)	116.8(6)
C(2)-C(3)-C(4)	121.0(7)
C(2)-C(3)-C(5)	119.9(7)
C(4)-C(3)-C(5)	119.1(7)
O(2)-C(4)-C(3)	128.2(7)
O(2)-C(4)-N(1)	116.4(7)
C(3)-C(4)-N(1)	115.4(7)
C(6)-C(5)-C(7)	118.1(7)
C(6)-C(5)-C(3)	121.8(7)
C(7)-C(5)-C(3)	120.1(7)
C(48)-C(47)-C(52)	119.2(10)
C(48)-C(47)-P(1)	118.4(8)

C(52)-C(47)-P(1)	122.4(8)
O(1)-C(2)-C(3)	128.0(7)
O(1)-C(2)-N(2)	115.7(7)
C(3)-C(2)-N(2)	116.3(7)
C(18)-C(17)-C(22)	122.3(8)
C(18)-C(17)-N(2)	120.0(8)
C(22)-C(17)-N(2)	117.7(8)
C(16)-C(11)-C(12)	125.2(9)
C(16)-C(11)-N(1)	117.2(8)
C(12)-C(11)-N(1)	117.6(9)
C(27)-C(26)-C(28)	109.4(15)
C(27)-C(26)-C(18)	113.3(11)
C(28)-C(26)-C(18)	113.1(11)
C(46)-C(41)-C(42)	117.5(9)
C(46)-C(41)-P(1)	121.7(8)
C(42)-C(41)-P(1)	120.5(7)
C(11)-C(16)-C(15)	115.2(10)
C(11)-C(16)-C(29)	123.2(9)
C(15)-C(16)-C(29)	121.5(10)
C(14)-C(15)-C(16)	122.3(12)
C(13)-C(12)-C(11)	115.5(11)
C(13)-C(12)-C(32)	120.7(11)
C(11)-C(12)-C(32)	123.8(9)
C(40)-C(35)-C(36)	119.9(11)
C(40)-C(35)-P(1)	121.0(9)
C(36)-C(35)-P(1)	119.1(7)
C(15)-C(14)-C(13)	120.9(10)
C(33)-C(32)-C(12)	112.2(11)
C(33)-C(32)-C(34)	111.8(11)
C(12)-C(32)-C(34)	112.2(10)
C(14)-C(13)-C(12)	120.5(12)
C(37)-C(36)-C(35)	119.1(11)
C(24)-C(23)-C(22)	113.3(10)
C(24)-C(23)-C(25)	111.0(10)
C(22)-C(23)-C(25)	111.1(11)
C(45)-C(44)-C(43)	119.4(10)
C(21)-C(22)-C(17)	116.9(10)
C(21)-C(22)-C(23)	120.9(10)
C(17)-C(22)-C(23)	122.1(8)
C(43)-C(42)-C(41)	122.2(10)
C(35)-C(40)-C(39)	120.0(13)
C(42)-C(43)-C(44)	119.8(10)
C(44)-C(45)-C(46)	120.3(11)
C(17)-C(18)-C(19)	118.2(10)
C(17)-C(18)-C(26)	121.8(8)
C(19)-C(18)-C(26)	119.8(10)

C(20)-C(19)-C(18)	121.1(12)
C(20)-C(21)-C(22)	120.7(11)
C(16)-C(29)-C(31)	112.3(11)
C(16)-C(29)-C(30)	111.2(11)
C(31)-C(29)-C(30)	109.5(11)
C(19)-C(20)-C(21)	120.7(10)
C(51)-C(52)-C(47)	121.9(13)
C(6)#1-C(7)-C(5)	120.6(7)
Cl(3)-C(90)-Cl(1)	110.3(6)
Cl(3)-C(90)-Cl(2)	111.4(6)
Cl(1)-C(90)-Cl(2)	109.7(6)
C(52)-C(51)-C(50)	118.7(12)
C(37)-C(38)-C(39)	121.1(13)
C(38)-C(37)-C(36)	120.7(13)
C(38)-C(39)-C(40)	119.1(12)
C(47)-C(48)-C(49)	120.7(11)
C(45)-C(46)-C(41)	120.8(11)
C(49)-C(50)-C(51)	121.1(12)
C(50)-C(49)-C(48)	118.4(13)
Cl(66)-Cl(6)-C(91)	65.2(17)
Cl(6)-Cl(66)-Cl(4)	127(2)
Cl(6)-Cl(66)-Cl(44)	120(2)
Cl(4)-Cl(66)-Cl(44)	8.4(12)
Cl(4)-C(91)-Cl(5)	120.9(15)
Cl(4)-C(91)-Cl(6)	101.0(13)
Cl(5)-C(91)-Cl(6)	104.6(10)
Cl(8)-C(92)-Cl(9)	111(2)
Cl(8)-C(92)-Cl(7)	107.2(19)
Cl(9)-C(92)-Cl(7)	106.3(19)
Cl(44)-Cl(4)-C(91)	89(4)
Cl(44)-Cl(4)-Cl(66)	143(5)
C(91)-Cl(4)-Cl(66)	53.7(14)
Cl(4)-Cl(44)-Cl(66)	29(4)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+2

Table 3B. Anisotropic displacement parameters (A^2 x 10^3) for **10**. The anisotropic 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}
Au(1)	37(1)	36(1)	35(1)	5(1)	-1(1)	4(1)
P(1)	43(1)	41(1)	42(1)	10(1)	-3(1)	3(1)
C(6)	24(3)	43(4)	38(4)	1(3)	0(3)	3(3)
O(2)	46(3)	58(3)	27(3)	-1(2)	1(2)	17(3)
N(1)	32(3)	43(3)	27(3)	3(3)	-1(2)	8(3)

C(1)	32(4)	34(4)	35(4)	4(3)	1(3)	-1(3)
N(2)	35(3)	35(3)	34(3)	2(3)	1(3)	4(3)
O(1)	48(3)	70(4)	35(3)	0(3)	6(3)	22(3)
C(3)	28(3)	40(4)	31(4)	3(3)	0(3)	6(3)
C(4)	32(4)	44(4)	36(4)	4(3)	2(3)	2(3)
C(5)	29(4)	37(4)	39(4)	0(3)	1(3)	4(3)
C(47)	61(6)	40(4)	52(5)	7(4)	-7(4)	-7(4)
C(2)	32(4)	39(4)	38(4)	2(3)	9(3)	2(3)
C(17)	40(4)	50(5)	36(4)	-4(3)	2(3)	7(4)
C(11)	53(5)	56(5)	24(4)	-3(3)	-3(3)	14(4)
C(26)	58(6)	46(5)	65(6)	10(4)	16(5)	-4(4)
C(41)	42(5)	45(4)	43(4)	9(4)	-3(4)	7(4)
C(16)	39(5)	69(6)	51(5)	7(4)	4(4)	15(4)
C(15)	56(6)	98(9)	45(5)	6(5)	14(4)	30(6)
C(12)	69(6)	55(5)	41(5)	-6(4)	-5(4)	18(5)
C(35)	43(5)	51(5)	53(5)	11(4)	0(4)	6(4)
C(14)	83(9)	87(9)	65(7)	-19(6)	8(6)	56(7)
C(32)	74(7)	51(5)	60(6)	-10(5)	-10(5)	0(5)
C(13)	87(9)	63(6)	58(6)	-6(5)	-12(6)	46(6)
C(36)	61(6)	74(7)	58(6)	12(5)	9(5)	7(5)
C(23)	69(7)	44(5)	66(6)	-6(4)	-6(5)	-9(5)
C(44)	51(6)	59(6)	75(7)	10(5)	7(5)	1(5)
C(22)	55(5)	52(5)	47(5)	-5(4)	-9(4)	4(4)
C(31)	70(9)	117(12)	122(12)	16(10)	8(8)	-36(9)
C(42)	67(6)	48(5)	54(5)	-1(4)	9(5)	2(5)
C(33)	124(13)	71(8)	81(9)	-21(7)	-38(8)	15(8)
C(40)	57(7)	60(6)	100(9)	10(6)	6(6)	26(5)
C(43)	75(7)	40(5)	67(6)	-5(4)	6(5)	-8(5)
C(28)	164(18)	55(7)	119(13)	27(8)	5(12)	-29(9)
C(45)	75(8)	93(8)	55(6)	15(6)	11(5)	-23(7)
C(18)	62(6)	47(5)	42(5)	5(4)	11(4)	3(4)
C(19)	128(12)	79(8)	41(6)	16(5)	21(6)	10(8)
C(21)	77(8)	86(8)	52(6)	-26(6)	-15(5)	6(6)
C(24)	71(8)	61(7)	132(12)	-5(7)	1(8)	-1(6)
C(29)	46(5)	84(8)	69(7)	13(6)	18(5)	-3(5)
C(20)	127(12)	102(10)	29(5)	1(6)	0(6)	6(9)
C(30)	92(10)	93(10)	101(10)	36(8)	10(8)	-1(8)
C(52)	56(6)	73(7)	63(6)	13(5)	-12(5)	-3(5)
C(7)	33(4)	41(4)	40(4)	10(3)	9(3)	7(3)
Cl(2)	69(2)	85(2)	87(2)	-6(2)	23(2)	-6(2)
C(90)	50(6)	65(6)	74(7)	-15(5)	2(5)	-8(5)
C(51)	71(8)	102(10)	68(7)	21(7)	-30(6)	-25(7)
C(38)	58(8)	119(12)	111(12)	-11(9)	29(8)	21(8)
C(37)	74(8)	99(10)	77(8)	5(7)	34(6)	18(7)
C(39)	82(9)	77(8)	119(12)	18(8)	28(8)	42(7)
Cl(1)	68(2)	105(2)	72(2)	-20(2)	13(1)	16(2)

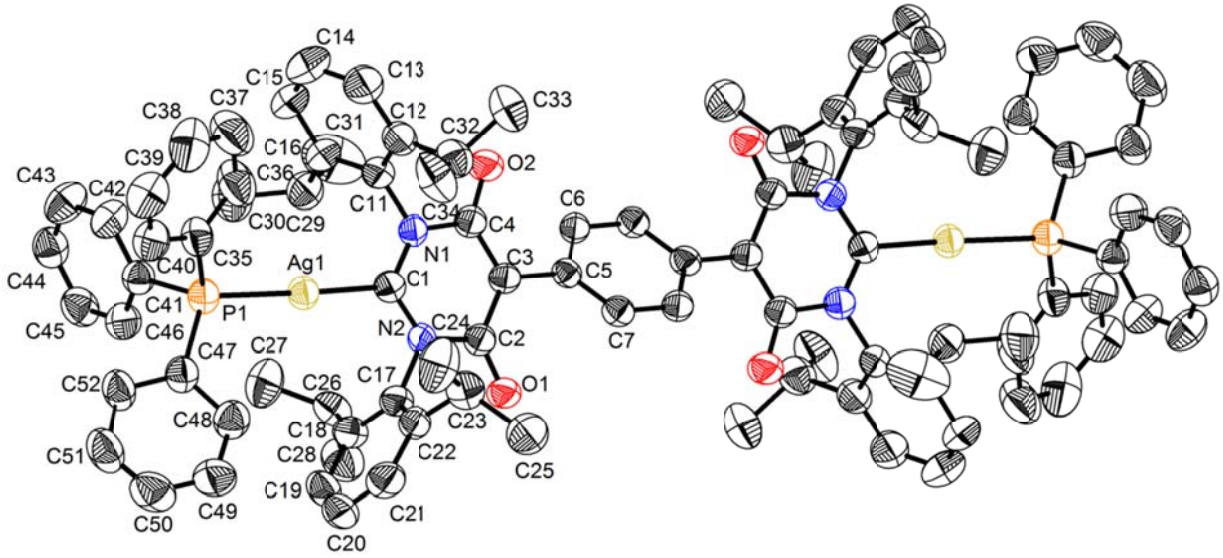
Cl(3)	110(3)	110(3)	106(3)	-17(2)	-4(2)	53(2)
C(48)	78(8)	53(6)	69(7)	1(5)	-19(6)	6(5)
C(46)	68(7)	75(7)	45(5)	17(5)	-6(5)	-16(5)
C(50)	99(11)	82(9)	82(9)	13(7)	-34(8)	-41(8)
C(49)	105(11)	62(7)	88(9)	-17(6)	-42(8)	10(7)
Cl(5)	109(5)	128(5)	154(6)	52(4)	9(4)	41(4)
Cl(6)	88(4)	158(7)	82(4)	12(4)	6(3)	7(4)
Cl(66)	50(14)	90(20)	62(15)	0(15)	15(11)	21(14)
Cl(7)	289(13)	118(5)	125(6)	-27(5)	-3(7)	-15(7)
C(34)	105(11)	84(9)	77(8)	13(7)	-6(7)	-22(8)
C(25)	71(8)	49(6)	159(15)	2(8)	-16(9)	-6(6)
C(91)	42(7)	74(9)	90(10)	1(8)	32(7)	19(6)
C(27)	63(10)	147(17)	240(30)	-65(18)	17(13)	-23(11)
C(92)	190(30)	180(30)	130(20)	-70(20)	90(20)	-30(30)
Cl(4)	120(20)	87(12)	92(10)	-42(9)	80(13)	-56(14)
Cl(44)	71(7)	114(9)	290(30)	-52(14)	70(12)	-19(6)
Cl(9)	286(19)	252(16)	233(14)	10(12)	-103(14)	-5(14)
Cl(8)	236(12)	140(7)	217(10)	-35(7)	112(9)	-1(7)
O(3W)	28(2)	28(2)	27(2)	2(1)	1(1)	1(1)

Table 4B. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **10**.

	x	y	z	U(eq)
H(6)	3096	5142	10355	42
H(26)	3402	6889	8114	67
H(15)	-1735	6749	10080	79
H(14)	-1234	7622	10281	94
H(32)	2995	7164	9441	75
H(13)	615	7961	10029	84
H(36)	-1929	7213	8733	77
H(23)	1185	5269	8134	72
H(44)	2086	8995	6664	74
H(31A)	-2289	6037	9286	155
H(31B)	-1769	5477	9076	155
H(31C)	-1404	6011	8729	155
H(42)	314	8362	8068	67
H(33A)	2790	8043	10261	141
H(33B)	4001	7773	10068	141
H(33C)	3133	7456	10501	141
H(40)	-2355	8363	7388	87
H(43)	1572	9000	7720	73
H(28A)	3998	7680	7651	169
H(28B)	2667	7535	7396	169
H(28C)	3755	7430	6965	169
H(45)	1313	8332	5982	89
H(19)	3131	6723	6443	98
H(21)	1059	5407	6436	87

H(24A)	-624	5597	7636	133
H(24B)	-717	4992	7860	133
H(24C)	-584	5125	7135	133
H(29)	194	5743	9447	79
H(20)	2041	6072	5899	104
H(30A)	-84	5678	10553	143
H(30B)	-942	5266	10172	143
H(30C)	-1470	5810	10424	143
H(52)	-3061	7578	6750	77
H(7)	5574	5440	9099	45
H(90)	4619	6009	10708	76
H(51)	-4014	7137	5906	98
H(38)	-4337	8387	8910	114
H(37)	-3378	7629	9297	99
H(39)	-3832	8770	7968	110
H(48)	-330	6527	6804	81
H(46)	7	7695	6335	75
H(50)	-3107	6378	5493	108
H(49)	-1255	6069	5933	105
H(34A)	1880	7741	8693	133
H(34B)	3249	7892	8854	133
H(34C)	2220	8217	9169	133
H(25A)	1089	4381	7777	141
H(25B)	2332	4637	7610	141
H(25C)	1278	4570	7074	141
H(91)	4825	5299	7511	81
H(27A)	5182	6613	7303	223
H(27B)	5083	6433	8017	223
H(27C)	5423	7035	7859	223
H(92)	-3295	4973	5835	195

3.3 Structural data for 11:



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.

Table 1C. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters (A^2 x 10^3) for **11**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ag(1)	4602(1)	3148(1)	1835(1)	80(1)
P(1)	5889(2)	2575(1)	2428(1)	82(1)
O(1)	2439(5)	3879(2)	-233(2)	83(2)
O(2)	1087(5)	4568(2)	1671(2)	91(2)
N(2)	3224(5)	3622(2)	715(2)	72(2)
N(1)	2566(5)	3950(2)	1627(3)	74(2)
C(1)	3333(6)	3626(2)	1337(3)	72(2)
C(28)	1911(14)	2272(5)	-169(6)	136(4)
C(26)	2511(9)	2522(4)	408(5)	102(3)
C(18)	3728(8)	2732(3)	283(4)	91(2)
C(17)	4086(7)	3275(3)	405(3)	82(2)
C(19)	4609(10)	2413(4)	20(5)	108(3)
C(3)	1638(6)	4280(3)	664(3)	72(2)
C(22)	5160(7)	3484(4)	268(4)	91(2)
C(2)	2398(6)	3932(3)	334(3)	73(2)
C(21)	5991(9)	3124(5)	8(5)	108(3)
C(23)	5498(8)	4072(4)	371(5)	102(3)
C(20)	5722(11)	2605(5)	-102(5)	114(3)
C(4)	1687(6)	4294(3)	1327(3)	76(2)

C(11)	2628(7)	3951(3)	2303(3)	79(2)
C(16)	2071(9)	3540(4)	2626(4)	98(2)
C(12)	3275(8)	4366(3)	2600(4)	93(2)
C(29)	1304(10)	3125(4)	2293(5)	110(3)
C(32)	3904(10)	4795(4)	2249(5)	107(3)
C(13)	3360(12)	4355(5)	3247(5)	123(3)
C(33)	3414(12)	5355(4)	2388(7)	130(4)
C(34)	5255(12)	4776(5)	2349(9)	152(5)
C(27)	2550(13)	2133(6)	945(6)	138(4)
C(5)	799(5)	4645(2)	320(3)	70(2)
C(6)	1123(5)	4912(3)	-213(3)	71(2)
C(7)	-354(6)	4736(3)	532(3)	73(2)
C(25)	5762(14)	4373(6)	-255(7)	145(5)
C(35)	6653(8)	2916(3)	3089(4)	94(2)
C(47)	7038(7)	2238(3)	1994(4)	89(2)
C(41)	5005(7)	2043(3)	2765(4)	83(2)
C(48)	7332(9)	2445(4)	1412(5)	105(3)
C(52)	7573(10)	1773(4)	2211(6)	112(3)
C(46)	4505(10)	1647(4)	2381(5)	105(3)
C(51)	8471(12)	1533(5)	1854(8)	139(4)
C(40)	7663(9)	2715(4)	3394(5)	107(3)
C(42)	4717(10)	2039(5)	3374(4)	108(3)
C(43)	3938(10)	1663(5)	3609(5)	119(3)
C(44)	3472(8)	1277(4)	3220(5)	105(3)
C(15)	2149(14)	3550(5)	3265(4)	128(4)
C(45)	3756(10)	1270(4)	2607(5)	109(3)
C(39)	8215(12)	2976(6)	3882(6)	127(4)
C(38)	7748(16)	3445(6)	4077(8)	156(6)
C(36)	6158(16)	3376(4)	3317(7)	149(6)
C(49)	8226(12)	2191(5)	1093(6)	130(4)
C(50)	8750(11)	1747(6)	1312(7)	134(4)
C(14)	2803(15)	3947(6)	3585(5)	145(5)
C(24)	6562(13)	4145(6)	852(8)	153(5)
C(37)	6631(17)	3642(5)	3847(8)	158(6)
C(30)	1480(20)	2568(5)	2589(9)	182(8)
C(31)	-1(16)	3280(9)	2268(12)	200(10)
Cl(17)	9447(2)	1683(1)	4850(2)	119(1)
Cl(18)	8599(4)	960(2)	3886(2)	151(2)
Cl(19)	10377(3)	1739(1)	3614(1)	122(1)
C(100)	9834(9)	1309(4)	4192(5)	103(3)
Cl(8)	9113(6)	5508(3)	2443(4)	240(3)
Cl(9)	8484	4453	2950	203(6)
Cl(39)	8224	4582	2533	377(16)
Cl(10)	10428(8)	5022(5)	3392(3)	264(4)
C(103)	9546(12)	4906(6)	2705(7)	147(5)
Cl(21)	4214(10)	6029(5)	4066(5)	187(4)

Cl(22)	6511(15)	5445(4)	3971(6)	209(5)
Cl(24)	2155(14)	5269(6)	4831(6)	212(5)
Cl(25)	839(16)	4301(6)	5069(6)	238(7)
Cl(23)	5390(20)	5783(6)	5159(5)	303(12)
C(102)	1863	4779	5450	360(40)
C(101)	5007	5565	4392	165(11)

Table 2C. Bond lengths [Å] and angles [deg] for **11**.

Ag(1)-C(1)	2.110(6)
Ag(1)-P(1)	2.364(2)
P(1)-C(41)	1.820(8)
P(1)-C(47)	1.821(9)
P(1)-C(35)	1.837(9)
O(1)-C(2)	1.226(8)
O(2)-C(4)	1.225(9)
N(2)-C(1)	1.337(9)
N(2)-C(2)	1.436(8)
N(2)-C(17)	1.474(9)
N(1)-C(1)	1.349(9)
N(1)-C(4)	1.437(9)
N(1)-C(11)	1.449(9)
C(28)-C(26)	1.519(15)
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(28)-H(28C)	0.9700
C(26)-C(18)	1.494(14)
C(26)-C(27)	1.504(15)
C(26)-H(26)	0.9900
C(18)-C(19)	1.404(12)
C(18)-C(17)	1.430(12)
C(17)-C(22)	1.353(12)
C(19)-C(20)	1.369(17)
C(19)-H(19)	0.9400
C(3)-C(4)	1.423(10)
C(3)-C(2)	1.424(9)
C(3)-C(5)	1.482(9)
C(22)-C(21)	1.423(12)
C(22)-C(23)	1.525(13)
C(21)-C(20)	1.344(16)
C(21)-H(21)	0.9400
C(23)-C(24)	1.556(17)
C(23)-C(25)	1.577(15)
C(23)-H(23)	0.9900
C(20)-H(20)	0.9400

C(11)-C(16)	1.398(11)
C(11)-C(12)	1.401(11)
C(16)-C(15)	1.370(13)
C(16)-C(29)	1.505(15)
C(12)-C(13)	1.390(14)
C(12)-C(32)	1.499(14)
C(29)-C(31)	1.51(2)
C(29)-C(30)	1.534(16)
C(29)-H(29)	0.9900
C(32)-C(34)	1.519(17)
C(32)-C(33)	1.532(14)
C(32)-H(32)	0.9900
C(13)-C(14)	1.408(19)
C(13)-H(13)	0.9400
C(33)-H(33A)	0.9700
C(33)-H(33B)	0.9700
C(33)-H(33C)	0.9700
C(34)-H(34A)	0.9700
C(34)-H(34B)	0.9700
C(34)-H(34C)	0.9700
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(27)-H(27C)	0.9700
C(5)-C(6)	1.383(9)
C(5)-C(7)	1.404(9)
C(6)-C(7)#1	1.390(9)
C(6)-H(6)	0.9400
C(7)-C(6)#1	1.390(9)
C(7)-H(7)	0.9400
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(25)-H(25C)	0.9700
C(35)-C(36)	1.369(16)
C(35)-C(40)	1.378(13)
C(47)-C(52)	1.376(12)
C(47)-C(48)	1.404(13)
C(41)-C(42)	1.359(12)
C(41)-C(46)	1.390(13)
C(48)-C(49)	1.386(15)
C(48)-H(48)	0.9400
C(52)-C(51)	1.420(16)
C(52)-H(52)	0.9400
C(46)-C(45)	1.359(14)
C(46)-H(46)	0.9400
C(51)-C(50)	1.33(2)
C(51)-H(51)	0.9400

C(40)-C(39)	1.360(16)
C(40)-H(40)	0.9400
C(42)-C(43)	1.387(14)
C(42)-H(42)	0.9400
C(43)-C(44)	1.362(16)
C(43)-H(43)	0.9400
C(44)-C(45)	1.367(15)
C(44)-H(44)	0.9400
C(15)-C(14)	1.39(2)
C(15)-H(15)	0.9400
C(45)-H(45)	0.9400
C(39)-C(38)	1.35(2)
C(39)-H(39)	0.9400
C(38)-C(37)	1.41(2)
C(38)-H(38)	0.9400
C(36)-C(37)	1.403(18)
C(36)-H(36)	0.9400
C(49)-C(50)	1.328(19)
C(49)-H(49)	0.9400
C(50)-H(50)	0.9400
C(14)-H(14)	0.9400
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(24)-H(24C)	0.9700
C(37)-H(37)	0.9400
C(30)-H(30A)	0.9700
C(30)-H(30B)	0.9700
C(30)-H(30C)	0.9700
C(31)-H(31A)	0.9700
C(31)-H(31B)	0.9700
C(31)-H(31C)	0.9700
Cl(17)-C(100)	1.760(11)
Cl(18)-C(100)	1.740(11)
Cl(19)-C(100)	1.766(9)
C(100)-H(100)	0.9900
Cl(8)-C(103)	1.665(18)
Cl(9)-Cl(39)	0.9845(2)
Cl(9)-C(103)	1.736(15)
Cl(10)-C(103)	1.766(18)
C(103)-H(103)	0.9900
Cl(21)-C(101)	1.600(10)
Cl(22)-C(101)	1.965(13)
Cl(22)-C(102)#2	2.235(16)
Cl(24)-C(102)	1.842(15)
Cl(25)-C(102)	1.824(14)
Cl(23)-C(101)	1.772(10)

C(102)-H(10A)	0.9800
C(102)-H(10B)	0.9800
C(101)-H(101)	0.9900
C(1)-Ag(1)-P(1)	175.23(17)
C(41)-P(1)-C(47)	106.0(4)
C(41)-P(1)-C(35)	105.8(4)
C(47)-P(1)-C(35)	106.9(4)
C(41)-P(1)-Ag(1)	108.9(2)
C(47)-P(1)-Ag(1)	115.4(3)
C(35)-P(1)-Ag(1)	113.1(3)
C(1)-N(2)-C(2)	126.8(5)
C(1)-N(2)-C(17)	114.8(5)
C(2)-N(2)-C(17)	118.4(5)
C(1)-N(1)-C(4)	125.9(6)
C(1)-N(1)-C(11)	117.1(5)
C(4)-N(1)-C(11)	117.0(5)
N(2)-C(1)-N(1)	115.5(6)
N(2)-C(1)-Ag(1)	122.4(4)
N(1)-C(1)-Ag(1)	122.2(5)
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(18)-C(26)-C(27)	111.4(9)
C(18)-C(26)-C(28)	112.0(9)
C(27)-C(26)-C(28)	111.1(10)
C(18)-C(26)-H(26)	107.4
C(27)-C(26)-H(26)	107.4
C(28)-C(26)-H(26)	107.4
C(19)-C(18)-C(17)	114.3(9)
C(19)-C(18)-C(26)	122.3(9)
C(17)-C(18)-C(26)	123.4(7)
C(22)-C(17)-C(18)	124.7(7)
C(22)-C(17)-N(2)	118.4(7)
C(18)-C(17)-N(2)	116.9(7)
C(20)-C(19)-C(18)	122.5(10)
C(20)-C(19)-H(19)	118.7
C(18)-C(19)-H(19)	118.7
C(4)-C(3)-C(2)	120.8(6)
C(4)-C(3)-C(5)	118.9(6)
C(2)-C(3)-C(5)	120.2(6)
C(17)-C(22)-C(21)	116.3(9)
C(17)-C(22)-C(23)	123.8(7)
C(21)-C(22)-C(23)	120.0(8)

O(1)-C(2)-C(3)	127.3(6)
O(1)-C(2)-N(2)	117.4(6)
C(3)-C(2)-N(2)	115.3(5)
C(20)-C(21)-C(22)	121.9(10)
C(20)-C(21)-H(21)	119.0
C(22)-C(21)-H(21)	119.0
C(22)-C(23)-C(24)	112.8(9)
C(22)-C(23)-C(25)	112.7(9)
C(24)-C(23)-C(25)	110.3(10)
C(22)-C(23)-H(23)	106.9
C(24)-C(23)-H(23)	106.9
C(25)-C(23)-H(23)	106.9
C(21)-C(20)-C(19)	120.1(8)
C(21)-C(20)-H(20)	119.9
C(19)-C(20)-H(20)	119.9
O(2)-C(4)-C(3)	128.0(6)
O(2)-C(4)-N(1)	116.2(6)
C(3)-C(4)-N(1)	115.7(6)
C(16)-C(11)-C(12)	123.1(7)
C(16)-C(11)-N(1)	119.5(7)
C(12)-C(11)-N(1)	117.4(7)
C(15)-C(16)-C(11)	118.1(10)
C(15)-C(16)-C(29)	120.1(9)
C(11)-C(16)-C(29)	121.5(8)
C(13)-C(12)-C(11)	117.1(9)
C(13)-C(12)-C(32)	120.1(9)
C(11)-C(12)-C(32)	122.8(8)
C(16)-C(29)-C(31)	112.0(10)
C(16)-C(29)-C(30)	111.1(12)
C(31)-C(29)-C(30)	110.8(14)
C(16)-C(29)-H(29)	107.6
C(31)-C(29)-H(29)	107.6
C(30)-C(29)-H(29)	107.6
C(12)-C(32)-C(34)	113.1(10)
C(12)-C(32)-C(33)	111.7(9)
C(34)-C(32)-C(33)	111.3(9)
C(12)-C(32)-H(32)	106.8
C(34)-C(32)-H(32)	106.8
C(33)-C(32)-H(32)	106.8
C(12)-C(13)-C(14)	121.0(11)
C(12)-C(13)-H(13)	119.5
C(14)-C(13)-H(13)	119.5
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5

H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(6)-C(5)-C(7)	117.7(6)
C(6)-C(5)-C(3)	121.7(5)
C(7)-C(5)-C(3)	120.7(6)
C(5)-C(6)-C(7)#1	122.2(6)
C(5)-C(6)-H(6)	118.9
C(7)#1-C(6)-H(6)	118.9
C(6)#1-C(7)-C(5)	120.1(6)
C(6)#1-C(7)-H(7)	120.0
C(5)-C(7)-H(7)	120.0
C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(36)-C(35)-C(40)	118.1(9)
C(36)-C(35)-P(1)	118.6(8)
C(40)-C(35)-P(1)	123.2(7)
C(52)-C(47)-C(48)	119.7(9)
C(52)-C(47)-P(1)	121.4(7)
C(48)-C(47)-P(1)	118.8(6)
C(42)-C(41)-C(46)	117.5(8)
C(42)-C(41)-P(1)	122.8(7)
C(46)-C(41)-P(1)	119.5(6)
C(49)-C(48)-C(47)	118.1(10)
C(49)-C(48)-H(48)	120.9
C(47)-C(48)-H(48)	120.9
C(47)-C(52)-C(51)	118.7(10)
C(47)-C(52)-H(52)	120.7
C(51)-C(52)-H(52)	120.7
C(45)-C(46)-C(41)	121.1(9)
C(45)-C(46)-H(46)	119.5

C(41)-C(46)-H(46)	119.5
C(50)-C(51)-C(52)	120.0(11)
C(50)-C(51)-H(51)	120.0
C(52)-C(51)-H(51)	120.0
C(39)-C(40)-C(35)	122.1(12)
C(39)-C(40)-H(40)	119.0
C(35)-C(40)-H(40)	119.0
C(41)-C(42)-C(43)	122.0(10)
C(41)-C(42)-H(42)	119.0
C(43)-C(42)-H(42)	119.0
C(44)-C(43)-C(42)	119.0(10)
C(44)-C(43)-H(43)	120.5
C(42)-C(43)-H(43)	120.5
C(43)-C(44)-C(45)	120.0(9)
C(43)-C(44)-H(44)	120.0
C(45)-C(44)-H(44)	120.0
C(16)-C(15)-C(14)	121.2(11)
C(16)-C(15)-H(15)	119.4
C(14)-C(15)-H(15)	119.4
C(46)-C(45)-C(44)	120.4(9)
C(46)-C(45)-H(45)	119.8
C(44)-C(45)-H(45)	119.8
C(38)-C(39)-C(40)	118.8(13)
C(38)-C(39)-H(39)	120.6
C(40)-C(39)-H(39)	120.6
C(39)-C(38)-C(37)	122.6(12)
C(39)-C(38)-H(38)	118.7
C(37)-C(38)-H(38)	118.7
C(35)-C(36)-C(37)	122.6(12)
C(35)-C(36)-H(36)	118.7
C(37)-C(36)-H(36)	118.7
C(50)-C(49)-C(48)	121.5(12)
C(50)-C(49)-H(49)	119.3
C(48)-C(49)-H(49)	119.3
C(49)-C(50)-C(51)	121.9(11)
C(49)-C(50)-H(50)	119.0
C(51)-C(50)-H(50)	119.0
C(15)-C(14)-C(13)	119.4(9)
C(15)-C(14)-H(14)	120.3
C(13)-C(14)-H(14)	120.3
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5

C(36)-C(37)-C(38)	114.8(14)
C(36)-C(37)-H(37)	122.6
C(38)-C(37)-H(37)	122.6
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(29)-C(31)-H(31A)	109.5
C(29)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(29)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
Cl(18)-C(100)-Cl(17)	110.6(5)
Cl(18)-C(100)-Cl(19)	109.1(6)
Cl(17)-C(100)-Cl(19)	110.2(5)
Cl(18)-C(100)-H(100)	109.0
Cl(17)-C(100)-H(100)	109.0
Cl(19)-C(100)-H(100)	109.0
Cl(39)-Cl(9)-C(103)	72.2(6)
Cl(8)-C(103)-Cl(9)	119.5(8)
Cl(8)-C(103)-Cl(10)	106.3(9)
Cl(9)-C(103)-Cl(10)	102.7(9)
Cl(8)-C(103)-H(103)	109.2
Cl(9)-C(103)-H(103)	109.2
Cl(10)-C(103)-H(103)	109.2
C(101)-Cl(22)-C(102)#2	118.4(6)
Cl(25)-C(102)-Cl(24)	103.6(6)
Cl(25)-C(102)-H(10A)	111.1
Cl(24)-C(102)-H(10A)	111.0
Cl(25)-C(102)-H(10B)	111.0
Cl(24)-C(102)-H(10B)	111.0
H(10A)-C(102)-H(10B)	109.0
Cl(21)-C(101)-Cl(23)	107.2(8)
Cl(21)-C(101)-Cl(22)	112.3(6)
Cl(23)-C(101)-Cl(22)	107.1(9)
Cl(21)-C(101)-H(101)	110.1
Cl(23)-C(101)-H(101)	110.1
Cl(22)-C(101)-H(101)	110.1

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z #2 -x+1,-y+1,-z+1

Table 3C. Anisotropic displacement parameters (A^2 x 10^3) for **11**. The anisotropic 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}
Ag(1)	79(1)	76(1)	83(1)	9(1)	5(1)	7(1)
P(1)	79(2)	78(1)	89(2)	12(1)	4(1)	3(1)
O(1)	82(3)	95(3)	72(3)	-2(2)	6(2)	21(2)
O(2)	89(3)	103(4)	80(3)	-3(2)	7(2)	24(3)
N(2)	67(3)	75(3)	74(3)	5(2)	8(2)	9(2)
N(1)	71(3)	73(3)	77(3)	4(2)	6(2)	1(2)
C(1)	65(3)	71(3)	79(4)	3(3)	7(3)	-3(2)
C(28)	149(10)	114(7)	142(9)	-22(7)	-30(8)	4(7)
C(26)	109(6)	83(5)	115(6)	-18(4)	9(5)	6(4)
C(18)	102(5)	91(5)	81(4)	-7(3)	4(4)	14(4)
C(17)	82(4)	88(4)	75(4)	-2(3)	9(3)	13(3)
C(19)	120(7)	95(5)	107(6)	-4(4)	-9(5)	43(5)
C(3)	63(3)	79(4)	76(3)	6(3)	12(2)	4(3)
C(22)	82(4)	103(5)	89(4)	8(4)	15(3)	22(4)
C(2)	66(3)	78(4)	74(4)	3(3)	6(2)	4(3)
C(21)	82(5)	140(9)	102(6)	14(5)	23(4)	28(5)
C(23)	75(4)	109(6)	124(6)	7(5)	21(4)	-1(4)
C(20)	119(8)	117(7)	108(6)	4(5)	13(5)	58(6)
C(4)	70(3)	81(4)	77(4)	5(3)	9(3)	7(3)
C(11)	82(4)	79(4)	77(4)	0(3)	6(3)	8(3)
C(16)	116(6)	98(5)	80(4)	8(4)	25(4)	3(4)
C(12)	102(5)	85(4)	91(5)	-6(3)	-5(4)	11(4)
C(29)	113(7)	99(6)	120(7)	16(5)	37(6)	-7(5)
C(32)	115(7)	89(5)	117(6)	-10(4)	-2(5)	-8(4)
C(13)	149(9)	120(7)	98(6)	-8(5)	-10(6)	15(7)
C(33)	128(8)	88(6)	172(11)	0(6)	-13(8)	5(5)
C(34)	118(8)	95(6)	244(17)	-6(8)	11(9)	3(6)
C(27)	137(10)	139(9)	136(9)	32(7)	-14(7)	-30(8)
C(5)	63(3)	69(3)	78(3)	-2(2)	7(2)	5(2)
C(6)	58(3)	78(4)	79(3)	-2(3)	10(2)	3(2)
C(7)	67(3)	77(3)	75(3)	4(3)	11(3)	5(3)
C(25)	157(11)	130(9)	152(10)	21(8)	59(9)	3(8)
C(35)	103(5)	73(4)	106(5)	9(4)	-11(4)	-6(4)
C(47)	84(4)	87(4)	97(5)	12(4)	4(3)	4(3)
C(41)	74(4)	83(4)	90(4)	8(3)	3(3)	4(3)
C(48)	98(6)	107(6)	112(6)	15(5)	13(5)	1(4)
C(52)	97(6)	99(6)	140(8)	22(5)	23(5)	19(4)
C(46)	117(7)	96(5)	104(6)	-2(4)	13(5)	-7(5)
C(51)	121(8)	113(7)	185(12)	14(8)	28(8)	35(6)
C(40)	99(6)	110(6)	110(6)	14(5)	-9(5)	-9(5)
C(42)	117(7)	122(7)	85(5)	9(4)	2(4)	-22(5)
C(43)	112(7)	148(9)	97(6)	15(6)	4(5)	-36(6)
C(44)	89(5)	93(5)	133(7)	17(5)	16(5)	-2(4)

C(15)	186(12)	121(7)	78(5)	13(5)	31(6)	6(7)
C(45)	119(7)	80(5)	128(7)	-9(4)	8(5)	-13(4)
C(39)	118(8)	140(9)	122(8)	13(7)	-17(6)	-36(7)
C(38)	179(14)	127(9)	156(11)	24(8)	-62(10)	-50(9)
C(36)	202(14)	91(6)	148(10)	-17(6)	-62(10)	17(7)
C(49)	128(8)	133(9)	131(8)	-1(7)	43(7)	8(7)
C(50)	104(7)	133(9)	168(12)	-12(8)	43(7)	13(6)
C(14)	195(14)	168(11)	72(5)	3(6)	9(6)	7(10)
C(24)	133(10)	158(11)	167(11)	45(9)	-18(8)	-51(8)
C(37)	195(15)	109(8)	166(12)	-27(8)	-37(11)	24(8)
C(30)	260(20)	95(7)	195(15)	27(8)	64(15)	-24(10)
C(31)	125(11)	205(17)	270(30)	-76(17)	33(14)	-46(12)
Cl(17)	102(2)	123(2)	132(2)	7(1)	26(1)	6(1)
Cl(18)	142(3)	149(3)	161(3)	20(2)	1(2)	-54(2)
Cl(19)	109(2)	140(2)	119(2)	26(2)	16(1)	-19(1)
C(100)	95(5)	104(6)	109(6)	21(4)	14(4)	10(4)
Cl(8)	179(5)	250(7)	290(8)	75(6)	2(5)	66(5)
Cl(9)	189(10)	139(6)	291(13)	-40(7)	130(9)	-42(6)
Cl(39)	113(7)	330(20)	690(40)	-220(30)	68(15)	-48(10)
Cl(10)	235(7)	380(12)	178(5)	51(6)	32(5)	71(7)
C(103)	112(8)	171(12)	160(11)	-39(9)	51(8)	4(8)
Cl(21)	188(8)	198(9)	174(7)	50(7)	-16(6)	-11(7)
Cl(22)	289(15)	163(7)	179(8)	-3(6)	71(9)	7(8)
Cl(24)	261(14)	207(10)	168(8)	-41(7)	2(8)	5(9)
Cl(25)	307(16)	215(11)	199(10)	-47(8)	117(11)	-88(11)
Cl(23)	530(30)	224(12)	143(7)	43(7)	-122(12)	-174(16)
C(102)	360(40)	360(40)	360(40)	-1(5)	16(5)	-1(5)
C(101)	167(12)	166(12)	163(12)	-1(5)	4(5)	-1(5)

Table 4C. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **11**.

	x	y	z	U(eq)
H(28A)	1895	2531	-507	204
H(28B)	1099	2170	-79	204
H(28C)	2355	1956	-289	204
H(26)	2015	2831	530	123
H(19)	4428	2053	-78	129
H(21)	6751	3252	-90	129
H(23)	4798	4251	548	123
H(20)	6299	2374	-262	137
H(29)	1566	3103	1859	132
H(32)	3731	4726	1800	128
H(13)	3796	4624	3462	147
H(33A)	2547	5344	2373	195

H(33B)	3683	5607	2079	195
H(33C)	3701	5468	2799	195
H(34A)	5464	4836	2786	228
H(34B)	5616	5053	2100	228
H(34C)	5547	4426	2225	228
H(27A)	2827	1786	804	207
H(27B)	1755	2095	1104	207
H(27C)	3092	2267	1273	207
H(6)	1889	4853	-364	86
H(7)	-606	4559	891	88
H(25A)	6478	4226	-428	217
H(25B)	5877	4753	-171	217
H(25C)	5091	4326	-550	217
H(48)	6933	2747	1242	127
H(52)	7349	1618	2588	134
H(46)	4688	1638	1957	126
H(51)	8868	1223	2002	167
H(40)	7980	2386	3261	128
H(42)	5055	2299	3645	130
H(43)	3736	1673	4029	143
H(44)	2954	1016	3374	126
H(15)	1755	3285	3491	153
H(45)	3432	1004	2340	131
H(39)	8909	2834	4079	152
H(38)	8182	3648	4378	187
H(36)	5475	3519	3109	179
H(49)	8466	2336	714	156
H(50)	9335	1580	1077	161
H(14)	2871	3942	4023	174
H(24A)	6322	4030	1260	230
H(24B)	6792	4521	869	230
H(24C)	7235	3931	726	230
H(37)	6236	3930	4034	189
H(30A)	2328	2505	2672	273
H(30B)	1163	2296	2306	273
H(30C)	1066	2553	2977	273
H(31A)	-342	3206	2667	300
H(31B)	-423	3074	1945	300
H(31C)	-77	3660	2175	300
H(100)	10467	1048	4317	123
H(103)	10042	4732	2391	176
H(10A)	2603	4602	5597	434
H(10B)	1493	4953	5804	434
H(101)	4544	5227	4405	199

Table 5C. Torsion angles [deg] for **11·**.

C(1)-Ag(1)-P(1)-C(41)	10(2)
C(1)-Ag(1)-P(1)-C(47)	129(2)
C(1)-Ag(1)-P(1)-C(35)	-107(2)
C(2)-N(2)-C(1)-N(1)	1.1(9)
C(17)-N(2)-C(1)-N(1)	178.6(6)
C(2)-N(2)-C(1)-Ag(1)	-179.7(5)
C(17)-N(2)-C(1)-Ag(1)	-2.1(8)
C(4)-N(1)-C(1)-N(2)	-1.6(9)
C(11)-N(1)-C(1)-N(2)	177.9(6)
C(4)-N(1)-C(1)-Ag(1)	179.1(5)
C(11)-N(1)-C(1)-Ag(1)	-1.4(8)
P(1)-Ag(1)-C(1)-N(2)	-116(2)
P(1)-Ag(1)-C(1)-N(1)	63(2)
C(27)-C(26)-C(18)-C(19)	71.5(12)
C(28)-C(26)-C(18)-C(19)	-53.6(12)
C(27)-C(26)-C(18)-C(17)	-110.1(10)
C(28)-C(26)-C(18)-C(17)	124.8(9)
C(19)-C(18)-C(17)-C(22)	2.0(12)
C(26)-C(18)-C(17)-C(22)	-176.5(8)
C(19)-C(18)-C(17)-N(2)	-176.6(7)
C(26)-C(18)-C(17)-N(2)	4.9(11)
C(1)-N(2)-C(17)-C(22)	-87.7(8)
C(2)-N(2)-C(17)-C(22)	90.0(8)
C(1)-N(2)-C(17)-C(18)	90.9(8)
C(2)-N(2)-C(17)-C(18)	-91.3(8)
C(17)-C(18)-C(19)-C(20)	0.8(13)
C(26)-C(18)-C(19)-C(20)	179.3(9)
C(18)-C(17)-C(22)-C(21)	-2.7(12)
N(2)-C(17)-C(22)-C(21)	175.9(7)
C(18)-C(17)-C(22)-C(23)	176.6(8)
N(2)-C(17)-C(22)-C(23)	-4.8(12)
C(4)-C(3)-C(2)-O(1)	179.4(7)
C(5)-C(3)-C(2)-O(1)	-2.0(11)
C(4)-C(3)-C(2)-N(2)	-2.3(9)
C(5)-C(3)-C(2)-N(2)	176.3(6)
C(1)-N(2)-C(2)-O(1)	179.3(6)
C(17)-N(2)-C(2)-O(1)	1.8(9)
C(1)-N(2)-C(2)-C(3)	0.8(9)
C(17)-N(2)-C(2)-C(3)	-176.6(6)
C(17)-C(22)-C(21)-C(20)	0.7(14)
C(23)-C(22)-C(21)-C(20)	-178.7(9)
C(17)-C(22)-C(23)-C(24)	117.1(11)
C(21)-C(22)-C(23)-C(24)	-63.7(12)
C(17)-C(22)-C(23)-C(25)	-117.3(10)

C(21)-C(22)-C(23)-C(25)	62.0(12)
C(22)-C(21)-C(20)-C(19)	1.9(16)
C(18)-C(19)-C(20)-C(21)	-2.7(15)
C(2)-C(3)-C(4)-O(2)	-179.5(7)
C(5)-C(3)-C(4)-O(2)	1.9(11)
C(2)-C(3)-C(4)-N(1)	1.9(9)
C(5)-C(3)-C(4)-N(1)	-176.7(6)
C(1)-N(1)-C(4)-O(2)	-178.6(7)
C(11)-N(1)-C(4)-O(2)	1.9(9)
C(1)-N(1)-C(4)-C(3)	0.2(10)
C(11)-N(1)-C(4)-C(3)	-179.3(6)
C(1)-N(1)-C(11)-C(16)	-80.3(9)
C(4)-N(1)-C(11)-C(16)	99.2(8)
C(1)-N(1)-C(11)-C(12)	98.4(8)
C(4)-N(1)-C(11)-C(12)	-82.0(8)
C(12)-C(11)-C(16)-C(15)	1.0(14)
N(1)-C(11)-C(16)-C(15)	179.8(9)
C(12)-C(11)-C(16)-C(29)	175.1(8)
N(1)-C(11)-C(16)-C(29)	-6.2(12)
C(16)-C(11)-C(12)-C(13)	0.6(13)
N(1)-C(11)-C(12)-C(13)	-178.1(8)
C(16)-C(11)-C(12)-C(32)	177.8(9)
N(1)-C(11)-C(12)-C(32)	-0.9(12)
C(15)-C(16)-C(29)-C(31)	80.4(16)
C(11)-C(16)-C(29)-C(31)	-93.6(15)
C(15)-C(16)-C(29)-C(30)	-44.1(15)
C(11)-C(16)-C(29)-C(30)	142.0(11)
C(13)-C(12)-C(32)-C(34)	62.5(14)
C(11)-C(12)-C(32)-C(34)	-114.7(11)
C(13)-C(12)-C(32)-C(33)	-64.0(13)
C(11)-C(12)-C(32)-C(33)	118.8(10)
C(11)-C(12)-C(13)-C(14)	-0.9(16)
C(32)-C(12)-C(13)-C(14)	-178.2(12)
C(4)-C(3)-C(5)-C(6)	138.9(7)
C(2)-C(3)-C(5)-C(6)	-39.8(9)
C(4)-C(3)-C(5)-C(7)	-40.2(9)
C(2)-C(3)-C(5)-C(7)	141.2(7)
C(7)-C(5)-C(6)-C(7)#1	0.5(11)
C(3)-C(5)-C(6)-C(7)#1	-178.6(6)
C(6)-C(5)-C(7)-C(6)#1	-0.5(10)
C(3)-C(5)-C(7)-C(6)#1	178.6(6)
C(41)-P(1)-C(35)-C(36)	-96.9(11)
C(47)-P(1)-C(35)-C(36)	150.5(10)
Ag(1)-P(1)-C(35)-C(36)	22.3(11)
C(41)-P(1)-C(35)-C(40)	78.9(9)
C(47)-P(1)-C(35)-C(40)	-33.7(9)

Ag(1)-P(1)-C(35)-C(40)	-161.9(7)
C(41)-P(1)-C(47)-C(52)	-37.2(9)
C(35)-P(1)-C(47)-C(52)	75.3(9)
Ag(1)-P(1)-C(47)-C(52)	-157.9(8)
C(41)-P(1)-C(47)-C(48)	139.3(7)
C(35)-P(1)-C(47)-C(48)	-108.2(8)
Ag(1)-P(1)-C(47)-C(48)	18.7(8)
C(47)-P(1)-C(41)-C(42)	131.8(8)
C(35)-P(1)-C(41)-C(42)	18.5(9)
Ag(1)-P(1)-C(41)-C(42)	-103.4(8)
C(47)-P(1)-C(41)-C(46)	-54.2(8)
C(35)-P(1)-C(41)-C(46)	-167.5(7)
Ag(1)-P(1)-C(41)-C(46)	70.6(7)
C(52)-C(47)-C(48)-C(49)	-4.7(16)
P(1)-C(47)-C(48)-C(49)	178.7(9)
C(48)-C(47)-C(52)-C(51)	4.1(17)
P(1)-C(47)-C(52)-C(51)	-179.4(10)
C(42)-C(41)-C(46)-C(45)	0.0(15)
P(1)-C(41)-C(46)-C(45)	-174.2(8)
C(47)-C(52)-C(51)-C(50)	-2(2)
C(36)-C(35)-C(40)-C(39)	-4.4(17)
P(1)-C(35)-C(40)-C(39)	179.7(9)
C(46)-C(41)-C(42)-C(43)	-1.1(16)
P(1)-C(41)-C(42)-C(43)	173.0(9)
C(41)-C(42)-C(43)-C(44)	1.6(19)
C(42)-C(43)-C(44)-C(45)	-1.1(18)
C(11)-C(16)-C(15)-C(14)	-2.4(18)
C(29)-C(16)-C(15)-C(14)	-176.6(12)
C(41)-C(46)-C(45)-C(44)	0.5(16)
C(43)-C(44)-C(45)-C(46)	0.1(17)
C(35)-C(40)-C(39)-C(38)	0.9(19)
C(40)-C(39)-C(38)-C(37)	8(2)
C(40)-C(35)-C(36)-C(37)	-1(2)
P(1)-C(35)-C(36)-C(37)	175.4(14)
C(47)-C(48)-C(49)-C(50)	4(2)
C(48)-C(49)-C(50)-C(51)	-2(2)
C(52)-C(51)-C(50)-C(49)	1(2)
C(16)-C(15)-C(14)-C(13)	2(2)
C(12)-C(13)-C(14)-C(15)	0(2)
C(35)-C(36)-C(37)-C(38)	8(3)
C(39)-C(38)-C(37)-C(36)	-12(3)
Cl(39)-Cl(9)-C(103)-Cl(8)	51.0(9)
Cl(39)-Cl(9)-C(103)-Cl(10)	168.3(8)
C(102)#2-Cl(22)-C(101)-Cl(21)	145.3(6)
C(102)#2-Cl(22)-C(101)-Cl(23)	27.9(7)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z #2 -x+1,-y+1,-z+1