SUPPORTING INFORMATION

Luminescent, Three-Coordinate Azadipyrromethene Complexes of d^{10} Copper, Silver, and Gold

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Contents

Experimental Methods

Abbreviations: OTf = trifluoromethanesulfonate. DIPEA = diisopropylethylamine. THF = tetrahydrofuran. 2-MeTHF = 2-methyltetrahydrofuran.

General. PPh_3, PEt_3 AgOTf, diisopropylethylamine, and $(CuOTf)_2$·toluene were obtained commercially and used as received. PPh_3AgOTf[1] and (3,5-diphenyl-1*H*-pyrrol-2-yl)(3,5-diphenylpyrrol-2-ylidene)amine] (**1**)[2] were prepared as previously described. Air-sensitive solids were handled and weighed in an inert-atmosphere glovebox operating at <10 ppm O_2.[3] Reactions involving air-sensitive materials were carried out under an atmosphere of Argon using standard Schlenk-line techniques; solvents for such reactions were purified with an M-Braun SPS and purged with argon prior to use.[4] ^1H and ^{31}P NMR spectra were recorded on a Varian AS-400 spectrometer, operating at 400 MHz and 161.8 MHz respectively. Microanalyses were performed by Quantitative Technologies Inc. and by Robertson Microlit Laboratories. Emission measurements were made in degassed solvents. Steady state emission spectra were recorded on a Cary Eclipse fluorescence spectrometer or on an automated Photon Technology International (PTI) QM 4 fluorimeter equipped with a 150-W Xe arc lamp and a Hamamatsu R928 photomultiplier tube. Excitation light was excluded with appropriate glass filters. Sample solutions were added to a quartz EPR tube, freeze pump thaw degassed (4 cycles, 1×10^{-5} Torr) and flame sealed. Low temperature emission spectra were recorded in rigid solvent glass at 77 K by immersion of the sealed EPR tubes into a liquid nitrogen-filled dewar. Integrated emission quantum yields[5] were determined in dry-deoxygenated chloroform at 23 ± 2 °C relative to $(Bu_4N)_2[Mo_6Cl_{14}]$ as a standard (ϕ_{em} = 0.19, 436-nm excitation in CH_3CN).[6] A 435.8 nm wavelength was used to excited samples. Quantum yields were corrected as follows:

$$\phi_s = \phi_r \left(\frac{A_r \eta_s^2 D_s}{A_s \eta_r^2 D_r} \right), \tag{1}$$

where the s and r indices designate the sample and reference samples, respectively, *A* is the absorbance at λ_{exc}, η is the average refractive index of the appropriate solution, and *D* is the integrated area under the corrected emission spectrum.[7] Absorption spectra were obtained with a Cary 5 absorption spectrometer.

Compound 2. PPh_3CuOTf was generated *in situ* by stirring $(CuOTF)_2$·toluene (28 mg, 0.054 mmol) and PPh_3 (28 mg, 0.11 mmol) in 5 mL of THF for 20 min at room temperature. To the resulting solution was added a solution of **1** (48 mg, 0.11 mmol) in 7 mL THF via syringe,

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[2] Gorman, A.; Killoran, J.; O'Shea, C.; Kenna, T.; Gallagher, W. M.; O'Shea, D. F. *J. Am. Chem. Soc.* **2004**, *126,* 10619-10631.
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[5] Demas, J. N.; Crosby, G. A. *J. Phys. Chem.* **1971**, *75*, 991–1024.
[6] Maverick, A. W.; Najdzionek, J. S.; MacKenzie, D.; Nocera, D. G.; Gray, H. B. *J. Am. Chem. Soc.* **1983**, *105*, 1878-1882.
[7] Gray, T. G.; Rudzinski, C. M.; Meyer, E. E.; Holm, R. H.; Nocera, D. G. *J. Am. Chem. Soc.* **2003**, *125*, 4755-4770.

followed by DIPEA (0.16 mL, 0.98 mmol). The reaction mixture was stirred at room temperature for 1 h, at which time all volatiles were removed *in vacuo.* The resulting residue was dried *in vacuo* overnight to give a bluish-black solid, which taken up in ca. 4 mL toluene, filtered through celite, and crystallized by vapor diffusion of pentane in the glovebox. Yield: 75 mg (88 %). ^{1}H NMR ($CDCl_3$): δ 8.04 (dd, 4H), 7.93 (dd, 4H), 7.27-7.40 (m, 9H), 7.24 (s, 2H), 7.17 (t, 6H), 6.91-7.00 (m, 12H). ^{31}P NMR ($CDCl_3$): δ 3.8 (s, br) ppm. UV-Vis ($CHCl_3$): λ (ε) 305 (38000), 597 (38000) nm. Emission ($CHCl_3$, λ_{ex} = 550 nm): λ 642 nm. Anal. Calcd. for $C_{50}H_{37}N_3PCu$: C, 77.55; H, 4.82; N, 5.43. Found: C, 77.55; H, 4.79; N, 5.30.

Compound 3. PPh_3AgOTf (58 mg, 0.11 mmol) and **1** (50 mg, 0.11 mmol) were dissolved in 12 mL THF, and DIPEA (0.16 mL, 0.98 mmol) was added via syringe. After stirring for 1 h at room temperature, the solvent was stripped via rotary evaporation. The resulting residue was taken up in 20 mL benzene, and washed with 2 x 20 mL H_2O. The organic layer was dried with $MgSO_4$ and evaporated to dryness. The product was crystallized from a concentrated THF solution via room temperature vapor diffusion of pentane. Yield: 51 mg (62 %). ^{1}H NMR ($CDCl_3$): δ 8.03 (dd, 4H), 7.96 (dd, 4H), 7.30-7.37 (m, 9H), 7.23 (s, 2H), 7.18 (td, 6H), 6.84-6.90 (m, 12H). ^{31}P NMR ($CDCl_3$): δ 14.4 (s, br) ppm. UV-Vis ($CHCl_3$): λ (ε) 306 (30000), 615 (65000) nm. Emission ($CHCl_3$, λ_{ex} = 550 nm): λ 647 nm. Anal. Calcd. for $C_{50}H_{37}N_3PAg$: C, 73.35; H, 4.56; N, 5.13. Found: C, 73.08; H, 4.41; N, 5.13.

Compound 4. Sodium *tert*-butoxide (18 mg, 0.18 mmol) was suspended in 3 mL of THF, and this slurry was added to a 2 mL THF solution of **1** (47 mg, 0.11 mmol). The resultant suspension was stirred for 8 h in a glove box, and the solvent was removed in vacuo. A small amount of THF (~ 1 mL) was added to the flask to soften the residue, which was scraped into the THF with a spatula. Toluene (10 mL) was added, followed by $(PPh_3)AuCl$ (51 mg, 0.10 mmol). The mixture was stirred for 48 h under an inert gas, and filtered in air. The filtrate (which was always contaminated with a small amount of free azadipyrromethene) was reduced to dryness via rotary evaporation, and a minimum of benzene was added. The benzene suspension was filtered, and pentane vapor was diffused. After 1-2 volume equivalents of pentane were diffused, the mother liquor was dumped into pentane, and allowed to stand for a day or more. Gold-colored crystals formed in erratic yields (26-54%). ^{1}H NMR (C_6D_6): δ 8.26 (dd, 4H, CH), 8.09-8.12 (m, 4H, CH), 7.35 (s, 2H, CH), 6.78-7.38 (m, 27H, CH) ppm. ^{31}P NMR (C_6D_6): δ 30.7 ppm. UV-Vis ($CHCl_3$): λ (ε) 304 (40000), 600 (45000) nm. Emission ($CHCl_3$, λ_{ex} = 550 nm): λ = 645 nm. Anal. Calcd. for $C_{50}H_{37}AuN_3P$: C, 66.15; H, 4.11; N, 4.63. Found: C, 65.96; H, 3.92, N, 4.43.

X-Ray Structure Determinations. Single crystal X-ray data were collected on a Bruker AXS SMART APEX CCD diffractometer using monochromatic Mo Kα radiation with the omega scan technique. The unit cells were determined using SMART[8] and SAINT+.[9] Data collection for all crystals was conducted at 100 K (–173.5°C). All structures were solved by direct methods and refined by full matrix least squares against F^2 with all reflections using SHELXTL.[10]

[8] Bruker Advanced X-ray Solutions, *SMART for WNT/2000* (Version 5.628), Bruker AXS Inc., Madison, Wisconsin: USA, 1997-2002.
[9] Bruker Advanced X-ray Solutions, *SAINT* (Version 6.45), Bruker AXS Inc., Madison, Wisconsin: USA, 1997-2003.
[10] Bruker Advanced X-ray Solutions *SHELXTL* (Version 6.10), Bruker AXS Inc., Madison, Wisconsin: USA, 2000.

Refinement of extinction coefficients was found to be insignificant. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in standard calculated positions and all hydrogen atoms were refined with an isotropic displacement parameter 1.2 times that of the adjacent carbon atom. Absorption corrections were applied using SADABS. For complex **3** the data set was corrected using the program SQUEEZE.

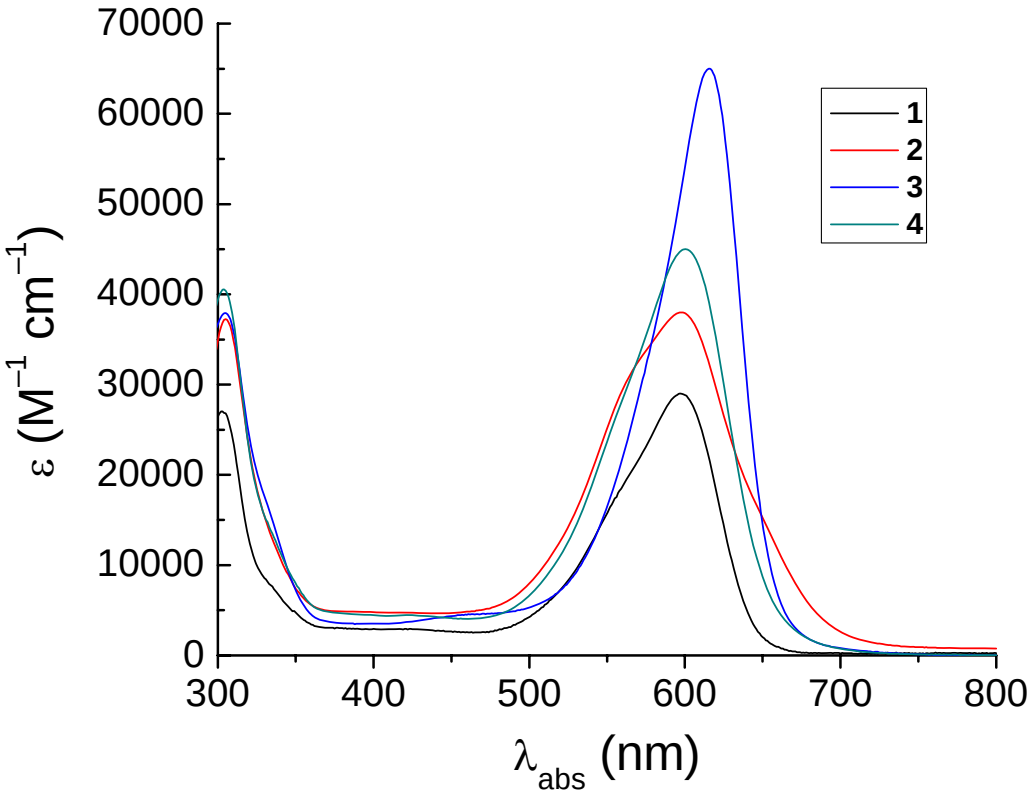

Figure S1. UV-vis absorption spectra (25 °C, $CHCl_3$) from 300 to 800 nm of neutral (protonated) ligand **1** and complexes **2**–**4**.

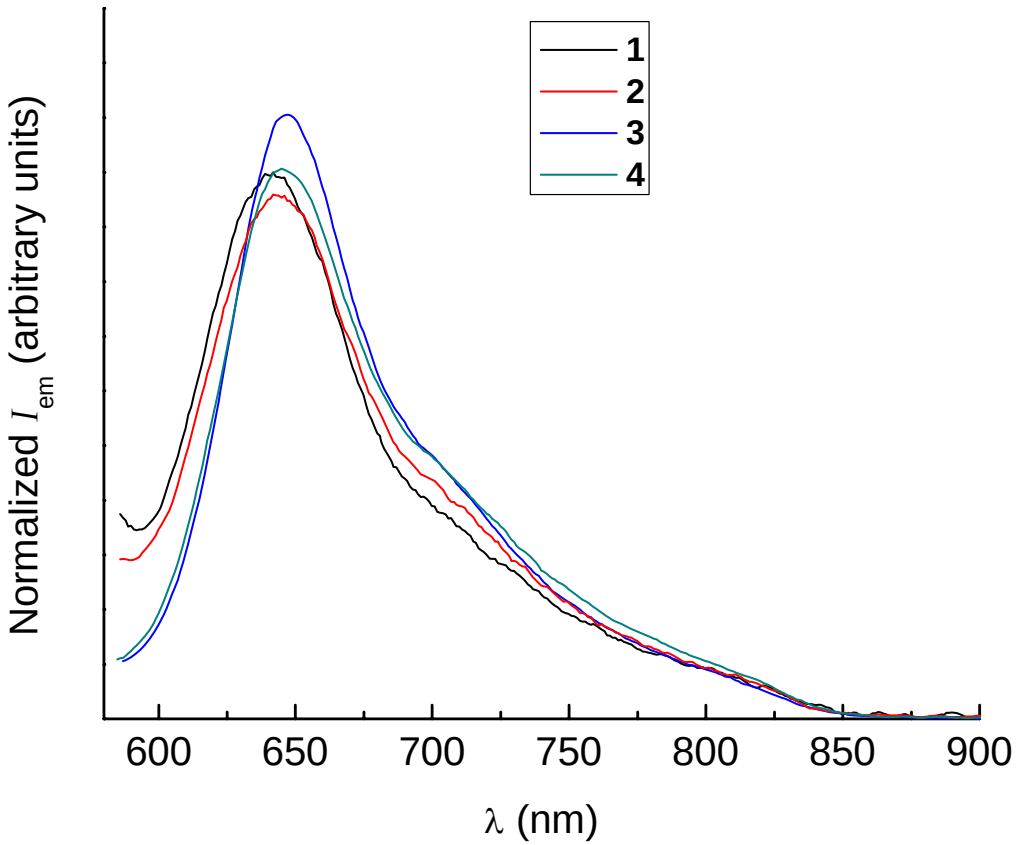

Figure S2. Emission spectra (550-nm excitation, 25 °C, $CHCl_3$) neutral (protonated) ligand **1** and complexes **2**–**4**.

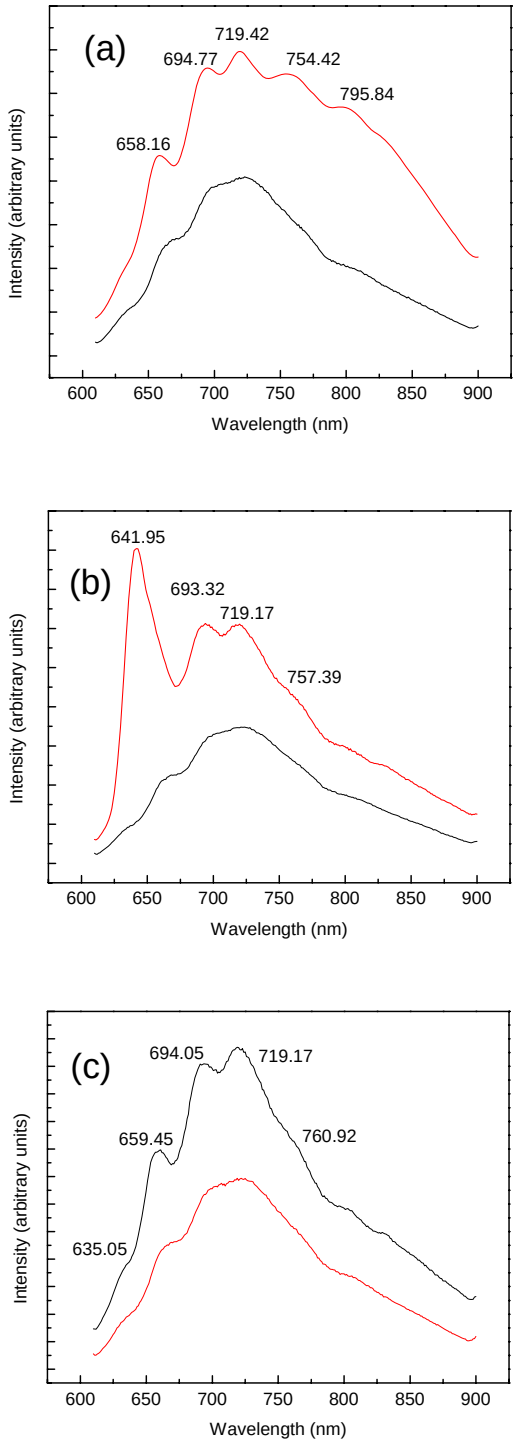

Figure S3. Room-temperature (298±2 K, black) and low-temperature (77 K, red) emission spectra in 2-MeTHF glass: (a) **2**, (b), **3**, and (c) **4**. Local maxima of vibronic peaks at 77 K are indicated.

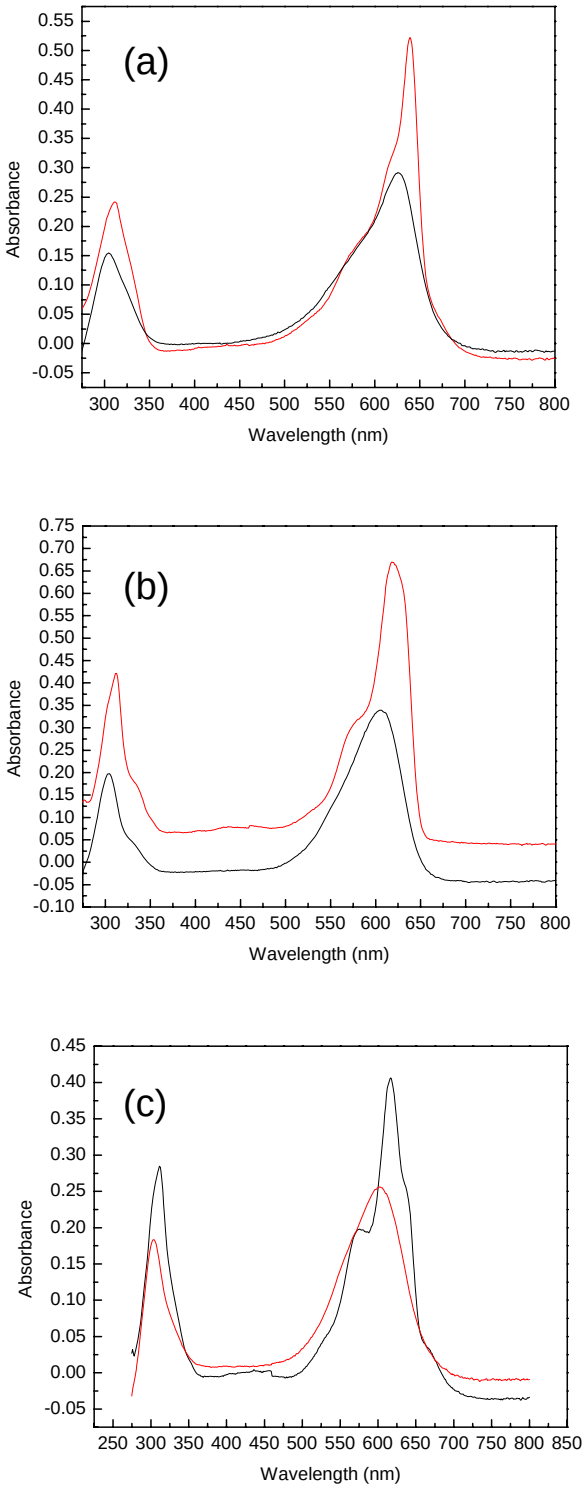

Figure S4. Room-temperature (298±2 K, black) and low-temperature (77 K, red) absorption spectra in 2-MeTHF: (a) **2**, (b), **3**, and (c) **4**. Local maxima of vibronic peaks at 77 K are indicated. Concentration of all solutions is 2×10^{-5} M.

X-Ray Structural Data for **2**

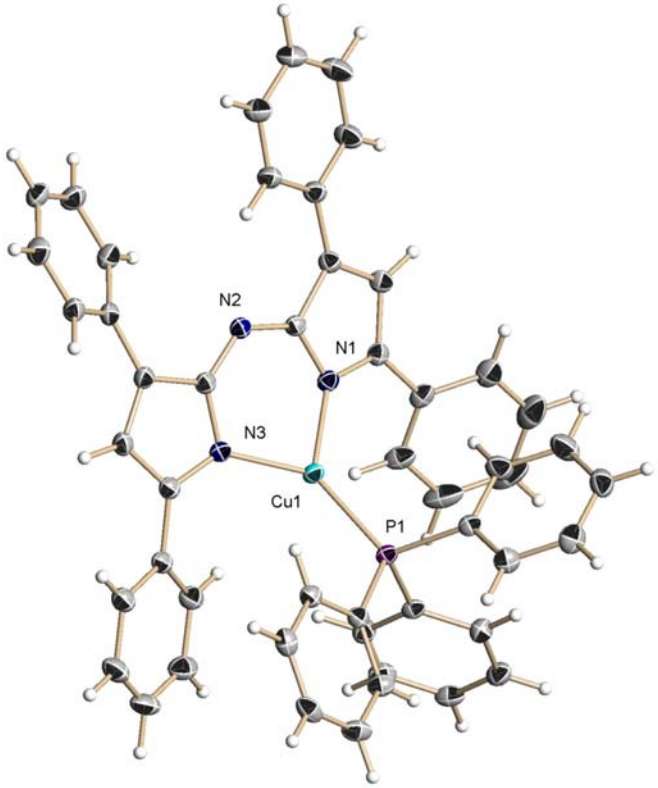

Figure S5. Thermal ellipsoid plot of $(Ph_3P)Cu^I$(tetraphenylazadipyrromethene) (**2**). Ellipsoids are drawn at 50% probability; data were collected at 100 K.

Table S1. Crystal data and structure refinement for **2**.

Identification code: 06mz229m

Empirical formula: C50 H37 Cu N3 P

Formula weight: 774.34

Temperature: 100(2) K

Wavelength: 0.71073 Å

Crystal system: Monoclinic

Space group: $P2_1/n$

Unit cell dimensions:

a = 12.2778(8) Å, α = 90°

b = 12.9304(8) Å, β = 92.5540(10)°

c = 23.6398(15) Å, γ = 90°

Volume, Z: 3749.3(4) $Å^3$, 4

Density (calculated): 1.372 g/m^3

Absorption coefficient: 0.666 mm^{-1}

F(000): 1608

Crystal size: 0.57 × 0.44 × 0.14

Crystal shape, colour: plate, black

θ range for data collection: 1.72 to 28.28°

Limiting indices: $-16 \leq h \leq 14$, $-14 \leq k \leq 17$, $-18 \leq l \leq 31$

Reflections collected: 31895

Independent reflections: 9282 (R(int) = 0.0283)

Completeness to θ = 28.28°: 99.8 %

Absorption correction: multi-scan

Max. and min. transmission: 0.911 and 0.758

Refinement method: Full-matrix least-squares on F^2

Data / restraints / parameters: 9282 / 0 / 496

Goodness-of-fit on F^2: 1.023

Final R indices [$I>2\sigma(I)$]: R1 = 0.0374, wR2 = 0.0936

R indices (all data): R1 = 0.0497, wR2 = 0.1009

Largest diff. peak and hole: 0.489 and -0.260 e × $Å^{-3}$

Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors.

Table S1 (continued). Crystal data and structure refinement for **2**.

Treatment of hydrogen atoms:
All hydrogen atoms were placed geometrically and were refined with an isotropic displacement parameter 1.5 (methyl) or 1.2 times (all others) that of the neighboring carbon atom.

Table S2. Atomic coordinates [× 10^4] and equivalent isotropic displacement parameters [Å^2 × 10^3] for **2**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	7930(1)	9751(2)	6671(1)	28(1)
C(2)	7860(2)	10541(2)	7062(1)	41(1)
C(3)	7361(2)	10374(2)	7568(1)	49(1)
C(4)	6930(2)	9412(2)	7683(1)	43(1)
C(5)	6992(2)	8619(2)	7295(1)	30(1)
C(6)	7502(1)	8779(2)	6783(1)	23(1)
C(7)	7569(1)	7929(1)	6380(1)	20(1)
C(8)	6813(1)	7096(1)	6316(1)	22(1)
C(9)	7148(1)	6480(1)	5882(1)	20(1)
C(10)	8124(1)	6979(1)	5686(1)	19(1)
C(11)	9538(1)	7060(1)	5035(1)	19(1)
C(12)	10008(1)	6639(1)	4535(1)	20(1)
C(13)	10911(1)	7237(1)	4447(1)	22(1)
C(14)	10965(1)	8015(1)	4874(1)	20(1)
C(15)	11741(1)	8877(1)	4903(1)	21(1)
C(16)	12742(1)	8799(2)	4643(1)	26(1)
C(17)	13477(2)	9612(2)	4665(1)	31(1)
C(18)	13228(2)	10519(2)	4938(1)	33(1)
C(19)	12233(2)	10618(2)	5190(1)	31(1)
C(20)	11497(1)	9803(1)	5173(1)	25(1)
C(21)	6630(1)	5514(1)	5681(1)	22(1)
C(22)	5613(2)	5227(2)	5878(1)	30(1)
C(23)	5107(2)	4316(2)	5708(1)	35(1)
C(24)	5594(2)	3665(2)	5334(1)	31(1)
C(25)	6602(2)	3929(2)	5132(1)	29(1)
C(26)	7116(1)	4841(2)	5304(1)	25(1)
C(27)	9552(1)	5799(1)	4179(1)	20(1)
C(28)	10238(1)	5133(1)	3897(1)	23(1)
C(29)	9819(2)	4367(2)	3538(1)	27(1)
C(30)	8704(2)	4252(2)	3454(1)	27(1)
C(31)	8010(2)	4904(2)	3734(1)	28(1)
C(32)	8425(1)	5670(2)	4091(1)	24(1)
C(33)	12408(1)	8911(1)	6578(1)	19(1)
C(34)	12770(1)	8217(1)	6175(1)	21(1)
C(35)	13863(1)	8200(2)	6043(1)	25(1)
C(36)	14601(1)	8870(2)	6312(1)	26(1)
C(37)	14249(1)	9551(2)	6715(1)	27(1)
C(38)	13156(1)	9579(1)	6848(1)	24(1)
C(39)	10745(1)	10217(1)	6988(1)	19(1)
C(40)	10542(1)	11019(1)	6605(1)	24(1)
C(41)	10422(2)	12025(2)	6795(1)	28(1)
C(42)	10493(1)	12245(1)	7369(1)	25(1)
C(43)	10685(2)	11457(1)	7752(1)	25(1)
C(44)	10805(1)	10446(1)	7566(1)	23(1)
C(45)	10872(1)	8145(1)	7366(1)	19(1)
C(46)	11776(1)	7920(2)	7724(1)	26(1)
C(47)	11645(2)	7419(2)	8234(1)	30(1)

Table S2 (continued).

C(48)	10617(2)	7144(2)	8399(1)	30(1)
C(49)	9719(2)	7355(2)	8045(1)	36(1)
C(50)	9845(2)	7841(2)	7531(1)	30(1)
Cu(1)	9882(1)	8395(1)	6016(1)	18(1)
N(1)	8368(1)	7852(1)	6013(1)	19(1)
N(2)	8658(1)	6649(1)	5248(1)	19(1)
N(3)	10154(1)	7901(1)	5237(1)	19(1)
P(1)	10955(1)	8909(1)	6720(1)	17(1)

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S3. Bond lengths [Å] and angles [deg] for **2**.

C(1)-C(2)	1.383(3)	C(28)-C(29)	1.388(3)
C(1)-C(6)	1.392(3)	C(28)-H(28)	0.9500
C(1)-H(1)	0.9500	C(29)-C(30)	1.382(3)
C(2)-C(3)	1.385(4)	C(29)-H(29)	0.9500
C(2)-H(2)	0.9500	C(30)-C(31)	1.387(3)
C(3)-C(4)	1.384(4)	C(30)-H(30)	0.9500
C(3)-H(3)	0.9500	C(31)-C(32)	1.384(3)
C(4)-C(5)	1.380(3)	C(31)-H(31)	0.9500
C(4)-H(4)	0.9500	C(32)-H(32)	0.9500
C(5)-C(6)	1.403(3)	C(33)-C(38)	1.395(2)
C(5)-H(5)	0.9500	C(33)-C(34)	1.396(2)
C(6)-C(7)	1.460(2)	C(33)-P(1)	1.8299(16)
C(7)-N(1)	1.342(2)	C(34)-C(35)	1.392(2)
C(7)-C(8)	1.425(2)	C(34)-H(34)	0.9500
C(8)-C(9)	1.375(2)	C(35)-C(36)	1.388(3)
C(8)-H(8)	0.9500	C(35)-H(35)	0.9500
C(9)-C(10)	1.455(2)	C(36)-C(37)	1.380(3)
C(9)-C(21)	1.472(2)	C(36)-H(36)	0.9500
C(10)-N(2)	1.320(2)	C(37)-C(38)	1.392(2)
C(10)-N(1)	1.393(2)	C(37)-H(37)	0.9500
C(11)-N(2)	1.323(2)	C(38)-H(38)	0.9500
C(11)-N(3)	1.396(2)	C(39)-C(40)	1.392(2)
C(11)-C(12)	1.445(2)	C(39)-C(44)	1.396(2)
C(12)-C(13)	1.375(2)	C(39)-P(1)	1.8280(17)
C(12)-C(27)	1.470(2)	C(40)-C(41)	1.386(3)
C(13)-C(14)	1.425(2)	C(40)-H(40)	0.9500
C(13)-H(13)	0.9500	C(41)-C(42)	1.384(3)
C(14)-N(3)	1.351(2)	C(41)-H(41)	0.9500
C(14)-C(15)	1.466(2)	C(42)-C(43)	1.377(3)
C(15)-C(20)	1.395(3)	C(42)-H(42)	0.9500
C(15)-C(16)	1.402(2)	C(43)-C(44)	1.389(3)
C(16)-C(17)	1.385(3)	C(43)-H(43)	0.9500
C(16)-H(16)	0.9500	C(44)-H(44)	0.9500
C(17)-C(18)	1.379(3)	C(45)-C(50)	1.393(2)
C(17)-H(17)	0.9500	C(45)-C(46)	1.396(2)
C(18)-C(19)	1.389(3)	C(45)-P(1)	1.8256(18)
C(18)-H(18)	0.9500	C(46)-C(47)	1.384(3)
C(19)-C(20)	1.388(3)	C(46)-H(46)	0.9500
C(19)-H(19)	0.9500	C(47)-C(48)	1.384(3)
C(20)-H(20)	0.9500	C(47)-H(47)	0.9500
C(21)-C(26)	1.399(2)	C(48)-C(49)	1.382(3)
C(21)-C(22)	1.403(2)	C(48)-H(48)	0.9500
C(22)-C(23)	1.382(3)	C(49)-C(50)	1.382(3)
C(22)-H(22)	0.9500	C(49)-H(49)	0.9500
C(23)-C(24)	1.377(3)	C(50)-H(50)	0.9500
C(23)-H(23)	0.9500	Cu(1)-N(1)	1.9871(14)
C(24)-C(25)	1.389(3)	Cu(1)-N(3)	1.9917(14)
C(24)-H(24)	0.9500	Cu(1)-P(1)	2.1800(5)
C(25)-C(26)	1.390(3)		
C(25)-H(25)	0.9500	C(2)-C(1)-C(6)	120.26(19)
C(26)-H(26)	0.9500	C(2)-C(1)-H(1)	119.9
C(27)-C(28)	1.395(2)	C(6)-C(1)-H(1)	119.9
C(27)-C(32)	1.400(2)	C(1)-C(2)-C(3)	120.4(2)

Table S3 (continued).

C(1)-C(2)-H(2)	119.8	C(19)-C(20)-H(20)	119.6
C(3)-C(2)-H(2)	119.8	C(15)-C(20)-H(20)	119.6
C(4)-C(3)-C(2)	119.8(2)	C(26)-C(21)-C(22)	117.32(16)
C(4)-C(3)-H(3)	120.1	C(26)-C(21)-C(9)	122.96(15)
C(2)-C(3)-H(3)	120.1	C(22)-C(21)-C(9)	119.71(16)
C(5)-C(4)-C(3)	120.3(2)	C(23)-C(22)-C(21)	121.61(18)
C(5)-C(4)-H(4)	119.9	C(23)-C(22)-H(22)	119.2
C(3)-C(4)-H(4)	119.9	C(21)-C(22)-H(22)	119.2
C(4)-C(5)-C(6)	120.3(2)	C(24)-C(23)-C(22)	120.35(18)
C(4)-C(5)-H(5)	119.9	C(24)-C(23)-H(23)	119.8
C(6)-C(5)-H(5)	119.9	C(22)-C(23)-H(23)	119.8
C(1)-C(6)-C(5)	118.94(17)	C(23)-C(24)-C(25)	119.32(18)
C(1)-C(6)-C(7)	121.53(16)	C(23)-C(24)-H(24)	120.3
C(5)-C(6)-C(7)	119.53(17)	C(25)-C(24)-H(24)	120.3
N(1)-C(7)-C(8)	111.50(15)	C(24)-C(25)-C(26)	120.55(18)
N(1)-C(7)-C(6)	122.82(15)	C(24)-C(25)-H(25)	119.7
C(8)-C(7)-C(6)	125.67(15)	C(26)-C(25)-H(25)	119.7
C(9)-C(8)-C(7)	107.56(15)	C(25)-C(26)-C(21)	120.85(16)
C(9)-C(8)-H(8)	126.2	C(25)-C(26)-H(26)	119.6
C(7)-C(8)-H(8)	126.2	C(21)-C(26)-H(26)	119.6
C(8)-C(9)-C(10)	105.04(15)	C(28)-C(27)-C(32)	118.00(16)
C(8)-C(9)-C(21)	126.42(15)	C(28)-C(27)-C(12)	120.48(15)
C(10)-C(9)-C(21)	128.52(15)	C(32)-C(27)-C(12)	121.46(16)
N(2)-C(10)-N(1)	126.51(15)	C(29)-C(28)-C(27)	121.13(16)
N(2)-C(10)-C(9)	123.51(15)	C(29)-C(28)-H(28)	119.4
N(1)-C(10)-C(9)	109.95(14)	C(27)-C(28)-H(28)	119.4
N(2)-C(11)-N(3)	128.40(15)	C(30)-C(29)-C(28)	120.17(17)
N(2)-C(11)-C(12)	121.53(15)	C(30)-C(29)-H(29)	119.9
N(3)-C(11)-C(12)	110.06(14)	C(28)-C(29)-H(29)	119.9
C(13)-C(12)-C(11)	105.46(15)	C(29)-C(30)-C(31)	119.45(17)
C(13)-C(12)-C(27)	128.14(15)	C(29)-C(30)-H(30)	120.3
C(11)-C(12)-C(27)	126.25(15)	C(31)-C(30)-H(30)	120.3
C(12)-C(13)-C(14)	107.56(15)	C(32)-C(31)-C(30)	120.54(17)
C(12)-C(13)-H(13)	126.2	C(32)-C(31)-H(31)	119.7
C(14)-C(13)-H(13)	126.2	C(30)-C(31)-H(31)	119.7
N(3)-C(14)-C(13)	111.13(15)	C(31)-C(32)-C(27)	120.71(17)
N(3)-C(14)-C(15)	123.31(16)	C(31)-C(32)-H(32)	119.6
C(13)-C(14)-C(15)	125.42(15)	C(27)-C(32)-H(32)	119.6
C(20)-C(15)-C(16)	118.16(16)	C(38)-C(33)-C(34)	119.18(15)
C(20)-C(15)-C(14)	121.47(16)	C(38)-C(33)-P(1)	123.00(13)
C(16)-C(15)-C(14)	120.35(17)	C(34)-C(33)-P(1)	117.81(12)
C(17)-C(16)-C(15)	120.79(19)	C(35)-C(34)-C(33)	120.18(16)
C(17)-C(16)-H(16)	119.6	C(35)-C(34)-H(34)	119.9
C(15)-C(16)-H(16)	119.6	C(33)-C(34)-H(34)	119.9
C(18)-C(17)-C(16)	120.35(18)	C(36)-C(35)-C(34)	120.20(17)
C(18)-C(17)-H(17)	119.8	C(36)-C(35)-H(35)	119.9
C(16)-C(17)-H(17)	119.8	C(34)-C(35)-H(35)	119.9
C(17)-C(18)-C(19)	119.73(18)	C(37)-C(36)-C(35)	119.83(16)
C(17)-C(18)-H(18)	120.1	C(37)-C(36)-H(36)	120.1
C(19)-C(18)-H(18)	120.1	C(35)-C(36)-H(36)	120.1
C(20)-C(19)-C(18)	120.14(19)	C(36)-C(37)-C(38)	120.44(17)
C(20)-C(19)-H(19)	119.9	C(36)-C(37)-H(37)	119.8
C(18)-C(19)-H(19)	119.9	C(38)-C(37)-H(37)	119.8
C(19)-C(20)-C(15)	120.81(17)	C(37)-C(38)-C(33)	120.17(17)

Table S3 (continued).

C(37)-C(38)-H(38)	119.9	C(46)-C(47)-H(47)	119.7
C(33)-C(38)-H(38)	119.9	C(48)-C(47)-H(47)	119.7
C(40)-C(39)-C(44)	118.56(16)	C(49)-C(48)-C(47)	119.40(18)
C(40)-C(39)-P(1)	119.19(13)	C(49)-C(48)-H(48)	120.3
C(44)-C(39)-P(1)	122.24(13)	C(47)-C(48)-H(48)	120.3
C(41)-C(40)-C(39)	120.46(17)	C(50)-C(49)-C(48)	120.31(18)
C(41)-C(40)-H(40)	119.8	C(50)-C(49)-H(49)	119.8
C(39)-C(40)-H(40)	119.8	C(48)-C(49)-H(49)	119.8
C(42)-C(41)-C(40)	120.46(18)	C(49)-C(50)-C(45)	120.85(17)
C(42)-C(41)-H(41)	119.8	C(49)-C(50)-H(50)	119.6
C(40)-C(41)-H(41)	119.8	C(45)-C(50)-H(50)	119.6
C(43)-C(42)-C(41)	119.64(17)	N(1)-Cu(1)-N(3)	94.49(6)
C(43)-C(42)-H(42)	120.2	N(1)-Cu(1)-P(1)	130.08(4)
C(41)-C(42)-H(42)	120.2	N(3)-Cu(1)-P(1)	133.13(4)
C(42)-C(43)-C(44)	120.34(17)	C(7)-N(1)-C(10)	105.89(14)
C(42)-C(43)-H(43)	119.8	C(7)-N(1)-Cu(1)	133.03(12)
C(44)-C(43)-H(43)	119.8	C(10)-N(1)-Cu(1)	117.79(10)
C(43)-C(44)-C(39)	120.53(17)	C(10)-N(2)-C(11)	127.67(15)
C(43)-C(44)-H(44)	119.7	C(14)-N(3)-C(11)	105.74(14)
C(39)-C(44)-H(44)	119.7	C(14)-N(3)-Cu(1)	135.27(12)
C(50)-C(45)-C(46)	118.48(17)	C(11)-N(3)-Cu(1)	117.09(11)
C(50)-C(45)-P(1)	118.14(13)	C(45)-P(1)-C(39)	101.35(8)
C(46)-C(45)-P(1)	123.20(13)	C(45)-P(1)-C(33)	104.17(8)
C(47)-C(46)-C(45)	120.32(17)	C(39)-P(1)-C(33)	102.49(8)
C(47)-C(46)-H(46)	119.8	C(45)-P(1)-Cu(1)	114.81(6)
C(45)-C(46)-H(46)	119.8	C(39)-P(1)-Cu(1)	117.19(5)
C(46)-C(47)-C(48)	120.62(17)	C(33)-P(1)-Cu(1)	114.91(6)

Table S4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(h a^*)^2 U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
C(1)	17(1)	29(1)	38(1)	-9(1)	0(1)	2(1)
C(2)	24(1)	35(1)	63(2)	-23(1)	0(1)	-1(1)
C(3)	30(1)	61(2)	57(2)	-38(1)	2(1)	1(1)
C(4)	29(1)	67(2)	35(1)	-21(1)	7(1)	3(1)
C(5)	21(1)	41(1)	29(1)	-6(1)	3(1)	3(1)
C(6)	14(1)	30(1)	24(1)	-6(1)	-2(1)	5(1)
C(7)	16(1)	24(1)	19(1)	0(1)	-1(1)	2(1)
C(8)	17(1)	25(1)	23(1)	0(1)	2(1)	1(1)
C(9)	16(1)	22(1)	22(1)	1(1)	1(1)	0(1)
C(10)	16(1)	21(1)	19(1)	1(1)	-1(1)	0(1)
C(11)	18(1)	21(1)	18(1)	1(1)	-1(1)	0(1)
C(12)	20(1)	23(1)	17(1)	0(1)	0(1)	-1(1)
C(13)	21(1)	28(1)	19(1)	0(1)	3(1)	-1(1)
C(14)	18(1)	23(1)	19(1)	3(1)	-2(1)	0(1)

Table S4 (continued).

C(15)	19(1)	26(1)	19(1)	6(1)	-3(1)	-3(1)
C(16)	23(1)	31(1)	25(1)	4(1)	1(1)	-3(1)
C(17)	23(1)	38(1)	33(1)	10(1)	2(1)	-6(1)
C(18)	28(1)	32(1)	39(1)	9(1)	-5(1)	-12(1)
C(19)	32(1)	24(1)	36(1)	3(1)	-6(1)	-4(1)
C(20)	22(1)	26(1)	26(1)	4(1)	-2(1)	-2(1)
C(21)	19(1)	23(1)	23(1)	1(1)	0(1)	-1(1)
C(22)	26(1)	29(1)	36(1)	-3(1)	10(1)	-3(1)
C(23)	26(1)	32(1)	45(1)	-1(1)	11(1)	-8(1)
C(24)	28(1)	26(1)	38(1)	-1(1)	0(1)	-8(1)
C(25)	26(1)	27(1)	34(1)	-4(1)	2(1)	-3(1)
C(26)	21(1)	27(1)	26(1)	-2(1)	2(1)	-5(1)
C(27)	22(1)	23(1)	15(1)	1(1)	1(1)	-1(1)
C(28)	21(1)	28(1)	20(1)	-1(1)	2(1)	-1(1)
C(29)	32(1)	27(1)	23(1)	-3(1)	4(1)	4(1)
C(30)	35(1)	26(1)	21(1)	-3(1)	-2(1)	-5(1)
C(31)	24(1)	34(1)	26(1)	-3(1)	-3(1)	-3(1)
C(32)	23(1)	30(1)	21(1)	-3(1)	-1(1)	2(1)
C(33)	16(1)	20(1)	20(1)	3(1)	-1(1)	0(1)
C(34)	19(1)	22(1)	21(1)	3(1)	-1(1)	1(1)
C(35)	23(1)	30(1)	23(1)	4(1)	3(1)	7(1)
C(36)	16(1)	30(1)	32(1)	12(1)	2(1)	2(1)
C(37)	19(1)	23(1)	38(1)	4(1)	-5(1)	-3(1)
C(38)	20(1)	22(1)	30(1)	-2(1)	-2(1)	1(1)
C(39)	14(1)	19(1)	22(1)	-3(1)	-1(1)	0(1)
C(40)	26(1)	25(1)	22(1)	0(1)	-3(1)	0(1)
C(41)	28(1)	22(1)	33(1)	4(1)	-4(1)	-1(1)
C(42)	17(1)	20(1)	36(1)	-6(1)	1(1)	0(1)
C(43)	25(1)	26(1)	25(1)	-7(1)	2(1)	-1(1)
C(44)	24(1)	24(1)	22(1)	-1(1)	-1(1)	1(1)
C(45)	20(1)	17(1)	21(1)	-2(1)	0(1)	1(1)
C(46)	20(1)	29(1)	28(1)	1(1)	-1(1)	4(1)
C(47)	28(1)	32(1)	29(1)	3(1)	-5(1)	7(1)
C(48)	39(1)	27(1)	25(1)	4(1)	3(1)	0(1)
C(49)	26(1)	45(1)	38(1)	11(1)	3(1)	-7(1)
C(50)	20(1)	37(1)	33(1)	7(1)	-3(1)	-4(1)
Cu(1)	16(1)	21(1)	18(1)	-3(1)	-1(1)	-1(1)
N(1)	17(1)	21(1)	19(1)	-1(1)	-1(1)	0(1)
N(2)	17(1)	20(1)	18(1)	1(1)	-1(1)	0(1)
N(3)	17(1)	21(1)	19(1)	0(1)	-1(1)	-2(1)
P(1)	15(1)	19(1)	19(1)	-2(1)	-1(1)	0(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **2**.

	x	y	z	U(eq)
H(1)	8272	9872	6324	34
H(2)	8155	11202	6983	49
H(3)	7316	10919	7835	59
H(4)	6589	9297	8030	52
H(5)	6689	7962	7375	36
H(8)	6191	6986	6533	26
H(13)	11409	7147	4154	27
H(16)	12917	8182	4449	31
H(17)	14157	9544	4492	38
H(18)	13735	11075	4953	40
H(19)	12056	11245	5374	37
H(20)	10820	9876	5348	30
H(22)	5263	5668	6135	36
H(23)	4420	4139	5850	41
H(24)	5243	3042	5214	37
H(25)	6943	3482	4874	35
H(26)	7807	5009	5163	30
H(28)	11006	5204	3952	27
H(29)	10299	3922	3349	32
H(30)	8416	3732	3206	33
H(31)	7243	4823	3681	34
H(32)	7940	6114	4278	29
H(34)	12268	7754	5991	25
H(35)	14105	7728	5767	30
H(36)	15346	8861	6219	31
H(37)	14756	10004	6903	32
H(38)	12920	10054	7124	29
H(40)	10485	10876	6211	29
H(41)	10290	12568	6530	33
H(42)	10409	12935	7497	29
H(43)	10736	11606	8146	30
H(44)	10930	9907	7834	28
H(46)	12485	8111	7617	31
H(47)	12266	7262	8472	36
H(48)	10529	6813	8753	36
H(49)	9011	7165	8155	44
H(50)	9224	7969	7287	36

X-ray Structural Data for **3**

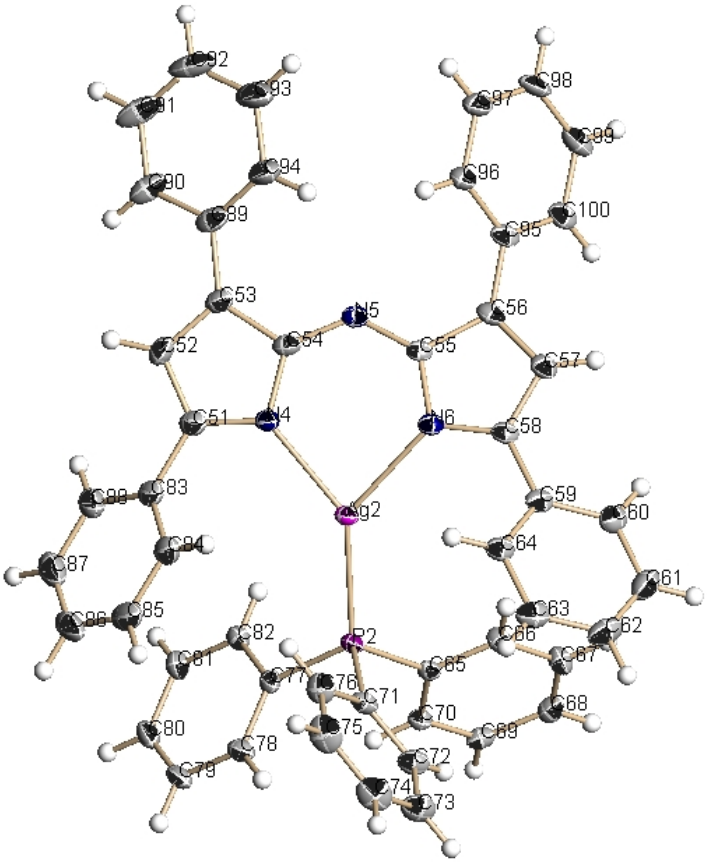

Figure S6. Thermal ellipsoid plot of $(Ph_3P)Ag^I$(tetraphenylazadipyrromethene) (**3**). Ellipsoids are drawn at 50% probability; data were collected at 100 K.

Table S6. Crystal data and structure refinement for **3**.

Identification code: JB061206

Empirical formula: C50 H37 Ag N3 P

Formula weight: 818.67

Temperature: 100(2) K

Wavelength: 0.71073 Å

Crystal system: Triclinic

Space group: P$\bar{1}$

Unit cell dimensions:

a = 15.0342(2) Å, α = 89.4080(10)°

b = 17.0484(3) Å, β = 77.7770(10)°

c = 26.9464(4) Å, γ = 70.7410(10)°

Volume, Z: 6359.03(17) Å^3, 6

Density (calculated): 1.283 Mg/m^3

Absorption coefficient: 0.550 mm^{-1}

F(000): 2520

Crystal size: 0.27 × 0.24 × 0.10 mm

Crystal shape, color: trapezoid, purple

θ range for data collection: 3.15 to 27.50°

Limiting indices: $-19 \leq h \leq 19$, $-22 \leq k \leq 21$, $-33 \leq l \leq 35$

Reflections collected: 66123

Independent reflections: 27307 (R(int) = 0.0335)

Completeness to θ = 25°: 95.2 %

Absorption correction: multi-scan

Max. and min. transmission: 0.9471 and 0.8657

Refinement method: Full-matrix least-squares on F^2

Data / restraints / parameters: 27307 / 954 / 1486

Goodness-of-fit on F^2: 1.681

Final R indices [$I>2\sigma(I)$]: R1 = 0.0369, wR2 = 0.0645

R indices (all data): R1 = 0.0500, wR2 = 0.0629

Largest diff. peak and hole: 0.924 and -0.767 e × Å^{-3}

Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit are based on F^2, conventional R-factors R are based

Table S6 (continued).

on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors

Treatment of hydrogen atoms:
All hydrogen atoms were placed geometrically and were refined with an isotropic displacement parameter 1.5 (methyl) or 1.2 times (all others) that of the neighboring carbon atom.

Table S7. Atomic coordinates [× 10^4] and equivalent isotropic displacement parameters [$Å^2$ × 10^3] for **3**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ag1	0.405551(14)	0.172793(12)	0.971474(8)	0.02904(5)
Ag2	0.620248(12)	0.365208(11)	0.748755(7)	0.01926(5)
Ag3	0.895352(12)	0.315869(11)	0.479884(7)	0.01635(4)
P3	0.75857(4)	0.27524(4)	0.48876(2)	0.01538(13)
P2	0.72606(4)	0.22990(4)	0.72036(2)	0.01744(13)
P1	0.30178(5)	0.31187(4)	0.97783(3)	0.03299(18)
N4	0.46330(13)	0.43825(12)	0.76879(7)	0.0205(5)
N6	0.63544(13)	0.49298(11)	0.75680(7)	0.0189(4)
N7	0.93512(13)	0.41384(11)	0.51684(7)	0.0158(4)
N9	1.05267(13)	0.27022(11)	0.44472(7)	0.0168(4)
N1	0.54722(15)	0.11685(12)	0.99481(8)	0.0259(5)
C115	0.70347(15)	0.29217(14)	0.43356(8)	0.0161(5)
C121	0.78119(15)	0.16437(13)	0.49665(9)	0.0165(5)
C126	0.72994(16)	0.13351(14)	0.53683(9)	0.0199(5)
C58	0.71794(17)	0.51029(14)	0.74659(9)	0.0203(5)
C65	0.82129(15)	0.22478(14)	0.66456(9)	0.0171(5)
N8	1.10612(13)	0.33326(11)	0.50851(7)	0.0171(4)
C69	0.92011(16)	0.16525(15)	0.58217(9)	0.0227(6)
C122	0.85499(16)	0.10837(14)	0.46075(9)	0.0242(6)
C127	0.66425(15)	0.32794(13)	0.54386(8)	0.0150(5)
C105	1.12058(15)	0.27919(14)	0.46990(9)	0.0167(5)
C70	0.84675(16)	0.16642(14)	0.62382(9)	0.0188(5)
C128	0.56727(16)	0.33826(14)	0.54729(9)	0.0204(5)
C106	1.21367(16)	0.21603(14)	0.44904(9)	0.0188(5)
C145	1.30431(16)	0.20010(15)	0.46655(9)	0.0223(6)
C107	1.19805(16)	0.17125(14)	0.41216(9)	0.0207(5)
C5	0.54878(17)	0.01517(14)	0.90255(9)	0.0222(6)
C131	0.62205(16)	0.39943(14)	0.62653(9)	0.0198(5)
C120	0.66258(16)	0.23749(15)	0.41748(9)	0.0221(6)
C104	1.02455(16)	0.39336(14)	0.52985(9)	0.0165(5)
C129	0.49791(17)	0.37882(15)	0.59047(9)	0.0238(6)
C132	0.69136(16)	0.35834(13)	0.58388(9)	0.0175(5)
N2	0.62228(14)	0.01619(12)	0.92167(8)	0.0215(5)
N3	0.44949(14)	0.05681(12)	0.92145(8)	0.0235(5)
C95	0.55534(17)	0.71698(15)	0.72451(10)	0.0238(6)
C103	1.01803(16)	0.45043(14)	0.57129(9)	0.0185(5)
C56	0.60580(17)	0.62907(14)	0.73392(9)	0.0219(6)
C119	0.62663(17)	0.24974(15)	0.37333(9)	0.0254(6)
C108	1.09952(16)	0.20510(14)	0.41038(9)	0.0184(5)
C55	0.56271(16)	0.56576(14)	0.74934(9)	0.0191(5)
N5	0.46904(13)	0.57898(12)	0.75598(7)	0.0189(4)
C46	0.73706(17)	-0.06083(15)	0.81860(9)	0.0220(5)
C6	0.56209(16)	-0.03584(14)	0.85683(9)	0.0210(5)
C45	0.65500(16)	-0.08330(14)	0.82264(9)	0.0205(5)
C49	0.74658(18)	-0.19314(15)	0.75712(10)	0.0268(6)
C48	0.82721(17)	-0.16989(15)	0.75355(9)	0.0257(6)
C50	0.66083(17)	-0.15077(14)	0.79114(9)	0.0248(6)

Table S7 (continued).

C4	0.62377(17)	0.05689(14)	0.96259(9)	0.0234(6)
C3	0.71330(18)	0.04910(15)	0.97758(9)	0.0260(6)
C71	0.79161(17)	0.17527(14)	0.76708(9)	0.0210(5)
C67	0.94535(18)	0.27892(15)	0.62209(10)	0.0267(6)
C66	0.87070(17)	0.28146(15)	0.66320(9)	0.0230(6)
C57	0.70256(17)	0.59296(14)	0.73142(9)	0.0239(6)
C72	0.88976(18)	0.12933(15)	0.75460(10)	0.0261(6)
C101	0.87652(16)	0.48024(14)	0.54752(9)	0.0175(5)
C102	0.92539(16)	0.50463(14)	0.58118(9)	0.0186(5)
C130	0.52553(17)	0.40965(14)	0.62998(9)	0.0227(6)
C52	0.29929(17)	0.47401(16)	0.78337(9)	0.0269(6)
C53	0.31809(17)	0.54731(15)	0.77716(9)	0.0242(6)
C110	1.08109(17)	0.08906(15)	0.36350(9)	0.0243(6)
C116	0.70814(15)	0.35986(14)	0.40469(9)	0.0190(5)
C59	0.80965(16)	0.45158(14)	0.75467(9)	0.0205(5)
C114	0.96679(16)	0.22597(15)	0.36365(9)	0.0204(5)
C47	0.82234(17)	-0.10386(15)	0.78449(9)	0.0256(6)
C113	0.91832(17)	0.19452(16)	0.33530(9)	0.0258(6)
C150	1.37527(18)	0.12056(16)	0.45712(10)	0.0297(6)
C118	0.63236(16)	0.31650(15)	0.34467(9)	0.0244(6)
C109	1.04893(16)	0.17360(14)	0.37884(9)	0.0188(5)
C2	0.68811(19)	0.10454(15)	1.01904(10)	0.0308(6)
C139	1.09229(16)	0.45003(15)	0.59923(9)	0.0199(5)
C135	0.63895(16)	0.53564(14)	0.50837(9)	0.0213(5)
C134	0.73705(16)	0.50682(13)	0.50538(9)	0.0185(5)
C136	0.57560(17)	0.57688(14)	0.55258(9)	0.0229(6)
C133	0.77380(16)	0.51737(13)	0.54726(9)	0.0174(5)
C54	0.42275(17)	0.52465(15)	0.76719(9)	0.0213(5)
C82	0.59818(16)	0.18952(15)	0.67389(9)	0.0216(5)
C64	0.81157(18)	0.38935(15)	0.78878(9)	0.0231(6)
C146	1.32414(17)	0.26056(16)	0.49266(10)	0.0269(6)
C140	1.08625(17)	0.52346(16)	0.62453(9)	0.0247(6)
C68	0.97015(17)	0.22092(15)	0.58144(9)	0.0231(6)
C138	0.70893(17)	0.56111(14)	0.59108(9)	0.0214(5)
C77	0.66931(16)	0.15865(14)	0.70169(9)	0.0185(5)
C81	0.55554(17)	0.13808(15)	0.65703(10)	0.0253(6)
C117	0.67296(16)	0.37208(15)	0.36079(9)	0.0227(6)
C63	0.89853(19)	0.33266(16)	0.79470(10)	0.0298(6)
C80	0.58212(18)	0.05534(16)	0.66831(10)	0.0286(6)
C143	1.23197(17)	0.37846(17)	0.63365(10)	0.0291(6)
C144	1.16675(17)	0.37713(16)	0.60439(9)	0.0249(6)
C8	0.40423(17)	0.03104(14)	0.89039(10)	0.0241(6)
C78	0.69541(17)	0.07550(14)	0.71285(9)	0.0234(6)
C89	0.24434(18)	0.63144(16)	0.78187(10)	0.0290(6)
C73	0.9351(2)	0.08620(16)	0.79131(11)	0.0321(7)
C100	0.59501(19)	0.75487(15)	0.68370(10)	0.0270(6)
C51	0.38932(17)	0.40885(15)	0.77763(9)	0.0247(6)
C60	0.89667(18)	0.45633(16)	0.72757(10)	0.0287(6)
C7	0.47151(17)	-0.02687(14)	0.85080(10)	0.0235(6)
C125	0.75389(17)	0.04820(15)	0.54096(10)	0.0261(6)
C76	0.74070(19)	0.17895(16)	0.81724(10)	0.0293(6)
C96	0.47005(17)	0.76432(15)	0.75760(10)	0.0267(6)
C83	0.40217(17)	0.32026(15)	0.78086(10)	0.0278(6)
C62	0.98413(19)	0.33790(17)	0.76722(11)	0.0343(7)

Table S7 (continued).

C1	0.58698(19)	0.14484(15)	1.02808(10)	0.0294(6)
C33	0.5304(2)	0.21211(16)	1.06755(10)	0.0345(7)
C9	0.29792(18)	0.06240(15)	0.89610(11)	0.0279(6)
C88	0.34677(19)	0.28629(17)	0.75830(10)	0.0323(7)
C14	0.23585(18)	0.10141(15)	0.94179(11)	0.0322(7)
C39	0.81179(18)	-0.00634(16)	0.95462(9)	0.0261(6)
C123	0.87650(19)	0.02348(15)	0.46469(10)	0.0332(7)
C137	0.61084(16)	0.59070(14)	0.59355(10)	0.0233(6)
C79	0.65127(18)	0.02425(15)	0.69636(10)	0.0273(6)
C74	0.8845(2)	0.08881(17)	0.84012(11)	0.0380(7)
C111	1.03231(18)	0.05816(16)	0.33544(10)	0.0309(6)
C142	1.22386(18)	0.45123(18)	0.65894(10)	0.0312(6)
C43	0.92367(19)	-0.13267(18)	0.90696(10)	0.0376(7)
C44	0.82955(18)	-0.08062(16)	0.92657(10)	0.0314(7)
C112	0.94997(18)	0.11059(16)	0.32116(10)	0.0306(6)
C148	1.47691(19)	0.16288(18)	0.50062(12)	0.0377(7)
C61	0.98367(19)	0.39988(17)	0.73397(11)	0.0344(7)
C84	0.46875(18)	0.26794(16)	0.80666(10)	0.0318(7)
C40	0.89033(19)	0.01370(17)	0.96132(10)	0.0312(7)
C13	0.13782(19)	0.13191(16)	0.94682(12)	0.0383(7).
C34	0.4346(2)	0.22579(17)	1.08939(10)	0.0374(7)
C97	0.42461(19)	0.84672(15)	0.74948(11)	0.0325(7)
C99	0.5490(2)	0.83785(16)	0.67641(11)	0.0334(7)
C75	0.7866(2)	0.13567(18)	0.85361(11)	0.0375(7)
C149	1.46082(18)	0.10333(17)	0.47341(11)	0.0364(7)
C141	1.15074(18)	0.52409(17)	0.65418(10)	0.0299(6).
C98	0.46389(19)	0.88339(16)	0.70914(11)	0.0339(7)
C124	0.82685(19)	-0.00696(16)	0.50506(10)	0.0329(7)
C10	0.25679(19)	0.05467(17)	0.85570(12)	0.0357(7)
C42	1.0003(2)	-0.11137(19)	0.91478(10)	0.0399(8)
C87	0.3588(2)	0.20264(18)	0.75976(11)	0.0410(7)
C85	0.4805(2)	0.18397(17)	0.80816(11)	0.0371(7)
C147	1.40733(19)	0.24202(18)	0.51046(11)	0.0361(7)
C90	0.15294(19)	0.64066(18)	0.77440(10)	0.0361(7)
C41	0.98413(19)	-0.03828(18)	0.94181(10)	0.0367(7)
C35	0.3835(2)	0.29393(19)	1.12457(11)	0.0461(9)
C86	0.4271(2)	0.15142(18)	0.78435(12)	0.0437(8)
C38	0.5753(2)	0.26531(18)	1.08262(11)	0.0464(9)
C12	0.0988(2)	0.12403(18)	0.90627(13)	0.0452(8)
C11	0.1579(2)	0.08540(18)	0.86091(13)	0.0447(8)
C94	0.2629(2)	0.70105(17)	0.79560(12)	0.0453(8)
C16	0.22420(18)	0.29401(16)	0.89566(10)	0.0298(6)
C17	0.15688(19)	0.31460(17)	0.86540(11)	0.0342(7)
C91	0.0819(2)	0.7181(2)	0.78035(11)	0.0448(9)
C92	0.1011(2)	0.7870(2)	0.79305(11)	0.0493(9)
C27	0.2343(2)	0.35659(17)	1.04120(12)	0.0389(8)
C15	0.2103(2)	0.34077(17)	0.93990(12)	0.0439(8)
C37	0.5222(3)	0.33184(19)	1.11765(12)	0.0587(11)
C93	0.1907(2)	0.77972(19)	0.80087(13)	0.0572(10)
C21	0.3770(2)	0.3741(2)	0.95550(14)	0.0570(10)
C28	0.2316(3)	0.43275(19)	1.06065(14)	0.0659(12)
C22	0.3649(3)	0.4244(2)	0.91648(14)	0.0710(12)
C29	0.1791(4)	0.4626(3)	1.10964(19)	0.0905(19)

Table S7 (continued).

C18	0.0759(2)	0.3831(2)	0.87932(14)	0.0730(13)
C32	0.1851(3)	0.3122(3)	1.07126(14)	0.0799(14)
C36	0.4265(3)	0.3471(2)	1.13760(11)	0.0552(11)
C20	0.1266(3)	0.4098(3)	0.95350(16)	0.115(2)
C30	0.1314(3)	0.4198(4)	1.1385(2)	0.111(2)
C19	0.0614(3)	0.4311(3)	0.92264(18)	0.135(3)
C23	0.4298(6)	0.4637(3)	0.89739(18)	0.120(2)
C31	0.1312(3)	0.3439(4)	1.11975(16)	0.116(2)
C24	0.5040(5)	0.4582(4)	0.9195(3)	0.181(3)
C25	0.169(6)	0.292(8)	0.409(11)	0.295(8)
C26	0.123(4)	0.207(6)	0.311(8)	0.228(6)

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S8. Bond lengths [Å] and angles [deg] for **3**.

Atom A	B	Dist
C1	N1	1.346
C1	C2	1.415
C1	C33	1.473
C2	H2	0.931
C2	C3	1.372
C2	C1	1.415
C3	C2	1.372
C3	C4	1.456
C3	C39	1.475
C4	N2	1.319
C4	N1	1.395
C4	C3	1.456
C5	N2	1.322
C5	N3	1.402
C5	C6	1.452
C6	C7	1.367
C6	C5	1.452
C6	C45	1.473
C7	H7	0.929
C7	C6	1.367
C7	C8	1.431
C8	N3	1.344
C8	C7	1.431
C8	C9	1.468
C9	C10	1.396
C9	C14	1.399
C9	C8	1.468
C10	H10	0.930
C10	C11	1.386
C10	C9	1.396
C11	H11	0.931
C11	C12	1.386
C11	C10	1.386
C12	H12	0.931
C12	C13	1.369
C12	C11	1.386
C13	H13	0.930
C13	C12	1.369
C13	C14	1.380
C14	H14	0.929
C14	C13	1.380
C14	C9	1.399
C15a	C20a	1.390
C15a	C16a	1.391
C15a	C16b	1.455
C15a	C20b	1.495
C15a	P1	1.800
C15b	C16a	1.336
C15b	C16b	1.394
C15b	C20b	1.407
C15b	C20a	1.483
C15b	P1	1.863
C16a	H16b	0.884
C16a	H16a	0.930
C16a	C15b	1.336
C16a	C17a	1.390
C16a	C15a	1.391
C16a	C17b	1.494
C16b	H16b	0.930
C16b	H16a	0.985
C16b	C17a	1.278
C16b	C17b	1.381
C16b	C15b	1.394
C16b	C15a	1.455
C17a	H17a	0.931
C17a	H17b	0.976
C17a	C16b	1.278
C17a	C16a	1.390
C17a	C18a	1.391
C17a	C18b	1.448
C17b	H17a	0.891
C17b	H17b	0.931
C17b	C18a	1.360
C17b	C18b	1.360
C17b	C16b	1.381
C17b	C16a	1.494
C18a	H18a	0.930
C18a	H18b	1.142
C18a	C17b	1.360
C18a	C19a	1.388
C18a	C17a	1.391
C18a	C19b	1.491
C18b	H18b	0.929
C18b	H18a	1.053
C18b	C17b	1.360
C18b	C19b	1.361
C18b	C17a	1.448
C18b	C19a	1.556
C19a	H19a	0.931
C19a	H19b	1.279
C19a	C18a	1.388
C19a	C20a	1.391
C19a	C20b	1.542
C19a	C18b	1.556
C19b	H19b	0.930
C19b	H19a	1.309
C19b	C18b	1.361
C19b	C20b	1.364
C19b	C18a	1.491
C19b	C20a	1.614
C20a	H20a	0.929
C20a	H20b	1.227
C20a	C15a	1.390

Table S8 (continued).

C20a	C19a	1.391
C20a	C15b	1.483
C20a	C19b	1.614
C20b	H20b	0.929
C20b	H20a	1.288
C20b	C19b	1.364
C20b	C15b	1.407
C20b	C15a	1.495
C20b	C19a	1.542
C21a	C26b	1.266
C21a	C22a	1.388
C21a	C26a	1.390
C21a	C22b	1.429
C21a	P1	1.891
C21b	C22a	1.360
C21b	C22b	1.390
C21b	C26b	1.390
C21b	C26a	1.625
C21b	P1	1.729
C22a	H22a	0.931
C22a	C23b	1.152
C22a	C21b	1.360
C22a	C21a	1.388
C22a	C23a	1.391
C22b	H22a	0.876
C22b	H22b	0.930
C22b	C21b	1.390
C22b	C23b	1.391
C22b	C21a	1.429
C23a	C24b	0.848
C23a	H23a	0.929
C23a	H23b	1.275
C23a	C24a	1.390
C23a	C22a	1.391
C23b	H23b	0.930
C23b	H23a	0.957
C23b	C22a	1.152
C23b	C24b	1.389
C23b	C22b	1.391
C24a	C24b	0.868
C24a	H24a	0.929
C24a	H24b	1.232
C24a	C23a	1.390
C24a	C25a	1.390
C24a	C25b	1.422
C24b	C23a	0.848
C24b	C24a	0.868
C24b	H24b	0.930
C24b	C23b	1.389
C24b	C25b	1.390
C25a	H25a	0.929
C25a	C25b	1.306
C25a	C24a	1.390
C25a	C26a	1.390
C25b	H25b	0.931
C25b	C25a	1.306
C25b	C24b	1.390
C25b	C26b	1.390
C25b	C24a	1.422
C26a	H26a	0.931
C26a	C26b	1.002
C26a	C25a	1.390
C26a	C21a	1.390
C26a	C21b	1.625
C26b	H26b	0.929
C26b	C26a	1.002
C26b	C21a	1.266
C26b	C21b	1.390
C26b	C25b	1.390
C27a	C28b	1.336
C27a	C28a	1.390
C27a	C32a	1.390
C27a	C32b	1.681
C27a	P1	1.739
C27b	C32a	1.143
C27b	C28b	1.390
C27b	C32b	1.390
C27b	C28a	1.517
C27b	P1	1.909
C28a	H28a	0.931
C28a	C27a	1.390
C28a	C29a	1.390
C28a	C27b	1.517
C28b	H28b	0.931
C28b	C29a	1.120
C28b	C27a	1.336
C28b	C29b	1.388
C28b	C27b	1.390
C29a	H29a	0.928
C29a	H29b	0.943
C29a	C28b	1.120
C29a	C28a	1.390
C29a	C30a	1.391
C29b	H29b	0.931
C29b	C28b	1.388
C29b	C30b	1.391
C30a	H30a	0.930
C30a	H30b	1.324
C30a	C31a	1.390
C30a	C29a	1.391
C30b	H30b	0.930
C30b	H30a	1.041
C30b	C31a	1.055
C30b	C31b	1.389
C30b	C29b	1.391
C31a	H31a	0.930
C31a	C30b	1.055
C31a	C32a	1.390

Table S8 (continued).

C31a	C30a	1.390
C31a	C32b	1.521
C31b	H31a	0.827
C31b	H31b	0.931
C31b	C30b	1.389
C31b	C32b	1.390
C31b	C32a	1.529
C32a	H32a	0.931
C32a	C27b	1.143
C32a	H32b	1.325
C32a	C31a	1.390
C32a	C27a	1.390
C32a	C31b	1.529
C32b	H32a	0.867
C32b	H32b	0.931
C32b	C27b	1.390
C32b	C31b	1.390
C32b	C31a	1.521
C32b	C27a	1.681
C33	C34	1.382
C33	C38	1.406
C33	C1	1.473
C34	H34	0.930
C34	C33	1.382
C34	C35	1.405
C35	H35	0.930
C35	C36	1.371
C35	C34	1.405
C36	H36	0.930
C36	C37	1.365
C36	C35	1.371
C37	H37	0.929
C37	C36	1.365
C37	C38	1.386
C38	H38	0.929
C38	C37	1.386
C38	C33	1.406
C39	C40	1.387
C39	C44	1.399
C39	C3	1.475
C40	H40	0.930
C40	C41	1.387
C40	C39	1.387
C41	H41	0.930
C41	C42	1.369
C41	C40	1.387
C42	H42	0.929
C42	C41	1.369
C42	C43	1.381
C43	H43	0.930
C43	C42	1.381
C43	C44	1.389
C44	H44	0.930
C44	C43	1.389
C44	C39	1.399
C45	C50	1.397
C45	C46	1.401
C45	C6	1.473
C46	H46	0.930
C46	C47	1.389
C46	C45	1.401
C47	H47	0.930
C47	C48	1.383
C47	C46	1.389
C48	H48	0.929
C48	C47	1.383
C48	C49	1.387
C49	H49	0.929
C49	C50	1.386
C49	C48	1.387
C50	H50	0.931
C50	C49	1.386
C50	C45	1.397
C51	N4	1.345
C51	C52	1.420
C51	C83	1.465
C52	H52	0.930
C52	C53	1.371
C52	C51	1.420
C53	C52	1.371
C53	C54	1.453
C53	C89	1.477
C54	N5	1.327
C54	N4	1.401
C54	C53	1.453
C55	N5	1.325
C55	N6	1.402
C55	C56	1.453
C56	C57	1.360
C56	C55	1.453
C56	C95	1.483
C57	H57	0.930
C57	C56	1.360
C57	C58	1.421
C58	N6	1.339
C58	C57	1.421
C58	C59	1.471
C59	C60	1.395
C59	C64	1.397
C59	C58	1.471
C60	H60	0.930
C60	C61	1.390
C60	C59	1.395
C61	H61	0.930
C61	C62	1.379
C61	C60	1.390
C62	H62	0.930
C62	C61	1.379

Table S8 (continued).

C62	C63	1.382
C63	H63	0.929
C63	C62	1.382
C63	C64	1.394
C64	H64	0.930
C64	C63	1.394
C64	C59	1.397
C65	C70	1.391
C65	C66	1.395
C65	P2	1.825
C66	H66	0.930
C66	C67	1.387
C66	C65	1.395
C67	H67	0.930
C67	C66	1.387
C67	C68	1.388
C68	H68	0.931
C68	C69	1.387
C68	C67	1.388
C69	H69	0.928
C69	C70	1.384
C69	C68	1.387
C70	H70	0.930
C70	C69	1.384
C70	C65	1.391
C71	C72	1.392
C71	C76	1.401
C71	P2	1.821
C72	H72	0.929
C72	C73	1.386
C72	C71	1.392
C73	H73	0.930
C73	C74	1.379
C73	C72	1.386
C74	H74	0.930
C74	C73	1.379
C74	C75	1.391
C75	H75	0.931
C75	C76	1.386
C75	C74	1.391
C76	H76	0.930
C76	C75	1.386
C76	C71	1.401
C77	C78	1.378
C77	C82	1.405
C77	P2	1.829
C78	H78	0.930
C78	C77	1.378
C78	C79	1.401
C79	H79	0.930
C79	C80	1.376
C79	C78	1.401
C80	H80	0.930
C80	C79	1.376
C80	C81	1.389
C81	H81	0.930
C81	C82	1.378
C81	C80	1.389
C82	H82	0.931
C82	C81	1.378
C82	C77	1.405
C83	C88	1.400
C83	C84	1.403
C83	C51	1.465
C84	H84	0.929
C84	C85	1.383
C84	C83	1.403
C85	H85	0.930
C85	C84	1.383
C85	C86	1.387
C86	H86	0.930
C86	C85	1.387
C86	C87	1.392
C87	H87	0.931
C87	C88	1.383
C87	C86	1.392
C88	H88	0.931
C88	C87	1.383
C88	C83	1.400
C89	C94	1.383
C89	C90	1.393
C89	C53	1.477
C90	H90	0.929
C90	C91	1.391
C90	C89	1.393
C91	H91	0.929
C91	C92	1.366
C91	C90	1.391
C92	H92	0.931
C92	C91	1.366
C92	C93	1.376
C93	H93	0.930
C93	C92	1.376
C93	C94	1.400
C94	H94	0.930
C94	C89	1.383
C94	C93	1.400
C95	C96	1.395
C95	C100	1.397
C95	C56	1.483
C96	H96	0.931
C96	C97	1.386
C96	C95	1.395
C97	H97	0.931
C97	C98	1.375
C97	C96	1.386
C98	H98	0.931
C98	C97	1.375

Table S8 (continued).

C98	C99	1.382
C99	H99	0.929
C99	C98	1.382
C99	C100	1.386
C100	H100	0.929
C100	C99	1.386
C100	C95	1.397
C101	N7	1.338
C101	C102	1.429
C101	C133	1.459
C102	H102	0.930
C102	C103	1.368
C102	C101	1.429
C103	C102	1.368
C103	C104	1.455
C103	C139	1.471
C104	N8	1.324
C104	N7	1.394
C104	C103	1.455
C105	N8	1.328
C105	N9	1.393
C105	C106	1.459
C106	C107	1.369
C106	C105	1.459
C106	C145	1.469
C107	H107	0.930
C107	C106	1.369
C107	C108	1.419
C108	N9	1.348
C108	C107	1.419
C108	C109	1.464
C109	C110	1.399
C109	C114	1.404
C109	C108	1.464
C110	H110	0.929
C110	C111	1.375
C110	C109	1.399
C111	H111	0.930
C111	C110	1.375
C111	C112	1.393
C112	H112	0.930
C112	C113	1.379
C112	C111	1.393
C113	H113	0.931
C113	C112	1.379
C113	C114	1.388
C114	H114	0.929
C114	C113	1.388
C114	C109	1.404
C115	C120	1.390
C115	C116	1.392
C115	P3	1.829
C116	H116	0.930
C116	C115	1.392
C116	C117	1.393
C117	H117	0.930
C117	C118	1.389
C117	C116	1.393
C118	H118	0.930
C118	C119	1.383
C118	C117	1.389
C119	H119	0.929
C119	C118	1.383
C119	C120	1.392
C120	H120	0.930
C120	C115	1.390
C120	C119	1.392
C121	C126	1.393
C121	C122	1.396
C121	P3	1.822
C122	H122	0.931
C122	C123	1.380
C122	C121	1.396
C123	H123	0.931
C123	C122	1.380
C123	C124	1.386
C124	H124	0.929
C124	C125	1.379
C124	C123	1.386
C125	H125	0.930
C125	C124	1.379
C125	C126	1.387
C126	H126	0.930
C126	C125	1.387
C126	C121	1.393
C127	C132	1.391
C127	C128	1.395
C127	P3	1.821
C128	H128	0.931
C128	C129	1.393
C128	C127	1.395
C129	H129	0.930
C129	C130	1.387
C129	C128	1.393
C130	H130	0.930
C130	C129	1.387
C130	C131	1.388
C131	H131	0.931
C131	C132	1.387
C131	C130	1.388
C132	H132	0.930
C132	C131	1.387
C132	C127	1.391
C133	C134	1.400
C133	C138	1.403
C133	C101	1.459
C134	H134	0.930
C134	C135	1.380

Table S8 (continued).

C134	C133	1.400
C135	H135	0.931
C135	C134	1.380
C135	C136	1.394
C136	H136	0.931
C136	C137	1.381
C136	C135	1.394
C137	H137	0.930
C137	C138	1.380
C137	C136	1.381
C138	H138	0.929
C138	C137	1.380
C138	C133	1.403
C139	C144	1.393
C139	C140	1.398
C139	C103	1.471
C140	H140	0.931
C140	C141	1.385
C140	C139	1.398
C141	H141	0.931
C141	C140	1.385
C141	C142	1.387
C142	H142	0.929
C142	C143	1.381
C142	C141	1.387
C143	H143	0.930
C143	C142	1.381
C143	C144	1.387
C144	H144	0.930
C144	C143	1.387
C144	C139	1.393
C145	C146	1.394
C145	C150	1.407
C145	C106	1.469
C146	H146	0.930
C146	C147	1.380
C146	C145	1.394
C147	H147	0.929
C147	C146	1.380
C147	C148	1.389
C148	H148	0.929
C148	C149	1.373
C148	C147	1.389
C149	H149	0.930
C149	C148	1.373
C149	C150	1.382
C150	H150	0.930
C150	C149	1.382
C150	C145	1.407
H2	C2	0.931
H7	C7	0.929
H10	C10	0.930
H11	C11	0.931
H12	C12	0.931
H13	C13	0.930
H14	C14	0.929
H16a	C16a	0.930
H16a	C16b	0.985
H16b	C16a	0.884
H16b	C16b	0.930
H17a	C17b	0.891
H17a	C17a	0.931
H17b	C17b	0.931
H17b	C17a	0.976
H18a	C18a	0.930
H18a	C18b	1.053
H18b	C18b	0.929
H18b	C18a	1.142
H19a	C19a	0.931
H19a	C19b	1.309
H19b	C19b	0.930
H19b	C19a	1.279
H20a	C20a	0.929
H20a	C20b	1.288
H20b	C20b	0.929
H20b	C20a	1.227
H22a	C22b	0.876
H22a	C22a	0.931
H22b	C22b	0.930
H23a	H23b	0.818
H23a	C23a	0.929
H23a	C23b	0.957
H23b	H23a	0.818
H23b	C23b	0.930
H23b	C23a	1.275
H24a	C24a	0.929
H24b	C24b	0.930
H24b	C24a	1.232
H25a	C25a	0.929
H25b	C25b	0.931
H26a	C26a	0.931
H26b	C26b	0.929
H28a	C28a	0.931
H28b	C28b	0.931
H29a	H29b	0.832
H29a	C29a	0.928
H29b	H29a	0.832
H29b	C29b	0.931
H29b	C29a	0.943
H30a	H30b	0.813
H30a	C30a	0.930
H30a	C30b	1.041
H30b	H30a	0.813
H30b	C30b	0.930
H30b	C30a	1.324
H31a	C31b	0.827
H31a	H31b	0.930
H31a	C31a	0.930

Table S8 (continued).

H31b	H31a	0.930
H31b	C31b	0.931
H32a	C32b	0.867
H32a	C32a	0.931
H32b	C32b	0.931
H32b	C32a	1.325
H34	C34	0.930
H35	C35	0.930
H36	C36	0.930
H37	C37	0.929
H38	C38	0.929
H40	C40	0.930
H41	C41	0.930
H42	C42	0.929
H43	C43	0.930
H44	C44	0.930
H46	C46	0.930
H47	C47	0.930
H48	C48	0.929
H49	C49	0.929
H50	C50	0.931
H52	C52	0.930
H57	C57	0.930
H60	C60	0.930
H61	C61	0.930
H62	C62	0.930
H63	C63	0.929
H64	C64	0.930
H66	C66	0.930
H67	C67	0.930
H68	C68	0.931
H69	C69	0.928
H70	C70	0.930
H72	C72	0.929
H73	C73	0.930
H74	C74	0.930
H75	C75	0.931
H76	C76	0.930
H78	C78	0.930
H79	C79	0.930
H80	C80	0.930
H81	C81	0.930
H82	C82	0.931
H84	C84	0.929
H85	C85	0.930
H86	C86	0.930
H87	C87	0.931
H88	C88	0.931
H90	C90	0.929
H91	C91	0.929
H92	C92	0.931
H93	C93	0.930
H94	C94	0.930
H96	C96	0.931
H97	C97	0.931
H98	C98	0.931
H99	C99	0.929
H100	C100	0.929
H102	C102	0.930
H107	C107	0.930
H110	C110	0.929
H111	C111	0.930
H112	C112	0.930
H113	C113	0.931
H114	C114	0.929
H116	C116	0.930
H117	C117	0.930
H118	C118	0.930
H119	C119	0.929
H120	C120	0.930
H122	C122	0.931
H123	C123	0.931
H124	C124	0.929
H125	C125	0.930
H126	C126	0.930
H128	C128	0.931
H129	C129	0.930
H130	C130	0.930
H131	C131	0.931
H132	C132	0.930
H134	C134	0.930
H135	C135	0.931
H136	C136	0.931
H137	C137	0.930
H138	C138	0.929
H140	C140	0.931
H141	C141	0.931
H142	C142	0.929
H143	C143	0.930
H144	C144	0.930
H146	C146	0.930
H147	C147	0.929
H148	C148	0.929
H149	C149	0.930
H150	C150	0.930
N1	C1	1.346
N1	C4	1.395
N1	Ag1	2.249
N2	C4	1.319
N2	C5	1.322
N3	C8	1.344
N3	C5	1.402
N3	Ag1	2.233
N4	C51	1.345
N4	C54	1.401
N4	Ag2	2.223
N5	C55	1.325
N5	C54	1.327

Table S8 (continued).

N6	C58	1.339
N6	C55	1.402
N6	Ag2	2.279
N7	C101	1.338
N7	C104	1.394
N7	Ag3	2.256
N8	C104	1.324
N8	C105	1.328
N9	C108	1.348
N9	C105	1.393
N9	Ag3	2.226
P1	C21b	1.729
P1	C27a	1.739
P1	C15a	1.800
P1	C15b	1.863
P1	C21a	1.891
P1	C27b	1.909
P1	Ag1	2.353
P2	C71	1.821
P2	C65	1.825
P2	C77	1.829
P2	Ag2	2.353
P3	C127	1.821
P3	C121	1.822
P3	C115	1.829
P3	Ag3	2.343
Ag1	N3	2.233
Ag1	N1	2.249
Ag1	P1	2.353
Ag2	N4	2.223
Ag2	N6	2.279
Ag2	P2	2.353
Ag3	N9	2.226
Ag3	N7	2.256
Ag3	P3	2.343

Atom A	B	C	Angle
N1	C1	C2	112.05
N1	C1	C33	123.02
C2	C1	C33	124.89
H2	C2	C3	126.47
H2	C2	C1	126.41
C3	C2	C1	107.12
C2	C3	C4	105.81
C2	C3	C39	125.93
C4	C3	C39	128.26
N2	C4	N1	128.52
N2	C4	C3	121.98
N1	C4	C3	109.27
N2	C5	N3	128.87
N2	C5	C6	121.58
N3	C5	C6	109.50
C7	C6	C5	105.67
C7	C6	C45	127.14
C5	C6	C45	127.12
H7	C7	C6	126.20
H7	C7	C8	126.23
C6	C7	C8	107.57
N3	C8	C7	111.23
N3	C8	C9	123.16
C7	C8	C9	125.55
C10	C9	C14	117.61
C10	C9	C8	120.60
C14	C9	C8	121.78
H10	C10	C11	119.70
H10	C10	C9	119.59
C11	C10	C9	120.71
H11	C11	C12	119.94
H11	C11	C10	119.92
C12	C11	C10	120.13
H12	C12	C13	119.95
H12	C12	C11	119.96
C13	C12	C11	120.09
H13	C13	C12	120.00
H13	C13	C14	120.05
C12	C13	C14	119.95
H14	C14	C13	119.28
H14	C14	C9	119.22
C13	C14	C9	121.50
C20a	C15a	C16a	119.98
C20a	C15a	C16b	116.30
C20a	C15a	C20b	29.59
C20a	C15a	P1	122.94
C16a	C15a	C16b	3.73
C16a	C15a	C20b	112.21
C16a	C15a	P1	117.01
C16b	C15a	C20b	108.74
C16b	C15a	P1	120.65
C20b	C15a	P1	120.35
C16a	C15b	C16b	4.05
C16a	C15b	C20b	121.79
C16a	C15b	C20a	117.25
C16a	C15b	P1	116.21
C16b	C15b	C20b	117.79
C16b	C15b	C20a	114.23
C16b	C15b	P1	120.26
C20b	C15b	C20a	29.68
C20b	C15b	P1	121.63
C20a	C15b	P1	113.72
H16b	C16a	H16a	21.07
H16b	C16a	C15b	129.93
H16b	C16a	C17a	110.97
H16b	C16a	C15a	125.18
H16b	C16a	C17b	112.58
H16a	C16a	C15b	118.78
H16a	C16a	C17a	120.05

Table S8 (continued).

H16a	C16a	C15a	119.95
H16a	C16a	C17b	119.59
C15b	C16a	C17a	118.95
C15b	C16a	C15a	14.81
C15b	C16a	C17b	117.48
C17a	C16a	C15a	120.00
C17a	C16a	C17b	5.55
C15a	C16a	C17b	120.13
H16b	C16b	H16a	19.85
H16b	C16b	C17a	117.39
H16b	C16b	C17b	119.25
H16b	C16b	C15b	119.39
H16b	C16b	C15a	115.16
H16a	C16b	C17a	126.13
H16a	C16b	C17b	125.73
H16a	C16b	C15b	109.77
H16a	C16b	C15a	110.45
C17a	C16b	C17b	6.05
C17a	C16b	C15b	122.85
C17a	C16b	C15a	123.37
C17b	C16b	C15b	121.35
C17b	C16b	C15a	123.63
C15b	C16b	C15a	14.13
H17a	C17a	H17b	7.34
H17a	C17a	C16b	119.70
H17a	C17a	C16a	119.99
H17a	C17a	C18a	120.02
H17a	C17a	C18b	115.58
H17b	C17a	C16b	126.82
H17b	C17a	C16a	127.09
H17b	C17a	C18a	112.88
H17b	C17a	C18b	109.73
C16b	C17a	C16a	0.77
C16b	C17a	C18a	120.28
C16b	C17a	C18b	119.84
C16a	C17a	C18a	119.99
C16a	C17a	C18b	119.88
C18a	C17a	C18b	21.84
H17a	C17b	H17b	7.81
H17a	C17b	C18a	126.81
H17a	C17b	C18b	127.65
H17a	C17b	C16b	113.38
H17a	C17b	C16a	113.57
H17b	C17b	C18a	119.01
H17b	C17b	C18b	120.54
H17b	C17b	C16b	120.59
H17b	C17b	C16a	120.77
C18a	C17b	C18b	22.93
C18a	C17b	C16b	115.29
C18a	C17b	C16a	115.02
C18b	C17b	C16b	118.87
C18b	C17b	C16a	118.69
C16b	C17b	C16a	0.32
H18a	C18a	H18b	33.80
H18a	C18a	C17b	116.10
H18a	C18a	C19a	120.04
H18a	C18a	C17a	119.98
H18a	C18a	C19b	117.26
H18b	C18a	C17b	105.04
H18b	C18a	C19a	117.49
H18b	C18a	C17a	111.67
H18b	C18a	C19b	97.23
C17b	C18a	C19a	123.49
C17b	C18a	C17a	7.14
C17b	C18a	C19b	112.33
C19a	C18a	C17a	119.98
C19a	C18a	C19b	31.97
C17a	C18a	C19b	112.97
H18b	C18b	H18a	36.72
H18b	C18b	C17b	119.58
H18b	C18b	C19b	119.38
H18b	C18b	C17a	122.72
H18b	C18b	C19a	119.26
H18a	C18b	C17b	107.60
H18a	C18b	C19b	119.10
H18a	C18b	C17a	106.89
H18a	C18b	C19a	99.74
C17b	C18b	C19b	121.05
C17b	C18b	C17a	6.14
C17b	C18b	C19a	112.07
C19b	C18b	C17a	117.62
C19b	C18b	C19a	30.88
C17a	C18b	C19a	106.46
H19a	C19a	H19b	51.68
H19a	C19a	C18a	119.91
H19a	C19a	C20a	120.01
H19a	C19a	C20b	120.62
H19a	C19a	C18b	118.36
H19b	C19a	C18a	104.90
H19b	C19a	C20a	111.21
H19b	C19a	C20b	89.26
H19b	C19a	C18b	88.66
C18a	C19a	C20a	120.08
C18a	C19a	C20b	111.59
C18a	C19a	C18b	20.14
C20a	C19a	C20b	28.81
C20a	C19a	C18b	117.61
C20b	C19a	C18b	100.10
H19b	C19b	H19a	50.42
H19b	C19b	C18b	119.51
H19b	C19b	C20b	119.24
H19b	C19b	C18a	120.12
H19b	C19b	C20a	117.58
H19a	C19b	C18b	107.95
H19a	C19b	C20b	108.51
H19a	C19b	C18a	92.18
H19a	C19b	C20a	87.00
C18b	C19b	C20b	121.24

Table S8 (continued).

C18b	C19b	C18a	21.23
C18b	C19b	C20a	115.65
C20b	C19b	C18a	116.22
C20b	C19b	C20a	27.31
C18a	C19b	C20a	101.62
H20a	C20a	H20b	50.97
H20a	C20a	C15a	120.00
H20a	C20a	C19a	120.04
H20a	C20a	C15b	122.41
H20a	C20a	C19b	120.52
H20b	C20a	C15a	106.19
H20b	C20a	C19a	110.60
H20b	C20a	C15b	97.19
H20b	C20a	C19b	88.37
C15a	C20a	C19a	119.96
C15a	C20a	C15b	13.72
C15a	C20a	C19b	111.18
C19a	C20a	C15b	115.79
C19a	C20a	C19b	29.66
C15b	C20a	C19b	101.12
H20b	C20b	H20a	48.41
H20b	C20b	C19b	120.22
H20b	C20b	C15b	120.28
H20b	C20b	C15a	117.61
H20b	C20b	C19a	119.28
H20a	C20b	C19b	114.82
H20a	C20b	C15b	104.43
H20a	C20b	C15a	92.85
H20a	C20b	C19a	90.82
C19b	C20b	C15b	119.51
C19b	C20b	C15a	120.36
C19b	C20b	C19a	31.16
C15b	C20b	C15a	13.64
C15b	C20b	C19a	111.27
C15a	C20b	C19a	104.87
C26b	C21a	C22a	104.53
C26b	C21a	C26a	44.02
C26b	C21a	C22b	126.49
C26b	C21a	P1	114.88
C22a	C21a	C26a	119.96
C22a	C21a	C22b	22.63
C22a	C21a	P1	122.53
C26a	C21a	C22b	129.67
C26a	C21a	P1	117.48
C22b	C21a	P1	109.52
C22a	C21b	C22b	23.21
C22a	C21b	C26b	99.55
C22a	C21b	C26a	107.04
C22a	C21b	P1	137.81
C22b	C21b	C26b	119.97
C22b	C21b	C26a	115.41
C22b	C21b	P1	121.37
C26b	C21b	C26a	37.83
C26b	C21b	P1	118.20
C26a	C21b	P1	114.23
H22a	C22a	C23b	101.85
H22a	C22a	C21b	110.03
H22a	C22a	C21a	120.07
H22a	C22a	C23a	119.83
C23b	C22a	C21b	146.81
C23b	C22a	C21a	135.95
C23b	C22a	C23a	22.23
C21b	C22a	C21a	10.89
C21b	C22a	C23a	129.93
C21a	C22a	C23a	120.10
H22a	C22b	H22b	70.25
H22a	C22b	C21b	111.37
H22a	C22b	C23b	88.44
H22a	C22b	C21a	120.79
H22b	C22b	C21b	120.07
H22b	C22b	C23b	119.93
H22b	C22b	C21a	126.00
C21b	C22b	C23b	120.01
C21b	C22b	C21a	10.56
C23b	C22b	C21a	113.36
C24b	C23a	H23a	106.32
C24b	C23a	H23b	143.68
C24b	C23a	C24a	36.40
C24b	C23a	C22a	121.59
H23a	C23a	H23b	39.83
H23a	C23a	C24a	119.99
H23a	C23a	C22a	120.05
H23b	C23a	C24a	135.69
H23b	C23a	C22a	93.01
C24a	C23a	C22a	119.95
H23b	C23b	H23a	51.37
H23b	C23b	C22a	136.47
H23b	C23b	C24b	119.95
H23b	C23b	C22b	120.02
H23a	C23b	C22a	147.04
H23a	C23b	C24b	72.02
H23a	C23b	C22b	158.63
C22a	C23b	C24b	101.36
C22a	C23b	C22b	22.78
C24b	C23b	C22b	120.03
C24b	C24a	H24a	106.68
C24b	C24a	H24b	48.92
C24b	C24a	C23a	35.40
C24b	C24a	C25a	121.75
C24b	C24a	C25b	70.00
H24a	C24a	H24b	57.76
H24a	C24a	C23a	119.92
H24a	C24a	C25a	120.09
H24a	C24a	C25b	125.92
H24b	C24a	C23a	70.99
H24b	C24a	C25a	149.05
H24b	C24a	C25b	99.04
C23a	C24a	C25a	119.99

Table S8 (continued).

C23a	C24a	C25b	88.97
C25a	C24a	C25b	55.31
C23a	C24b	C24a	108.20
C23a	C24b	H24b	118.40
C23a	C24b	C23b	2.29
C23a	C24b	C25b	121.56
C24a	C24b	H24b	86.36
C24a	C24b	C23b	109.60
C24a	C24b	C25b	74.06
H24b	C24b	C23b	120.04
H24b	C24b	C25b	120.00
C23b	C24b	C25b	119.96
H25a	C25a	C25b	123.42
H25a	C25a	C24a	120.02
H25a	C25a	C26a	120.01
C25b	C25a	C24a	63.59
C25b	C25a	C26a	83.83
C24a	C25a	C26a	119.97
H25b	C25b	C25a	91.33
H25b	C25b	C24b	120.04
H25b	C25b	C26b	119.91
H25b	C25b	C24a	106.42
C25a	C25b	C24b	95.06
C25a	C25b	C26b	83.44
C25a	C25b	C24a	61.10
C24b	C25b	C26b	120.05
C24b	C25b	C24a	35.95
C26b	C25b	C24a	121.76
H26a	C26a	C26b	112.14
H26a	C26a	C25a	119.92
H26a	C26a	C21a	120.06
H26a	C26a	C21b	117.44
C26b	C26a	C25a	95.90
C26b	C26a	C21a	61.38
C26b	C26a	C21b	58.28
C25a	C26a	C21a	120.02
C25a	C26a	C21b	122.50
C21a	C26a	C21b	4.47
H26b	C26b	C26a	89.97
H26b	C26b	C21a	122.54
H26b	C26b	C21b	120.00
H26b	C26b	C25b	120.02
C26a	C26b	C21a	74.60
C26a	C26b	C21b	83.89
C26a	C26b	C25b	96.38
C21a	C26b	C21b	9.99
C21a	C26b	C25b	116.58
C21b	C26b	C25b	119.98
C28b	C27a	C28a	21.26
C28b	C27a	C32a	99.19
C28b	C27a	C32b	105.24
C28b	C27a	P1	142.60
C28a	C27a	C32a	119.98
C28a	C27a	C32b	123.44
C28a	C27a	P1	121.80
C32a	C27a	C32b	18.12
C32a	C27a	P1	118.17
C32b	C27a	P1	111.00
C32a	C27b	C28b	109.78
C32a	C27b	C32b	23.13
C32a	C27b	C28a	129.19
C32a	C27b	P1	121.66
C28b	C27b	C32b	119.97
C28b	C27b	C28a	19.41
C28b	C27b	P1	123.47
C32b	C27b	C28a	137.37
C32b	C27b	P1	116.53
C28a	C27b	P1	105.62
H28a	C28a	C27a	119.94
H28a	C28a	C29a	120.02
H28a	C28a	C27b	129.03
C27a	C28a	C29a	120.04
C27a	C28a	C27b	11.35
C29a	C28a	C27b	110.53
H28b	C28b	C29a	94.39
H28b	C28b	C27a	107.73
H28b	C28b	C29b	120.03
H28b	C28b	C27b	119.94
C29a	C28b	C27a	157.26
C29a	C28b	C29b	27.45
C29a	C28b	C27b	144.27
C27a	C28b	C29b	131.99
C27a	C28b	C27b	13.03
C29b	C28b	C27b	120.03
H29a	C29a	H29b	52.81
H29a	C29a	C28b	138.61
H29a	C29a	C28a	120.00
H29a	C29a	C30a	120.06
H29b	C29a	C28b	156.87
H29b	C29a	C28a	162.51
H29b	C29a	C30a	69.61
C28b	C29a	C28a	19.72
C28b	C29a	C30a	100.95
C28a	C29a	C30a	119.93
H29b	C29b	C28b	120.05
H29b	C29b	C30b	119.91
C28b	C29b	C30b	120.04
H30a	C30a	H30b	37.40
H30a	C30a	C31a	120.06
H30a	C30a	C29a	119.92
H30b	C30a	C31a	84.93
H30b	C30a	C29a	151.99
C31a	C30a	C29a	120.03
H30b	C30b	H30a	48.33
H30b	C30b	C31a	134.75
H30b	C30b	C31b	120.05
H30b	C30b	C29b	119.98
H30a	C30b	C31a	149.82

Table S8 (continued).

H30a	C30b	C31b	166.80
H30a	C30b	C29b	72.02
C31a	C30b	C31b	30.38
C31a	C30b	C29b	99.14
C31b	C30b	C29b	119.97
H31a	C31a	C30b	95.60
H31a	C31a	C32a	119.97
H31a	C31a	C30a	120.06
H31a	C31a	C32b	108.65
C30b	C31a	C32a	141.63
C30b	C31a	C30a	28.29
C30b	C31a	C32b	137.53
C32a	C31a	C30a	119.98
C32a	C31a	C32b	21.69
C30a	C31a	C32b	127.52
H31a	C31b	H31b	63.56
H31a	C31b	C30b	78.83
H31a	C31b	C32b	129.64
H31a	C31b	C32a	114.92
H31b	C31b	C30b	119.98
H31b	C31b	C32b	120.04
H31b	C31b	C32a	132.61
C30b	C31b	C32b	119.99
C30b	C31b	C32a	104.65
C32b	C31b	C32a	21.56
H32a	C32a	C27b	121.48
H32a	C32a	H32b	31.47
H32a	C32a	C31a	120.04
H32a	C32a	C27a	119.92
H32a	C32a	C31b	100.68
C27b	C32a	H32b	109.86
C27b	C32a	C31a	117.74
C27b	C32a	C27a	8.77
C27b	C32a	C31b	128.05
H32b	C32a	C31a	117.13
H32b	C32a	C27a	113.34
H32b	C32a	C31b	90.00
C31a	C32a	C27a	120.04
C31a	C32a	C31b	27.92
C27a	C32a	C31b	134.37
H32a	C32b	H32b	47.04
H32a	C32b	C27b	104.37
H32a	C32b	C31b	115.74
H32a	C32b	C31a	112.92
H32a	C32b	C27a	100.09
H32b	C32b	C27b	119.95
H32b	C32b	C31b	120.05
H32b	C32b	C31a	140.58
H32b	C32b	C27a	117.71
C27b	C32b	C31b	120.00
C27b	C32b	C31a	96.37
C27b	C32b	C27a	4.37
C31b	C32b	C31a	28.06
C31b	C32b	C27a	122.11
C31a	C32b	C27a	97.39
C34	C33	C38	119.33
C34	C33	C1	121.95
C38	C33	C1	118.71
H34	C34	C33	120.35
H34	C34	C35	120.37
C33	C34	C35	119.28
H35	C35	C36	119.60
H35	C35	C34	119.58
C36	C35	C34	120.82
H36	C36	C37	120.08
H36	C36	C35	120.03
C37	C36	C35	119.89
H37	C37	C36	119.61
H37	C37	C38	119.59
C36	C37	C38	120.80
H38	C38	C37	120.17
H38	C38	C33	120.06
C37	C38	C33	119.77
C40	C39	C44	118.13
C40	C39	C3	119.53
C44	C39	C3	122.33
H40	C40	C41	119.33
H40	C40	C39	119.36
C41	C40	C39	121.31
H41	C41	C42	119.97
H41	C41	C40	119.96
C42	C41	C40	120.07
H42	C42	C41	120.13
H42	C42	C43	120.05
C41	C42	C43	119.82
H43	C43	C42	119.68
H43	C43	C44	119.77
C42	C43	C44	120.54
H44	C44	C43	119.88
H44	C44	C39	120.00
C43	C44	C39	120.12
C50	C45	C46	118.11
C50	C45	C6	120.46
C46	C45	C6	121.35
H46	C46	C47	119.67
H46	C46	C45	119.62
C47	C46	C45	120.71
H47	C47	C48	119.78
H47	C47	C46	119.70
C48	C47	C46	120.51
H48	C48	C47	120.28
H48	C48	C49	120.40
C47	C48	C49	119.32
H49	C49	C50	119.77
H49	C49	C48	119.71
C50	C49	C48	120.52
H50	C50	C49	119.57
H50	C50	C45	119.59

Table S8 (continued).

C49	C50	C45	120.83
N4	C51	C52	111.56
N4	C51	C83	122.80
C52	C51	C83	125.64
H52	C52	C53	126.31
H52	C52	C51	126.38
C53	C52	C51	107.30
C52	C53	C54	106.00
C52	C53	C89	125.35
C54	C53	C89	128.59
N5	C54	N4	127.36
N5	C54	C53	123.55
N4	C54	C53	108.98
N5	C55	N6	128.04
N5	C55	C56	123.27
N6	C55	C56	108.66
C57	C56	C55	106.26
C57	C56	C95	126.67
C55	C56	C95	127.03
H57	C57	C56	126.34
H57	C57	C58	126.33
C56	C57	C58	107.33
N6	C58	C57	111.58
N6	C58	C59	122.47
C57	C58	C59	125.77
C60	C59	C64	118.52
C60	C59	C58	120.09
C64	C59	C58	121.38
H60	C60	C61	119.73
H60	C60	C59	119.73
C61	C60	C59	120.53
H61	C61	C62	119.83
H61	C61	C60	119.92
C62	C61	C60	120.25
H62	C62	C61	119.85
H62	C62	C63	119.99
C61	C62	C63	120.16
H63	C63	C62	120.06
H63	C63	C64	120.05
C62	C63	C64	119.89
H64	C64	C63	119.69
H64	C64	C59	119.69
C63	C64	C59	120.63
C70	C65	C66	119.03
C70	C65	P2	122.77
C66	C65	P2	118.19
H66	C66	C67	119.73
H66	C66	C65	119.79
C67	C66	C65	120.49
H67	C67	C66	119.96
H67	C67	C68	120.05
C66	C67	C68	119.99
H68	C68	C69	120.15
H68	C68	C67	120.13
C69	C68	C67	119.73
H69	C69	C70	119.87
H69	C69	C68	119.83
C70	C69	C68	120.30
H70	C70	C69	119.74
H70	C70	C65	119.82
C69	C70	C65	120.44
C72	C71	C76	119.18
C72	C71	P2	122.61
C76	C71	P2	118.20
H72	C72	C73	119.90
H72	C72	C71	119.94
C73	C72	C71	120.16
H73	C73	C74	119.78
H73	C73	C72	119.70
C74	C73	C72	120.52
H74	C74	C73	120.00
H74	C74	C75	120.02
C73	C74	C75	119.97
H75	C75	C76	120.06
H75	C75	C74	120.01
C76	C75	C74	119.92
H76	C76	C75	119.93
H76	C76	C71	119.86
C75	C76	C71	120.21
C78	C77	C82	119.54
C78	C77	P2	123.16
C82	C77	P2	117.28
H78	C78	C77	119.83
H78	C78	C79	119.97
C77	C78	C79	120.20
H79	C79	C80	120.08
H79	C79	C78	120.19
C80	C79	C78	119.73
H80	C80	C79	119.82
H80	C80	C81	119.78
C79	C80	C81	120.40
H81	C81	C82	119.94
H81	C81	C80	119.97
C82	C81	C80	120.09
H82	C82	C81	119.98
H82	C82	C77	120.00
C81	C82	C77	120.02
C88	C83	C84	118.62
C88	C83	C51	119.42
C84	C83	C51	121.94
H84	C84	C85	119.75
H84	C84	C83	119.75
C85	C84	C83	120.49
H85	C85	C84	119.92
H85	C85	C86	119.85
C84	C85	C86	120.23
H86	C86	C85	120.04
H86	C86	C87	120.03

Table S8 (continued).

C85	C86	C87	119.94
H87	C87	C88	119.94
H87	C87	C86	120.03
C88	C87	C86	120.02
H88	C88	C87	119.62
H88	C88	C83	119.75
C87	C88	C83	120.63
C94	C89	C90	118.55
C94	C89	C53	121.78
C90	C89	C53	119.65
H90	C90	C91	119.73
H90	C90	C89	119.76
C91	C90	C89	120.51
H91	C91	C92	119.81
H91	C91	C90	119.83
C92	C91	C90	120.36
H92	C92	C91	119.95
H92	C92	C93	119.91
C91	C92	C93	120.13
H93	C93	C92	120.00
H93	C93	C94	120.08
C92	C93	C94	119.92
H94	C94	C89	119.76
H94	C94	C93	119.73
C89	C94	C93	120.51
C96	C95	C100	118.57
C96	C95	C56	120.89
C100	C95	C56	120.47
H96	C96	C97	119.71
H96	C96	C95	119.75
C97	C96	C95	120.53
H97	C97	C98	119.82
H97	C97	C96	119.84
C98	C97	C96	120.34
H98	C98	C97	120.06
H98	C98	C99	120.04
C97	C98	C99	119.91
H99	C99	C98	119.88
H99	C99	C100	119.77
C98	C99	C100	120.35
H100	C100	C99	119.87
H100	C100	C95	119.85
C99	C100	C95	120.28
N7	C101	C102	111.69
N7	C101	C133	122.44
C102	C101	C133	125.80
H102	C102	C103	126.50
H102	C102	C101	126.51
C103	C102	C101	106.99
C102	C103	C104	105.87
C102	C103	C139	125.40
C104	C103	C139	128.68
N8	C104	N7	127.86
N8	C104	C103	122.82
N7	C104	C103	109.30
N8	C105	N9	127.44
N8	C105	C106	123.42
N9	C105	C106	109.08
C107	C106	C105	105.58
C107	C106	C145	126.99
C105	C106	C145	127.30
H107	C107	C106	126.17
H107	C107	C108	126.06
C106	C107	C108	107.77
N9	C108	C107	111.15
N9	C108	C109	121.81
C107	C108	C109	126.94
C110	C109	C114	118.10
C110	C109	C108	120.19
C114	C109	C108	121.70
H110	C110	C111	119.55
H110	C110	C109	119.61
C111	C110	C109	120.84
H111	C111	C110	119.68
H111	C111	C112	119.78
C110	C111	C112	120.53
H112	C112	C113	120.18
H112	C112	C111	120.28
C113	C112	C111	119.54
H113	C113	C112	119.77
H113	C113	C114	119.93
C112	C113	C114	120.30
H114	C114	C113	119.64
H114	C114	C109	119.68
C113	C114	C109	120.67
C120	C115	C116	119.02
C120	C115	P3	122.39
C116	C115	P3	118.46
H116	C116	C115	119.69
H116	C116	C117	119.73
C115	C116	C117	120.58
H117	C117	C118	119.99
H117	C117	C116	120.06
C118	C117	C116	119.95
H118	C118	C119	120.17
H118	C118	C117	120.17
C119	C118	C117	119.66
H119	C119	C118	119.78
H119	C119	C120	119.80
C118	C119	C120	120.42
H120	C120	C115	119.82
H120	C120	C119	119.82
C115	C120	C119	120.35
C126	C121	C122	118.90
C126	C121	P3	123.79
C122	C121	P3	117.30
H122	C122	C123	119.76
H122	C122	C121	119.73

Table S8 (continued).

C123	C122	C121	120.50
H123	C123	C122	119.79
H123	C123	C124	119.84
C122	C123	C124	120.37
H124	C124	C125	120.26
H124	C124	C123	120.34
C125	C124	C123	119.40
H125	C125	C124	119.60
H125	C125	C126	119.57
C124	C125	C126	120.83
H126	C126	C125	120.02
H126	C126	C121	119.99
C125	C126	C121	119.98
C132	C127	C128	119.30
C132	C127	P3	118.15
C128	C127	P3	122.55
H128	C128	C129	119.97
H128	C128	C127	119.91
C129	C128	C127	120.13
H129	C129	C130	119.90
H129	C129	C128	119.88
C130	C129	C128	120.23
H130	C130	C129	120.14
H130	C130	C131	120.26
C129	C130	C131	119.60
H131	C131	C132	119.79
H131	C131	C130	119.82
C132	C131	C130	120.38
H132	C132	C131	119.77
H132	C132	C127	119.88
C131	C132	C127	120.35
C134	C133	C138	118.06
C134	C133	C101	122.19
C138	C133	C101	119.65
H134	C134	C135	119.66
H134	C134	C133	119.64
C135	C134	C133	120.70
H135	C135	C134	119.80
H135	C135	C136	119.79
C134	C135	C136	120.41
H136	C136	C137	120.27
H136	C136	C135	120.33
C137	C136	C135	119.40
H137	C137	C138	119.69
H137	C137	C136	119.78
C138	C137	C136	120.53
H138	C138	C137	119.56
H138	C138	C133	119.63
C137	C138	C133	120.82
C144	C139	C140	117.87
C144	C139	C103	122.54
C140	C139	C103	119.48
H140	C140	C141	119.44
H140	C140	C139	119.40
C141	C140	C139	121.16
H141	C141	C140	120.02
H141	C141	C142	119.88
C140	C141	C142	120.10
H142	C142	C143	120.25
H142	C142	C141	120.35
C143	C142	C141	119.40
H143	C143	C142	119.84
H143	C143	C144	119.65
C142	C143	C144	120.51
H144	C144	C143	119.48
H144	C144	C139	119.57
C143	C144	C139	120.94
C146	C145	C150	117.59
C146	C145	C106	122.80
C150	C145	C106	119.61
H146	C146	C147	119.72
H146	C146	C145	119.53
C147	C146	C145	120.74
H147	C147	C146	119.62
H147	C147	C148	119.61
C146	C147	C148	120.77
H148	C148	C149	120.38
H148	C148	C147	120.36
C149	C148	C147	119.26
H149	C149	C148	119.72
H149	C149	C150	119.82
C148	C149	C150	120.45
H150	C150	C149	119.45
H150	C150	C145	119.47
C149	C150	C145	121.07
C16a	H16a	C16b	5.89
C16a	H16b	C16b	6.52
C17b	H17a	C17a	10.68
C17b	H17b	C17a	10.11
C18a	H18a	C18b	30.84
C18b	H18b	C18a	27.92
C19a	H19a	C19b	37.18
C19b	H19b	C19a	38.45
C20a	H20a	C20b	34.67
C20b	H20b	C20a	37.23
C22b	H22a	C22a	35.54
H23b	H23a	C23a	93.47
H23b	H23a	C23b	62.62
C23a	H23a	C23b	33.44
H23a	H23b	C23b	66.02
H23a	H23b	C23a	46.69
C23b	H23b	C23a	22.24
C24b	H24b	C24a	44.72
H29b	H29a	C29a	64.51
H29a	H29b	C29b	102.48
H29a	H29b	C29a	62.69
C29b	H29b	C29a	40.55
H30b	H30a	C30a	98.59

Table S8 (continued).

H30b	H30a	C30b	58.73
C30a	H30a	C30b	39.88
H30a	H30b	C30b	72.95
H30a	H30b	C30a	44.02
C30b	H30b	C30a	28.95
C31b	H31a	H31b	63.65
C31b	H31a	C31a	47.72
H31b	H31a	C31a	111.37
H31a	H31b	C31b	52.79
C32b	H32a	C32a	36.25
C32b	H32b	C32a	20.82
C1	N1	C4	105.75
C1	N1	Ag1	131.48
C4	N1	Ag1	119.75
C4	N2	C5	130.10
C8	N3	C5	105.95
C8	N3	Ag1	131.68
C5	N3	Ag1	118.05
C51	N4	C54	106.13
C51	N4	Ag2	127.55
C54	N4	Ag2	125.75
C55	N5	C54	128.23
C58	N6	C55	106.12
C58	N6	Ag2	126.53
C55	N6	Ag2	121.26
C101	N7	C104	106.12
C101	N7	Ag3	128.12
C104	N7	Ag3	119.95
C104	N8	C105	127.93
C108	N9	C105	106.40
C108	N9	Ag3	126.10
C105	N9	Ag3	121.91
C21b	P1	C27a	105.25
C21b	P1	C15a	95.96
C21b	P1	C15b	106.92
C21b	P1	C21a	6.53
C21b	P1	C27b	111.35
C21b	P1	Ag1	105.59
C27a	P1	C15a	103.13
C27a	P1	C15b	100.31
C27a	P1	C21a	99.37
C27a	P1	C27b	8.30
C27a	P1	Ag1	121.29
C15a	P1	C15b	10.97
C15a	P1	C21a	100.28
C15a	P1	C27b	107.38
C15a	P1	Ag1	121.62
C15b	P1	C21a	111.25
C15b	P1	C27b	103.17
C15b	P1	Ag1	116.36
C21a	P1	C27b	105.21
C21a	P1	Ag1	106.98
C27b	P1	Ag1	113.40
C71	P2	C65	103.65
C71	P2	C77	104.11
C71	P2	Ag2	114.23
C65	P2	C77	103.31
C65	P2	Ag2	114.71
C77	P2	Ag2	115.37
C127	P3	C121	104.91
C127	P3	C115	107.07
C127	P3	Ag3	112.53
C121	P3	C115	102.43
C121	P3	Ag3	114.61
C115	P3	Ag3	114.30
N3	Ag1	N1	86.30
N3	Ag1	P1	139.25
N1	Ag1	P1	130.54
N4	Ag2	N6	82.89
N4	Ag2	P2	140.72
N6	Ag2	P2	135.77
N9	Ag3	N7	82.20
N9	Ag3	P3	140.64
N7	Ag3	P3	136.37

Table S9. Anisotropic displacement parameters [$Å^2 \times 10^3$] for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(h a^*)^2 U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
C(15A)	41(5)	24(5)	54(6)	-10(4)	-18(4)	1(3)
C(16A)	22(6)	19(6)	22(6)	7(4)	-7(4)	0(4)
C(17A)	19(4)	24(5)	27(5)	-14(4)	2(3)	-7(3)
C(18A)	30(4)	54(5)	41(4)	-4(4)	-14(3)	-5(3)
C(19A)	57(5)	60(5)	73(6)	-22(4)	-34(4)	21(4)
C(20A)	53(5)	49(5)	64(5)	-26(4)	-36(4)	12(3)
P(1)	30(1)	24(1)	37(1)	-2(1)	-11(1)	3(1)
C(15B)	20(3)	22(4)	27(4)	5(3)	-8(2)	-4(3)
C(16B)	32(7)	30(7)	42(8)	-11(5)	5(5)	-10(5)
C(17B)	39(6)	46(7)	39(7)	6(5)	-15(4)	-13(5)
C(18B)	23(3)	49(4)	40(4)	-6(3)	-7(3)	-7(3)
C(19B)	31(3)	52(4)	45(4)	-20(3)	-12(3)	10(3)
C(20B)	27(3)	44(4)	41(4)	-16(3)	-6(3)	3(3)
P(2)	19(1)	14(1)	17(1)	2(1)	-4(1)	-5(1)
P(3)	13(1)	16(1)	17(1)	-1(1)	-4(1)	-4(1)
C(21A)	69(6)	32(5)	62(6)	38(4)	-32(5)	-20(4)
C(22A)	81(5)	29(4)	35(4)	-4(3)	-20(4)	-28(4)
C(23A)	148(8)	87(6)	71(6)	44(5)	-66(6)	-87(6)
C(24A)	146(7)	107(6)	75(6)	27(5)	-43(5)	-100(5)
C(25A)	91(5)	95(5)	67(5)	45(4)	-41(4)	-74(4)
C(26A)	58(4)	54(4)	44(4)	27(3)	-26(3)	-33(3)
Ag(1)	28(1)	22(1)	26(1)	-2(1)	-1(1)	2(1)
C(21B)	45(5)	54(6)	65(6)	23(5)	-25(4)	-18(4)
C(22B)	28(3)	32(4)	37(3)	5(3)	-2(3)	-2(3)
C(23B)	63(5)	78(6)	68(5)	25(4)	-28(4)	-39(4)
C(24B)	99(6)	56(5)	101(7)	36(5)	0(5)	-49(4)
C(25B)	64(5)	97(6)	155(7)	44(6)	-17(5)	-42(4)
C(26B)	63(5)	64(5)	116(6)	50(5)	-23(4)	-23(4)
Ag(2)	20(1)	14(1)	19(1)	0(1)	-2(1)	-3(1)
C(27A)	36(4)	28(4)	37(4)	-3(3)	-21(3)	4(3)
C(28A)	68(6)	32(4)	33(4)	-5(3)	-23(4)	2(3)
C(29A)	59(5)	34(4)	45(5)	-3(3)	-21(4)	1(3)
C(30A)	45(5)	52(5)	39(4)	-14(4)	-10(3)	10(4)
C(31A)	44(4)	74(5)	51(4)	-10(4)	2(3)	-12(4)
C(32A)	48(4)	53(5)	49(5)	-26(4)	-8(3)	-8(4)
Ag(3)	12(1)	17(1)	19(1)	-1(1)	-3(1)	-5(1)
C(27B)	24(4)	25(4)	27(3)	-11(3)	-5(3)	-1(3)
C(28B)	43(4)	24(3)	27(4)	-3(3)	-17(3)	2(3)
C(29B)	37(4)	26(3)	27(4)	-14(3)	-11(3)	-1(3)
C(30B)	37(4)	65(5)	42(4)	-26(4)	-6(3)	-8(3)
C(31B)	61(5)	73(5)	43(4)	-8(4)	3(3)	-39(4)
C(32B)	38(4)	46(4)	35(3)	-8(3)	2(3)	-22(3)
C(1)	43(2)	23(1)	16(1)	2(1)	-8(1)	0(1)
C(2)	42(2)	26(1)	24(1)	1(1)	-15(1)	-4(1)
C(3)	33(1)	23(1)	21(1)	3(1)	-8(1)	-4(1)
C(4)	30(1)	19(1)	17(1)	2(1)	-5(1)	-1(1)

Table S9 (continued).

C(5)	24(1)	17(1)	20(1)	2(1)	0(1)	-4(1)
C(6)	25(1)	14(1)	24(1)	1(1)	-3(1)	-7(1)
C(7)	24(1)	18(1)	27(1)	-1(1)	-2(1)	-8(1)
C(8)	23(1)	18(1)	29(1)	4(1)	-1(1)	-7(1)
C(9)	24(1)	20(1)	38(2)	8(1)	-2(1)	-8(1)
C(10)	28(1)	34(2)	46(2)	0(1)	-4(1)	-11(1)
C(11)	29(2)	49(2)	61(2)	9(2)	-15(1)	-16(1)
C(12)	18(1)	38(2)	72(2)	10(2)	0(1)	-7(1)
C(13)	27(1)	30(2)	53(2)	8(1)	5(1)	-7(1)
C(14)	26(1)	24(1)	44(2)	6(1)	2(1)	-7(1)
C(33)	51(2)	23(1)	20(1)	0(1)	-13(1)	6(1)
C(34)	53(2)	26(1)	20(1)	2(1)	-7(1)	5(1)
C(35)	60(2)	39(2)	18(1)	4(1)	-6(1)	17(1)
C(36)	85(3)	34(2)	28(2)	-12(1)	-27(2)	17(2)
C(37)	88(3)	30(2)	43(2)	-13(1)	-40(2)	8(2)
C(38)	62(2)	32(2)	36(2)	-5(1)	-25(1)	3(1)
C(39)	30(1)	30(1)	17(1)	4(1)	-8(1)	-3(1)
C(40)	40(2)	32(2)	22(1)	5(1)	-15(1)	-9(1)
C(41)	30(1)	50(2)	28(1)	10(1)	-12(1)	-9(1)
C(42)	27(1)	53(2)	30(2)	0(1)	-6(1)	0(1)
C(43)	35(2)	40(2)	29(1)	-9(1)	-7(1)	1(1)
C(44)	29(1)	35(2)	27(1)	-2(1)	-10(1)	-1(1)
C(45)	21(1)	19(1)	22(1)	2(1)	-4(1)	-5(1)
C(46)	26(1)	21(1)	22(1)	-3(1)	-5(1)	-9(1)
C(47)	21(1)	33(1)	26(1)	0(1)	-6(1)	-11(1)
C(48)	21(1)	28(1)	23(1)	-2(1)	-1(1)	-1(1)
C(49)	31(1)	18(1)	28(1)	-6(1)	-5(1)	-5(1)
C(50)	24(1)	19(1)	31(1)	-2(1)	-7(1)	-6(1)
C(51)	26(1)	25(1)	23(1)	2(1)	0(1)	-8(1)
C(52)	20(1)	33(1)	26(1)	4(1)	-1(1)	-8(1)
C(53)	23(1)	27(1)	21(1)	3(1)	-2(1)	-4(1)
C(54)	25(1)	20(1)	16(1)	1(1)	-2(1)	-3(1)
C(55)	25(1)	15(1)	16(1)	-4(1)	-3(1)	-3(1)
C(56)	31(1)	15(1)	21(1)	-3(1)	-7(1)	-7(1)
C(57)	29(1)	18(1)	27(1)	-4(1)	-6(1)	-9(1)
C(58)	27(1)	18(1)	16(1)	-4(1)	-6(1)	-6(1)
C(59)	25(1)	17(1)	22(1)	-8(1)	-8(1)	-5(1)
C(60)	30(1)	28(1)	31(1)	-2(1)	-10(1)	-11(1)
C(61)	23(1)	40(2)	38(2)	-7(1)	-5(1)	-9(1)
C(62)	27(1)	34(2)	39(2)	-6(1)	-15(1)	1(1)
C(63)	37(2)	26(1)	29(1)	-1(1)	-15(1)	-5(1)
C(64)	27(1)	21(1)	22(1)	-4(1)	-7(1)	-7(1)
C(65)	18(1)	16(1)	17(1)	3(1)	-5(1)	-3(1)
C(66)	31(1)	20(1)	19(1)	0(1)	-4(1)	-11(1)
C(67)	30(1)	25(1)	27(1)	5(1)	-6(1)	-15(1)
C(68)	21(1)	29(1)	19(1)	6(1)	-3(1)	-6(1)
C(69)	22(1)	22(1)	21(1)	-2(1)	-7(1)	1(1)
C(70)	19(1)	16(1)	22(1)	1(1)	-7(1)	-4(1)
C(71)	29(1)	15(1)	22(1)	3(1)	-9(1)	-8(1)
C(72)	34(1)	21(1)	25(1)	2(1)	-12(1)	-6(1)
C(73)	34(1)	29(1)	36(2)	4(1)	-18(1)	-6(1)
C(74)	51(2)	38(2)	34(2)	13(1)	-24(1)	-19(1)
C(75)	53(2)	47(2)	21(1)	12(1)	-12(1)	-26(1)
C(76)	34(1)	34(1)	24(1)	7(1)	-7(1)	-14(1)

Table S9 (continued).

C(77)	19(1)	19(1)	16(1)	0(1)	1(1)	-8(1)
C(78)	26(1)	20(1)	26(1)	1(1)	-2(1)	-6(1)
C(79)	31(1)	15(1)	33(1)	2(1)	0(1)	-9(1)
C(80)	32(1)	25(1)	31(1)	-1(1)	-2(1)	-17(1)
C(81)	26(1)	28(1)	28(1)	3(1)	-7(1)	-14(1)
C(82)	23(1)	19(1)	24(1)	3(1)	-3(1)	-7(1)
C(83)	21(1)	24(1)	32(1)	4(1)	6(1)	-6(1)
C(84)	24(1)	31(1)	37(2)	10(1)	2(1)	-10(1)
C(85)	30(1)	30(2)	42(2)	11(1)	9(1)	-4(1)
C(86)	45(2)	27(2)	47(2)	4(1)	16(1)	-15(1)
C(87)	42(2)	37(2)	46(2)	0(1)	6(1)	-23(1)
C(88)	30(1)	30(1)	35(2)	2(1)	2(1)	-12(1)
C(89)	27(1)	29(1)	22(1)	5(1)	2(1)	0(1)
C(90)	28(1)	44(2)	26(1)	2(1)	-5(1)	1(1)
C(91)	33(2)	58(2)	28(2)	6(1)	-7(1)	14(1)
C(92)	41(2)	41(2)	36(2)	12(1)	8(1)	17(1)
C(93)	43(2)	29(2)	68(2)	3(2)	17(2)	2(1)
C(94)	28(2)	29(2)	63(2)	4(1)	8(1)	-1(1)
C(95)	29(1)	16(1)	28(1)	-4(1)	-12(1)	-8(1)
C(96)	29(1)	18(1)	37(2)	-1(1)	-8(1)	-9(1)
C(97)	28(1)	18(1)	53(2)	-5(1)	-11(1)	-5(1)
C(98)	39(2)	14(1)	55(2)	4(1)	-22(1)	-8(1)
C(99)	47(2)	22(1)	39(2)	8(1)	-17(1)	-18(1)
C(100)	35(1)	22(1)	30(1)	0(1)	-13(1)	-13(1)
C(101)	20(1)	16(1)	19(1)	4(1)	-4(1)	-7(1)
C(102)	21(1)	16(1)	20(1)	-1(1)	-3(1)	-8(1)
C(103)	20(1)	19(1)	21(1)	3(1)	-4(1)	-12(1)
C(104)	18(1)	17(1)	19(1)	3(1)	-4(1)	-10(1)
C(105)	14(1)	18(1)	20(1)	4(1)	-3(1)	-7(1)
C(106)	16(1)	18(1)	25(1)	4(1)	-3(1)	-5(1)
C(107)	16(1)	19(1)	24(1)	-1(1)	-1(1)	-2(1)
C(108)	17(1)	18(1)	18(1)	1(1)	-2(1)	-4(1)
C(109)	17(1)	23(1)	16(1)	-2(1)	1(1)	-6(1)
C(110)	23(1)	22(1)	24(1)	-5(1)	-4(1)	-2(1)
C(111)	34(1)	25(1)	30(1)	-8(1)	-4(1)	-7(1)
C(112)	33(1)	36(2)	25(1)	-7(1)	-9(1)	-13(1)
C(113)	24(1)	35(1)	18(1)	-1(1)	-5(1)	-6(1)
C(114)	20(1)	23(1)	16(1)	-1(1)	0(1)	-3(1)
C(115)	13(1)	18(1)	16(1)	-2(1)	-4(1)	-2(1)
C(116)	15(1)	20(1)	22(1)	-2(1)	-3(1)	-4(1)
C(117)	18(1)	26(1)	20(1)	4(1)	-4(1)	-3(1)
C(118)	18(1)	32(1)	19(1)	-2(1)	-7(1)	-1(1)
C(119)	24(1)	29(1)	26(1)	-6(1)	-9(1)	-8(1)
C(120)	23(1)	20(1)	22(1)	0(1)	-7(1)	-6(1)
C(121)	17(1)	15(1)	20(1)	0(1)	-9(1)	-4(1)
C(122)	24(1)	21(1)	25(1)	3(1)	-2(1)	-4(1)
C(123)	37(2)	18(1)	31(1)	-2(1)	0(1)	1(1)
C(124)	45(2)	16(1)	39(2)	4(1)	-9(1)	-6(1)
C(125)	32(1)	25(1)	29(1)	6(1)	-8(1)	-15(1)
C(126)	20(1)	21(1)	22(1)	2(1)	-6(1)	-8(1)
C(127)	15(1)	12(1)	18(1)	2(1)	-3(1)	-3(1)
C(128)	17(1)	23(1)	22(1)	0(1)	-6(1)	-6(1)
C(129)	15(1)	26(1)	26(1)	6(1)	-2(1)	-3(1)
C(130)	25(1)	19(1)	17(1)	2(1)	0(1)	-1(1)

Table S9 (continued).

C(131)	27(1)	17(1)	17(1)	2(1)	-7(1)	-5(1)
C(132)	18(1)	15(1)	21(1)	5(1)	-6(1)	-5(1)
C(133)	19(1)	12(1)	22(1)	2(1)	-4(1)	-4(1)
C(134)	22(1)	13(1)	20(1)	0(1)	-4(1)	-4(1)
C(135)	24(1)	16(1)	25(1)	2(1)	-10(1)	-5(1)
C(136)	17(1)	19(1)	31(1)	2(1)	-6(1)	-2(1)
C(137)	21(1)	19(1)	25(1)	-2(1)	-3(1)	-1(1)
C(138)	25(1)	18(1)	22(1)	-1(1)	-6(1)	-7(1)
C(139)	19(1)	26(1)	20(1)	1(1)	-3(1)	-13(1)
C(140)	25(1)	28(1)	24(1)	1(1)	-3(1)	-14(1)
C(141)	32(1)	38(2)	27(1)	-3(1)	-7(1)	-22(1)
C(142)	27(1)	51(2)	27(1)	4(1)	-11(1)	-24(1)
C(143)	22(1)	40(2)	30(1)	6(1)	-9(1)	-11(1)
C(144)	24(1)	29(1)	26(1)	1(1)	-6(1)	-13(1)
C(145)	17(1)	20(1)	31(1)	8(1)	-4(1)	-7(1)
C(146)	19(1)	25(1)	40(2)	6(1)	-6(1)	-10(1)
C(147)	28(1)	39(2)	52(2)	8(1)	-17(1)	-21(1)
C(148)	22(1)	44(2)	59(2)	22(1)	-20(1)	-16(1)
C(149)	23(1)	29(1)	57(2)	15(1)	-13(1)	-5(1)
C(150)	24(1)	23(1)	41(2)	8(1)	-10(1)	-7(1)
N(1)	35(1)	19(1)	19(1)	1(1)	-5(1)	1(1)
N(2)	25(1)	16(1)	20(1)	1(1)	-3(1)	-3(1)
N(3)	24(1)	18(1)	24(1)	3(1)	0(1)	-3(1)
N(4)	22(1)	17(1)	22(1)	2(1)	-1(1)	-5(1)
N(5)	23(1)	18(1)	15(1)	-2(1)	-3(1)	-4(1)
N(6)	21(1)	17(1)	17(1)	-2(1)	-5(1)	-3(1)
N(7)	16(1)	15(1)	19(1)	1(1)	-3(1)	-5(1)
N(8)	17(1)	18(1)	19(1)	5(1)	-4(1)	-9(1)
N(9)	16(1)	19(1)	17(1)	1(1)	-3(1)	-5(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3**.

	x	y	z	U(eq)
H(16A)	2767	2427	8906	27
H(17A)	1677	2796	8379	29
H(18A)	431	4067	8530	52
H(19A)	276	4968	9206	84
H(20A)	1367	4598	9733	71
H(16B)	2811	2548	8812	44
H(17B)	1622	2839	8350	49
H(18B)	175	3870	8656	46
H(19B)	-92	4617	9400	58
H(20B)	1004	4264	9907	50
H(22A)	3469	4108	8904	54
H(23A)	4497	4875	8684	100
H(24A)	5447	5011	9230	110
H(25A)	5369	4380	9998	84
H(26A)	4341	3613	10219	55
H(22B)	2835	4479	9146	42
H(23B)	3913	5114	8739	77
H(24B)	5468	4708	8877	100
H(25B)	5946	3666	9423	123
H(26B)	4868	3031	9830	96
H(28A)	2886	4577	10339	56
H(29A)	2041	5185	11142	58
H(30A)	1009	4597	11650	62
H(31A)	821	3400	11354	72
H(32A)	1666	2792	10551	63
H(28B)	2437	4667	10467	40
H(29B)	1546	5090	11291	38
H(30B)	906	4192	11777	60
H(31B)	1156	2871	11439	68
H(32B)	2047	2448	10614	47
H(2)	7298	1140	10375	37
H(7)	4562	-534	8254	28
H(10)	2967	284	8248	44
H(11)	1311	796	8334	54
H(12)	318	1455	9097	54
H(13)	975	1581	9776	47
H(14)	2622	1070	9696	40
H(34)	4045	1898	10810	45
H(35)	3189	3032	11396	58
H(36)	3921	3936	11598	67
H(37)	5535	3672	11272	68
H(38)	6412	2561	10687	55
H(40)	8805	637	9794	37
H(41)	10364	-236	9474	43
H(42)	10638	-1457	9017	48
H(43)	9351	-1816	8885	45

Table S10 (continued).

H(44)	7781	-955	9209	39
H(46)	7346	-162	8392	27
H(47)	8766	-879	7822	32
H(48)	8847	-1988	7306	32
H(49)	7493	-2380	7365	32
H(50)	6069	-1669	7931	30
H(52)	2383	4684	7900	33
H(57)	7496	6176	7213	29
H(60)	8973	4986	7051	35
H(61)	10422	4037	7154	41
H(62)	10432	2997	7708	42
H(63)	8993	2907	8174	36
H(64)	7535	3856	8078	28
H(66)	8537	3210	6901	27
H(67)	9786	3161	6219	32
H(68)	10196	2190	5539	29
H(69)	9353	1270	5548	28
H(70)	8153	1277	6244	23
H(72)	9250	1275	7214	32
H(73)	10007	547	7822	39
H(74)	9152	593	8646	45
H(75)	7523	1384	8871	45
H(76)	6753	2111	8264	36
H(78)	7433	545	7312	30
H(79)	6679	-317	7042	33
H(80)	5527	205	6569	34
H(81)	5083	1590	6380	31
H(82)	5789	2458	6667	27
H(84)	5048	2896	8228	39
H(85)	5245	1496	8254	46
H(86)	4357	940	7847	52
H(87)	3219	1801	7439	50
H(88)	3001	3205	7421	39
H(90)	1393	5941	7653	44
H(91)	210	7241	7755	56
H(92)	541	8398	7967	60
H(93)	2050	8270	8094	66
H(94)	3236	6963	8016	54
H(96)	4431	7402	7854	33
H(97)	3668	8776	7714	40
H(98)	4339	9393	7040	41
H(99)	5764	8628	6490	40
H(100)	6525	7246	6614	33
H(102)	8993	5499	6053	22
H(107)	12445	1261	3917	25
H(110)	11363	531	3723	30
H(111)	10544	12	3258	37
H(112)	9169	891	3025	37
H(113)	8631	2297	3258	32
H(114)	9444	2828	3730	25
H(116)	7346	3970	4154	24
H(117)	6755	4176	3417	27
H(118)	6102	3242	3147	29
H(119)	5990	2137	3631	31

Table S10 (continued).

H(120)	6589	1923	4364	26
H(122)	8904	1287	4341	29
H(123)	9255	-128	4401	39
H(124)	8425	-638	5080	41
H(125)	7204	278	5679	33
H(126)	6801	1699	5608	24
H(128)	5486	3180	5207	25
H(129)	4335	3857	5926	29
H(130)	4793	4373	6587	27
H(131)	6408	4200	6531	24
H(132)	7561	3508	5822	21
H(134)	7791	4803	4752	23
H(135)	6150	5266	4803	26
H(136)	5086	5952	5548	28
H(137)	5687	6196	6231	29
H(138)	7322	5712	6191	26
H(140)	10375	5726	6214	30
H(141)	11450	5734	6710	36
H(142)	12669	4512	6790	38
H(143)	12815	3294	6360	36
H(144)	11723	3276	5879	30
H(146)	12793	3145	4981	33
H(147)	14174	2820	5293	44
H(148)	15332	1505	5124	47
H(149)	15075	507	4657	44
H(150)	13647	790	4394	35

X-ray Structural Data for **4**

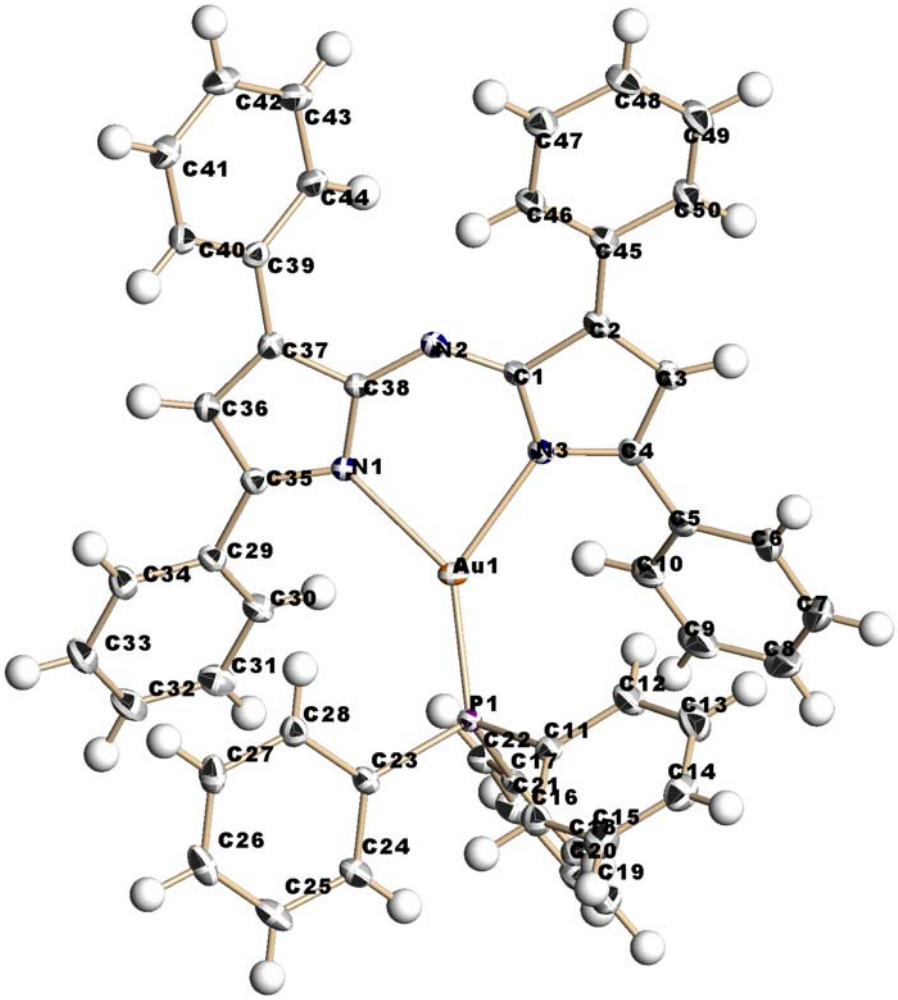

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Figure S7. Thermal ellipsoid plot of $(Ph_3P)Au^I$(tetraphenylazadipyrromethene) (**4**). Ellipsoids are drawn at 50% probability; data were collected at 100 K.

Table S11. Crystal data and structure refinement for **4.**

Identification code: JU092206

Empirical formula: C50 H37 Au P N3

Formula weight: 907.76

Temperature: 100(2) K

Wavelength: 0.71073 Å

Crystal system: Monoclinic

Space group: $P2_1/n$

Unit cell dimensions:

a = 12.3616(2) Å, α = 90°

b = 12.9923(2) Å, β = 90.6780(10)°

c = 23.7047(5) Å, γ = 90°

Volume, Z: 3806.84(12) $Å^3$, 4

Density (calculated): 1.584 Mg/m^3

Absorption coefficient: 3.947 mm^{-1}

F(000): 1808

Crystal size: 0.44 × 0.42 × 0.18 mm

Crystal shape, colour: irregular chunk, violet

θ range for data collection: 1.72 to 29.58°

Limiting indices: $-17 \leq h \leq 17$, $-17 \leq k \leq 18$, $-32 \leq l \leq 32$

Reflections collected: 119551

Independent reflections: 10670 (R(int) = 0.0232)

Completeness to θ = 29.58°: 99.9 %

Absorption correction: multi-scan

Max. and min. transmission: 0.2535 and 0.4939

Refinement method: Full-matrix least-squares on F^2

Data / restraints / parameters: 10670 / 0 / 496

Goodness-of-fit on F^2: 1.009

Final R indices [$I>2\sigma(I)$]: R1 = 0.0157, wR2 = 0.0401

R indices (all data): R1 = 0.0180, wR2 = 0.0413

Largest diff. peak and hole: 1.177 and -0.560 e × $Å^{-3}$

Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit are based on F^2, conventional R-factors R are based

on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors

Treatment of hydrogen atoms:
All hydrogen atoms were placed geometrically and were refined with an isotropic displacement parameter 1.5 (methyl) or 1.2 times (all others) that of the neighboring carbon atom.

Table S12. Atomic coordinates [× 10^4] and equivalent isotropic displacement parameters [$Å^2$ × 10^3] for **4.** U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Au1	501.928(4)	340.112(4)	108.096(2)	17.08(2)
P1	607.13(3)	393.96(3)	178.043(15)	14.67(6)
N1	512.30(9)	288.00(10)	18.03(5)	17.1(2)
N2	363.65(10)	163.36(9)	20.51(5)	17.0(2)
N3	332.58(9)	282.65(9)	97.11(5)	16.8(2)
C28	788.01(12)	331.66(11)	118.82(6)	20.1(3)
C27	896.85(13)	331.77(13)	104.68(7)	25.3(3)
C17	580.98(10)	524.60(11)	201.84(6)	16.3(2)
C29	675.38(11)	381.57(12)	-14.00(6)	18.4(3)
C6	204.32(13)	350.84(14)	230.70(8)	28.2(3)
C11	593.54(11)	318.76(11)	242.52(6)	17.2(3)
C4	254.75(11)	288.44(11)	136.03(6)	17.5(3)
C20	547.01(12)	727.42(12)	236.10(8)	25.2(3)
C2	212.65(11)	145.60(11)	85.67(6)	17.4(3)
C23	751.23(11)	394.87(11)	162.27(6)	17.1(3)
C15	664.38(14)	241.02(13)	327.82(7)	27.1(3)
C24	824.52(12)	458.10(12)	191.20(7)	21.9(3)
C16	680.96(12)	293.53(12)	277.49(7)	22.4(3)
C1	309.30(11)	196.34(11)	64.60(6)	16.4(2)
C19	569.75(13)	652.54(12)	275.56(7)	24.9(3)
C26	969.23(12)	394.50(13)	133.41(7)	26.6(3)
C3	179.79(11)	205.54(11)	130.38(6)	18.8(3)
C22	557.65(12)	600.84(12)	162.16(7)	22.8(3)
C18	585.77(12)	551.02(12)	258.84(6)	21.2(3)
C14	560.84(15)	214.62(13)	343.83(7)	28.4(3)
C10	290.65(12)	468.93(13)	166.81(8)	26.4(3)
C9	286.03(14)	545.05(16)	207.88(10)	40.8(5)
C30	650.32(12)	475.24(12)	12.01(6)	21.3(3)
C13	473.70(14)	239.30(15)	309.31(8)	33.0(4)
C25	933.54(12)	457.57(13)	176.71(8)	26.1(3)
C21	541.11(13)	701.95(13)	179.50(8)	27.7(3)
C12	489.57(13)	290.30(14)	258.69(7)	26.9(3)

Table S12, continued.

C5	250.18(11)	370.90(12)	177.94(7)	20.4(3)
C8	241.56(16)	524.44(19)	259.83(10)	49.2(6)
C7	200.93(15)	427.43(19)	271.23(9)	42.8(5)
C37	502.92(12)	159.66(11)	-50.21(6)	17.9(3)
C35	596.79(11)	296.91(11)	-17 16(6)	17.7(3)
C36	594.50(12)	217 71(12)	-59.03(6)	20.2(3)
C45	161.06(11)	50 23(11)	65 79(6)	18.8(3)
C47	158.78(13)	-107.46(13)	10 95(7)	25.4(3)
C46	210.72(12)	-17.47(12)	27.98(7)	21.2(3)
C34	777.24(12)	370.99(13)	-39.04(7)	22.9(3)
C32	826.40(13)	542.91(13)	-10.13(8)	28.2(3)
C31	725.08(13)	555 13(13)	13.76(7)	25.8(3)
C33	852.13(13)	450.99(13)	-36.44(7)	27.1(3)
C39	459.96(11)	75.12(11)	-85.08(6)	17.7(3)
C40	530.33(12)	7.15(12)	-111.89(6)	20.4(3)
C44	348.26(12)	62.70(12)	-93.95(6)	21.9(3)
C43	309.27(13)	-15.27(13)	-128.76(7)	25.7(3)
C38	452.3(11)	203.81(11)	-1.07(6)	16.6(2)
C50	58.0(13)	23.0(13)	86.9(7)	25.(3)
C48	57.32(13)	-132.52(13)	31.41(8)	27.4(3)
C49	7.73(13)	-67.18(13)	69.31(8)	28.6(3)
C42	379.74(14)	-81.54(12)	-155.65(7)	25.3(3)
C41	490.38(13)	-70.13(12)	-146 98(7)	24.5(3)

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S13. Bond lengths [Å] and angles [deg] for **4**.

Au1 P1 2.2088(3)	C10 C9 1.389(2)
Au1 N3 2.2349(12)	C10 C5 1.395(2)
Au1 N1 2.2448(12)	C9 C8 1.381(3)
P1 C17 1.8188(14)	C30 C31 1.390(2)
P1 C11 1.8234(15)	C13 C12 1.387(2)
P1 C23 1.8245(14)	C8 C7 1.385(4)
N2 C1 1.3207(18)	C37 C36 1.378(2)
N2 C38 1.3250(18)	C37 C38 1.4467(19)
N3 C4 1.3429(18)	C37 C39 1.470(2)
N3 C1 1.3888(18)	C35 C36 1.430(2)
N1 C35 1.3494(18)	C45 C50 1.406(2)
N1 C38 1.3933(18)	C45 C46 1.402(2)
C28 C27 1.391(2)	C47 C48 1.389(2)
C28 C23 1.398(2)	C47 C46 1.391(2)
C27 C26 1.384(3)	C34 C33 1.393(2)
C17 C22 1.394(2)	C32 C33 1.386(3)
C17 C18 1.395(2)	C32 C31 1.390(2)
C29 C30 1.401(2)	C39 C40 1.398(2)
C29 C34 1.405(2)	C39 C44 1.404(2)
C29 C35 1.469(2)	C40 C41 1.391(2)
C6 C7 1.384(3)	C44 C43 1.389(2)
C6 C5 1.404(2)	C43 C42 1.385(2)
C11 C16 1.393(2)	C50 C49 1.386(2)
C11 C12 1.395(2)	C48 C49 1.385(2)
C4 C3 1.426(2)	C42 C41 1.389(2)
C4 C5 1.463(2)	
C20 C21 1.383(3)	P1 Au1 N3 137.36(3)
C20 C19 1.376(2)	P1 Au1 N1 140.33(3)
C2 C3 1.380(2)	N3 Au1 N1 81.51(4)
C2 C1 1.4579(19)	C17 P1 C11 102.80(6)
C2 C45 1.469(2)	C17 P1 C23 103.59(6)
C23 C24 1.397(2)	C11 P1 C23 105.96(7)
C15 C14 1.383(2)	C17 P1 Au1 115.04(5)
C15 C16 1.392(2)	C11 P1 Au1 113.59(5)
C24 C25 1.395(2)	C23 P1 Au1 114.57(5)
C19 C18 1.392(2)	C1 N2 C38 127.46(13)
C26 C25 1.389(3)	C4 N3 C1 106.32(11)
C22 C21 1.392(2)	C4 N3 Au1 125.38(9)
C14 C13 1.383(3)	C1 N3 Au1 121.47(9)

Table S13, continued.

C35	N1	C38	106.16(12)
C35	N1	Au1	127.99(9)
C38	N1	Au1	120.65(9)
C27	C28	C23	120.08(15)
C26	C27	C28	120.25(15)
C22	C17	C18	119.02(14)
C22	C17	P1	119.33(11)
C18	C17	P1	121.64(11)
C30	C29	C34	118.36(14)
C30	C29	C35	121.57(13)
C34	C29	C35	120.04(14)
C7	C6	C5	120.05(18)
C16	C11	C12	118.99(14)
C16	C11	P1	123.12(11)
C12	C11	P1	117.81(12)
N3	C4	C3	111.29(13)
N3	C4	C5	122.78(13)
C3	C4	C5	125.93(13)
C21	C20	C19	119.88(15)
C3	C2	C1	104.94(12)
C3	C2	C45	126.28(13)
C1	C2	C45	128.76(13)
C24	C23	C28	119.51(13)
C24	C23	P1	122.17(11)
C28	C23	P1	118.30(11)
C14	C15	C16	120.21(15)
C23	C24	C25	119.96(15)
C15	C16	C11	120.29(14)
N2	C1	N3	126.66(13)
N2	C1	C2	123.44(13)
N3	C1	C2	109.89(12)
C20	C19	C18	120.32(15)
C27	C26	C25	120.13(14)
C2	C3	C4	107.54(12)
C21	C22	C17	120.07(15)
C19	C18	C17	120.30(15)
C13	C14	C15	119.82(15)
C9	C10	C5	119.99(17)
C8	C9	C10	120.46(19)
C31	C30	C29	120.77(14)
C14	C13	C12	120.38(16)
C26	C25	C24	120.06(15)
C20	C21	C22	120.40(15)
C13	C12	C11	120.30(15)
C10	C5	C6	119.18(15)
C10	C5	C4	121.58(14)
C6	C5	C4	119.24(15)
C7	C8	C9	119.99(17)
C8	C7	C6	120.32(19)
C36	C37	C38	105.55(12)
C36	C37	C39	127.99(13)
C38	C37	C39	126.34(13)
N1	C35	C36	111.00(12)
N1	C35	C29	123.30(13)
C36	C35	C29	125.59(13)
C37	C36	C35	107.34(12)
C50	C45	C46	117.69(14)
C50	C45	C2	119.44(14)
C46	C45	C2	122.85(13)
C48	C47	C46	120.75(15)
C47	C46	C45	120.56(14)
C33	C34	C29	120.45(15)
C33	C32	C31	119.64(15)
C30	C31	C32	120.30(16)
C32	C33	C34	120.46(15)
C40	C39	C44	118.40(14)
C40	C39	C37	120.34(13)
C44	C39	C37	121.22(13)
C41	C40	C39	120.64(14)
C43	C44	C39	120.44(14)
C42	C43	C44	120.72(15)
N2	C38	N1	128.70(13)
N2	C38	C37	121.38(13)
N1	C38	C37	109.90(12)
C49	C50	C45	121.39(15)
C49	C48	C47	119.44(15)
C48	C49	C50	120.17(15)
C43	C42	C41	119.28(15)
C42	C41	C40	120.51(15)

Table S14. Anisotropic displacement parameters [Å^2 × 10^3] for **4**. The anisotropic displacement factor exponent takes the form: -2 π2 [(h a*)^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Au1	17.22(3)	16.28(3)	17.64(3)	-2.37(2)	-3.81(2)	-1.38(2)
P1	12.15(14)	15.94(15)	15.91(15)	-2.30(12)	-0.40(12)	-0.32(12)
N2	15.3(5)	18.8(6)	16.9(6)	-0.1(4)	-0.3(4)	-0.6(4)
N3	13.9(5)	18.2(6)	18.1(5)	-2.1(4)	-0.2(4)	-0.7(4)
N1	15.7(5)	19.8(6)	15.7(5)	-1.7(4)	-0.2(4)	-2.3(4)
C28	18.0(6)	23.2(7)	19.1(7)	2.1(5)	0.7(5)	2.3(5)
C27	21.1(7)	31.6(8)	23.2(7)	5.8(6)	5.1(6)	8.0(6)
C17	12.2(5)	15.7(6)	20.8(6)	-2.5(5)	-0.9(5)	-0.4(5)
C29	17.2(6)	21.6(7)	16.3(6)	3.4(5)	-1.6(5)	-2.6(5)
C6	18.7(7)	39.7(10)	26.3(8)	-7.5(7)	3.9(6)	0.6(6)
C11	18.5(6)	15.4(6)	17.7(6)	-2.5(5)	0.1(5)	-0.4(5)
C4	14.2(6)	19.3(7)	18.9(6)	-0.5(5)	-1.0(5)	1.6(5)
C20	16.6(6)	17.9(7)	41.3(9)	-6.2(6)	1.0(6)	-1.3(5)
C2	13.8(6)	18.4(6)	20.0(7)	0.5(5)	-0.4(5)	-0.6(5)
C23	13.6(6)	18.2(6)	19.5(6)	1.9(5)	-0.2(5)	0.3(5)
C15	30.4(8)	26.4(8)	24.5(8)	3.4(6)	-2.3(6)	6.0(6)
C24	17.2(6)	19.9(7)	28.7(8)	-0.4(6)	-2.3(5)	-0.8(5)
C16	18.9(6)	24.5(7)	23.8(7)	2.1(6)	0.4(5)	3.4(6)
C1	13.4(5)	17.9(6)	17.9(6)	0.2(5)	-0.9(5)	-1.7(5)
C19	23.5(7)	24.7(8)	26.5(8)	-8 5(6)	3.4(6)	-1.7(6)
C26	14.6(6)	30.7(8)	34.5(9)	14.4(7)	3.4(6)	3.1(6)
C3	14.8(6)	20.1(7)	21.6(7)	-0.3(5)	2.4(5)	0.1(5)
C22	24.0(7)	21.1(7)	23.2(7)	0.6(6)	-3.6(6)	-2.0(6)
C18	23.2(7)	20.2(7)	20.3(7)	-2.5(5)	-0.7(5)	0.6(5)
C14	37.6(9)	24.2(8)	23.3(8)	3.9(6)	3.1(7)	-1.1(7)
C10	17.0(6)	25.6(8)	36.6(9)	-9.5(7)	0.7(6)	1.0(6)
C9	23.4(8)	33.7(9)	65.3(14)	-25.8(9)	5.3(8)	-3.9(7)
C30	18.3(6)	22.3(7)	23.2(7)	2.0(6)	-1.4(5)	-2.2(5)
C13	27.0(8)	40.3(10)	31.7(9)	7.6(8)	4.6(7)	-8.7(7)
C25	16.0(6)	23.8(7)	38.4(9)	6.7(7)	-4.2(6)	-3.7(5)
C21	27.0(7)	18.2(7)	37.6(9)	5.1(6)	-5.9(7)	-1.8(6)
C12	18.6(7)	34.5(9)	27.7(8)	5.1(7)	-1.0(6)	-4.4(6)
C5	11.9(6)	25.3(7)	24.0(7)	-6.3(6)	-1.4(5)	2.3(5)
C8	28.0(9)	61.3(14)	58.5(14)	-43.2(12)	7.2(9)	-4.5(9)
C7	28.4(9)	66.7(14)	33.6(10)	-24.6(10)	7.6(7)	-1.4(9)
C37	17.8(6)	20.8(7)	14.9(6)	-0.8(5)	0.1(5)	-0.5(5)
C35	16.6(6)	20.4(7)	16.2(6)	1.4(5)	-0.5(5)	-1.7(5)
C36	18.5(6)	25.2(7)	17.1(6)	-0.8(5)	2.2(5)	-1.6(5)
C45	16.4(6)	18.2(6)	21.7(7)	1.3(5)	-1.0(5)	-2.2(5)
C47	24.9(7)	22.3(7)	29.1(8)	-3.6(6)	0.2(6)	-2.6(6)
C46	18.3(6)	21.3(7)	24.1(7)	-1.4(6)	0.0000(5)	-2.8(5)
C34	21.2(7)	24.2(7)	23.4(7)	3.9(6)	2.9(6)	-2.0(6)
C32	23.1(7)	27.3(8)	34.2(9)	6.0(7)	-1.7(6)	-9.3(6)
C31	26.6(7)	19.8(7)	31.1(8)	1.4(6)	-3.0(6)	-2.8(6)
C33	19.5(7)	30.7(8)	31.2(8)	6.0(7)	3.5(6)	-4.4(6)
C39	20.5(6)	19.3(6)	13.1(6)	0.8(5)	-0.8(5)	-1.9(5)
C40	19.6(6)	22.6(7)	19.1(7)	0.8(5)	2.2(5)	0.5(5)
C44	20.7(7)	25.4(7)	19.5(7)	-4.2(6)	-2.5(5)	1.2(6)
C43	23.7(7)	29.1(8)	24.0(7)	-3.4(6)	-5.4(6)	-2.5(6)

C38	15.8(6)	18.7(6)	15.3(6)	-1.2(5)	-0.8(5)	-1.4(5)
C50	21.1(7)	23.7(7)	31.6(8)	-1.7(6)	6.3(6)	-3.8(6)
C48	25.3(7)	21.5(7)	35.2(9)	-0.9(7)	-1.4(7)	-7.6(6)
C49	21.5(7)	26.2(8)	38.2(9)	0.3(7)	5.8(6)	-7.9(6)
C42	33.7(8)	21.2(7)	21.0(7)	-4.3(6)	-4.1(6)	-3.0(6)
C41	29.6(8)	22.1(7)	21.8(7)	-2.2(6)	2.6(6)	2.2(6)

Table S15. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **4**.

	x	y	z	U(eq)
H28	7386	2886	989	24
H27	9216	2886	752	30
H6	1756	2846	2386	34
H20	5354	7965	2477	30
H15	7244	2233	3513	33
H24	8001	5014	2207	26
H16	7522	3123	2669	27
H19	5745	6702	3144	30
H26	10435	3944	1235	32
H3	1184	1937	1532	23
H22	5530	5838	1232	27
H18	6000	4995	2864	25
H14	5496	1796	3785	34
H10	3214	4837	1312	32
H9	3137	6117	2002	49
H30	5814	4843	286	26
H13	4025	2212	3203	40
H25	9834	5004	1965	31
H21	5257	7537	1523	33
H12	4294	3059	2349	32
H8	2388	5768	2877	59
H7	1706	4134	3070	51
H36	6465	2071	-876	24
H47	1931	-1523	-150	30
H46	2804	-18	139	25
H34	7952	3088	-579	28
H32	8777	5973	-84	34
H31	7068	6184	314	31
H33	9213	4425	-528	33
H40	6062	138	-1061	25
H44	2990	1079	-760	26
H43	2335	-232	-1342	31
H50	233	676	1118	31
H48	222	-1940	195	33
H49	-613	-843	839	34
H42	3527	-1342	-1798	30
H41	5392	-1155	-1652	29

Computational Methods

Spin-restricted Scalar-relativistic density-functional calculations were executed within the zero-order regular approximation, as implemented in the Amsterdam Density Functional package (ADF2004).[11–13] In these computations, the local density functional is that of Vosko, Wilk, and Nusair.[14] Geometries were optimized with the revised Perdew-Becke-Ernzerhof functional.[15,16] Scalar relativistic interactions were included within the zero-order regular approximation (ZORA).[17–20] Atomic orbitals of all atoms were constructed from triple-ζ basis sets of Slater orbitals (ADF database TZP) with one set of diffuse functions added. Core electronic shells (one or more principle quantum numbers below the valence level) were frozen for all atoms. The electron density was fitted with sets of auxiliary s, p, d, f, and g-functions centered on all nuclei, along with the Coulomb and exchange potentials, in every self-consistent field cycle. Geometries were optimized in the gas-phase (no inclusion of solvent) with the Broyden-Fletcher-Goldfarb-Shano algorithm; the convergence criterion was that successive energies differ by not more than 1×10^{-5} H (the default is 1×10^{-3} H). Analytical harmonic frequency calculations on $(H_3P)Ag(\mathbf{1})$ ($\mathbf{3'}$) returned a frequency $4.73i$ cm^{-1} corresponding to phenyl rotation. Tightening of convergence criteria did not eliminate this imaginary-frequency mode, and the structure was deemed converged. Vertical excitation energies were calculated with single-point time-dependent density-functional theory (TDDFT) calculations,[21–23] performed with the statistical average of model exchange-correlation potentials (SAOP)[24–26] at the geometry previously optimized with the rPBE functional. Solvation was treated implicitly with a conductor-like screening model (COSMO).[27] Basis sets for time-dependent calculations are those used in geometry optimization. Time-dependent calculations employed the Davidson algorithm; error tolerances in the square of the excitation energies and the trial-vector orthonormality cutoff were both set to 10^{-8}.

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Cartesian Coordinates of Optimized 3′

Atom	X	Y	Z (Angstrom)
1.Ag	11.690905	10.873963	14.426765
2.P	13.135465	11.722963	16.143063
3.H	13.067071	13.105007	16.477686
4.H	14.552523	11.647881	16.024289
5.H	13.044618	11.224368	17.473575
6.C	8.789146	12.593372	15.721760
7.H	9.284992	12.754645	14.763413
8.C	8.566711	13.670680	16.587549
9.H	8.914760	14.668435	16.309780
10.C	7.874277	13.479361	17.794396
11.H	7.693965	14.321624	18.465774
12.C	7.402620	12.198124	18.123401
13.H	6.862344	12.038191	19.059123
14.C	7.620254	11.120661	17.256797
15.H	7.256727	10.128175	17.528864
16.C	8.323142	11.295753	16.041148
17.C	8.508774	10.173872	15.106939
18.C	7.607788	9.075124	14.934225
19.H	6.699275	8.909453	15.505043
20.C	8.093512	8.291409	13.893584
21.C	9.320458	8.964330	13.444700
22.C	11.084193	9.104589	11.810408
23.C	11.671545	8.575481	10.573576
24.C	12.774056	9.381814	10.314524
25.H	13.409791	9.346343	9.434778
26.C	12.830926	10.376659	11.342779
27.C	13.775232	11.503968	11.391038
28.C	15.073717	11.384583	10.841079
29.H	15.390546	10.430015	10.417075
30.C	15.962425	12.465741	10.851559
31.H	16.961581	12.348052	10.426259
32.C	15.574913	13.696918	11.405226
33.H	16.265549	14.542880	11.404010
34.C	14.285706	13.835030	11.944860
35.H	13.964142	14.796648	12.351933
36.C	13.396605	12.753627	11.937105
37.H	12.379401	12.880096	12.310965
38.C	7.459099	7.073794	13.355769
39.C	6.055907	6.898943	13.464622
40.H	5.448116	7.696308	13.895692
41.C	5.430858	5.735321	13.003487
42.H	4.347249	5.630283	13.095560
43.C	6.190636	4.711051	12.414190
44.H	5.704397	3.801758	12.052854
45.C	7.579212	4.869897	12.293024
46.H	8.182641	4.082290	11.836205
47.C	8.207699	6.032463	12.757516
48.H	9.285763	6.140201	12.661133
49.C	11.196840	7.464628	9.727932
50.C	12.131000	6.684259	9.001638
51.H	13.198251	6.879539	9.123012
52.C	11.711668	5.652247	8.154693
53.H	12.453735	5.061109	7.612785

54.C	10.343155	5.371057	8.008336
55.H	10.013238	4.566788	7.346394
56.C	9.405327	6.133412	8.720880
57.H	8.337817	5.928610	8.612991
58.C	9.822924	7.166462	9.570143
59.H	9.084602	7.756235	10.109451
60.N	9.542620	10.104851	14.232651
61.N	10.011632	8.557400	12.381421
62.N	11.833216	10.208138	12.246267