Structural snapshots of a flexible Cu_2P_2 core that accomodates the oxidation states $Cu^{I}Cu^{I}$, $Cu^{1.5}Cu^{1.5}$, and $Cu^{II}Cu^{II}$

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Supporting Information

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(Fully-labelled drawings, crystal data and refinement, atomic coordinates and displacement parameters, bond lengths and angles, anisotropic parameters, and hydrogen coordinates and displacement parameters)

Experimental Section

General. All manipulations were carried out using standard Schlenk or glovebox techniques under a dinitrigen atmosphere. Unless otherwise noted, solvents were deoxygenated and dried by thoroughly sparging with N_2 gas followed by passage through an activated alumina column. Non-halogenated solvents were tested with a standard purple solution of sodium benzophenone ketyl in tetrahydrofuran in order to confirm effective oxygen and moisture removal. All reagents were purchased from commercial vendors and used without further purification unless otherwise stated. 2-diisopropylphosphinophenyl bromide,[1] mesitylcopper(I),[2] ferrocenium tetraphenylborate,[3] and ferrocenium tetrakis(3,5-bis(trifluoromethyl)phenyl)borate[3] were prepared according to literature procedures. Elemental analyses were performed by Desert Analytics, Tucson, AZ. Deuterated solvents were purchased from Cambridge Isotope Laboratories, Inc., degassed, and dried over activated 3-Å molecular sieves prior to use. X-ray diffraction studies were carried out at the Beckman Institute Crystallography Facility on a Brüker Smart 1000 CCD diffractometer and solved using SHELX v. 6.14.

Electrochemistry. Electrochemical measurements were carried out in a glovebox under a dinitrogen atmosphere in a one-compartment cell using a CH Instruments 600B electrochemical analyzer. A glassy carbon electrode was used as the working electrode for **3**. A platinum working electrode was used for **2**. Platinum wire was used as the auxillary electrodes in both cases. The reference electrode was $Ag/AgNO_3$ in THF. The ferrocene couple Fc^+/Fc was used as an external reference. Solutions (THF) of electrolyte (0.35 M tetra-*n*-butylammonium hexafluorophosphate) and analyte were also prepared under an inert atmosphere.

EPR measurements. X-band EPR spectra were obtained on a Brüker EMX spectrometer (controlled by Brüker Win EPR software v. 3.0) equipped with a rectangular cavity working in the TE_{102} mode. Variable temperature measurements were conducted with an Oxford continuous-flow helium cryostat (temperature range 3.6-300 K). Accurate frequency values were provided by a frequency counter built into the microwave bridge. Solution spectra were acquired in 2-methyltetrahydrofuran. Sample preparation was performed under a dinitrogen atmosphere in an EPR tube equipped with a ground glass joint.

Spectroscopic measurements. A Varian Mercury-300 spectrometer was used to record ^1H, ^{13}C, ^{19}F, and ^{31}P NMR spectra at ambient temperature. ^1H and ^{13}C chemical shifts were referenced to the residual solvent peaks. ^{19}F and ^{31}P chemical shifts were referenced to external hexafluorobenzene (δ = -165 ppm) and phosphoric acid (δ = 0 ppm) respectively. Emission spectra were recorded on a Spex Fluorolog-2 spectrofluorometer. Excitation for the luminescence lifetime experiments employed 8 ns pulses (at a repetition rate of 10 Hz) from a frequency-tripled Nd^{3+}:YAG laser (Quanta Ray Pro, Spectra Physics). The luminescence was dispersed through a monochrometer (Instruments SA DH-10) onto a photomultiplier tube (PMT)

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[1] (a) Talay, R.; Rehder, D. *Zeit. f. Natur., B: Anorg. Chemie* **1981**, *36*, 451. (b) Tamm, M.; Dreβel, B.; Baum, K.; Lügger, T.; Pape, T. *J. Organomet. Chem.* **2003**, *677*, 1.

[2] Eriksson, H.; Håkansson, M. *Organometallics* **1997**, *16*, 4243.

[3] Chavez, I.; *J. Organomet. Chem.* **2000**, *601*, 126.

(Hamamatsu R928). The PMT current was amplified and recorded with a transient digitizer (Tektronix). Optical spectroscopy measurements were taken on a Cary 50 UV/Vis Spectrophotometer using a 1-cm quartz cell or a Cary 500 UV/Vis/NIR Spectrophotometer using either a 2-cm or 1-cm quartz cell sealed with a Teflon stopper.

Synthesis of Bis(2-diisopropylphosphinophenyl)chlorophosphine. To a solution of 2-diisopropylphosphinophenyl bromide (0.767 g, 2.85 mmol) in 8 mL of Et_2O was added *n*-butyllithium (1.6 M solution in hexanes, 1.8 mL, 2.9 mmol) at -78 ºC. A white suspension was observed after the addition was complete, and the reaction was gradually warmed to room temperature and stirred for 1 h to give a pale orange, clear solution. The solution was cooled again to -78 ºC and added dropwise over 20 min to a cold (-78 ºC) solution of PCl_3 (0.196 g, 1.43 mmol) in 1.5 mL of Et_2O. The resulting yellow slurry was slowly warmed to room temperature, and after 2 h of stirring was filtered through Celite. Removal of the volatiles afforded a yellow, viscous oil that gradually solidified upon standing (16 h) to yield a yellow solid (0.572 g, 90%). ^{1}H (C_6D_6): δ 7.8 (m, 2H, Ar-*H*), 7.2 (m, 2H, Ar-*H*), 7.0 (m, 4H, Ar-*H*), 2.01 (m, 2H, C*H*$(CH_3)_2$), 1.91 (sept., J = 6.9 Hz, 2H, C*H*$(CH_3)_2$), 1.18 (dd, J = 7.2 and 14.9 Hz, 6H, CH(C*H*$_3)_2$), 1.01 (dd, J = 7.2 and 14.3 Hz, 6H, CH(C*H*$_3)_2$), 0.98 (dd, J = 7.2 and 13.5 Hz, 6H, CH(C*H*$_3)_2$), 0.73 (dd, J = 7.2 and 13.4 Hz, 6H, CH(C*H*$_3)_2$). ^{13}C{^{1}H} (C_6D_6): δ 150.4 (dd, $^1J_{PC}$ = 35.3 Hz, $^2J_{PC}$ = 35.4 Hz), 140.7 (dd, $^1J_{PC}$ = 21.0 Hz, $^2J_{PC}$ = 12.6 Hz), 133.4 (d, $^2J_{PC}$ = 10.6 Hz), 132.4 (d, $^2J_{PC}$ = 1.4 Hz), 130.0, 129.5, 26.2 (d, $^1J_{PC}$ = 14.9 Hz, *C*H$(CH_3)_2$), 24.5 (d, $^1J_{PC}$ = 14.9 Hz, *C*H$(CH_3)_2$), 21.0 (d, $^2J_{PC}$ = 14.9 Hz, CH(*C*H$_3)_2$), 20.6 (CH(*C*H$_3)_2$), 20.3 (CH(*C*H$_3)_2$), 19.9 (d, $^2J_{PC}$ = 7.2 Hz, CH(*C*H$_3)_2$). ^{31}P{^{1}H} (C_6D_6): δ 68.4 (t, $^3J_{PP}$ = 254.9 Hz, 1P, Ar_2*P*Cl), -3.6 (d, $^2J_{PP}$ = 254.7 Hz, 2P, ^{i}Pr$_2$*P*Ar). IR (KBr, cm^{-1}): 3046, 2955, 2865, 1458, 1381, 1232, 1174, 1019, 880.

Note: Often a mixture of chlorophosphine and bromophosphine products was observed and utilized without further purification.

Synthesis of Bis(2-diisopropylphosphinophenyl)phosphine, (PPP)H. To a suspension of $LiAlH_4$ (0.080 g, 2.11 mmol) in 10 mL of Et_2O (-30 ºC) was added dropwise a cold (-30 ºC) solution of bis(2-diisopropylphosphinophenyl)chlorophosphine (0.820 g, 1.81 mmol) in 30 mL of Et_2O. The reaction was warmed to room temperature and stirred for 4 h. The resulting mixture was filtered through silica and volatiles were removed, leaving a yellow oily residue. (Note: An exothermic reaction is obtained upon combining the reaction solution with silica, so only small portions should be filtered at a time to prevent excessive frothing.) This residue was dissolved in benzene and filtered again through silica. Removal of the volatiles yielded a colorless oil (0.720 g, 95%). ^{1}H (C_6D_6): δ 7.3 (m, 4H, Ar-*H*), 7.08 (dt, J = 1.7 and 7.4 Hz, 2H, Ar-*H*), 7.00 (dt, J = 0.8 and 6.6 Hz, 2H, Ar-*H*), 6.34 (dt, $^4J_{PH}$ = 10.5 Hz and $^1J_{PH}$ = 218.1 Hz, 1H, Ar_2P*H*), 2.07 (m, 4H, C*H*$(CH_3)_2$), 1.16 (dd, J = 6.6 and 14.3 Hz, 3H, CH(C*H*$_3)_2$), 1.12 (dd, J = 7.2 and 14.3 Hz, 3H, CH(C*H*$_3)_2$), 0.97 (dd, J = 5.2 and 6.5 Hz, 3H, CH(C*H*$_3)_2$), 0.93 (dd, J = 5.2 and 6.5 Hz, 3H, CH(C*H*$_3)_2$). ^{13}C{^{1}H} (C_6D_6): δ 146.8 (dd, $^1J_{PC}$ = 21.0 Hz, $^2J_{PC}$ = 12.6 Hz), 141.5 (dd, $^1J_{PC}$ = 35.3 Hz, $^2J_{PC}$ = 35.4 Hz), 136.2 (d, $^2J_{PC}$ = 2.3 Hz), 136.1 (d, $^2J_{PC}$ = 4.6 Hz), 132.7, 132.6 (d, $^2J_{PC}$ = 1.7 Hz), 129.3, 25.3 (dd, $^1J_{PC}$ = 15.5 Hz, $^4J_{PC}$ = 1.4 Hz, *C*H$(CH_3)_2$), 24.6 (dd, $^1J_{PC}$ = 14.9 Hz, $^4J_{PC}$ = 2.3 Hz, *C*H$(CH_3)_2$), 20.8 (d, $^2J_{PC}$ = 20.1 Hz, CH(*C*H$_3)_2$), 20.6 (d, $^2J_{PC}$ = 19.5 Hz, CH(*C*H$_3)_2$), 20.3 (d, $^2J_{PC}$ = 12.6 Hz, CH(*C*H$_3)_2$), 19.9 (d, $^2J_{PC}$ = 10.3 Hz, CH(*C*H$_3)_2$). ^{31}P (C_6D_6): δ 0.3 (d, $^3J_{PP}$ = 135.8 Hz, 1P, ^{i}Pr$_2$*P*Ar), -46.7 (dt, $^3J_{PP}$ = 135.8 Hz, $^1J_{PH}$ = 219.7 Hz, 1P, Ar_2*P*H). IR (KBr, cm^{-1}): 3052, 2957, 2870, 2282, 1574, 1519, 1444, 1427, 1363, 1152, 1033. Anal. Calcd for $C_{24}H_{57}P_3$: C, 68.88; H, 8.91. Found: C, 68.72; H, 8.61.

Synthesis of {(PPP)Cu}$_2$ (3). A solution of bis(2-diisopropylphosphinophenyl)phosphine (1.05 g, 2.51 mmol) in 5 mL of THF was added to solid mesitylcopper(I) (0.461 g, 2.51 mmol) at room temperature. The resulting red-orange solution was stirred for 2.5 h and then concentrated *in vacuo* to a red-orange solid. 10 mL of petroleum ether was added and the suspension was stirred for 5 min at -78 °C, after which the cold solution was filtered through a sintered glass frit. The collected solids were washed with petroleum ether (3 x 2 mL) and dried under vacuum, giving analytically pure {(PPP)Cu}$_2$ as a fine red-orange powder (0.752 g, 65%). X-ray quality crystals were grown by cooling a CH_2Cl_2/petroleum ether solution to -30 °C. ^{1}H (C_6D_6): δ 7.87 (br d, *J* = 6.6 Hz, 4H, Ar-*H*), 7.25 (br d, *J* = 5.2 Hz, 4H, Ar-*H*), 7.07 (dd, *J* = 7.3 Hz, 4H, Ar-*H*), 6.93 (dd, *J* = 6.9 Hz, 4H, Ar-*H*), 2.15 (br sept., *J* = 6.3 Hz, 4H, C*H*(CH_3)$_2$), 1.95 (br sept., *J* = 6.3 Hz, 4H, C*H*(CH_3)$_2$), 1.19 (dd, *J* = 7.2 Hz and 14.6 Hz, 6H, CH(C*H*$_3$)$_2$), 1.10 (dd, *J* = 6.9 Hz and 9.8 Hz, 6H, CH(C*H*$_3$)$_2$), 1.03 (dd, *J* = 6.3 Hz and 11.8 Hz, 6H, CH(C*H*$_3$)$_2$), 0.76 (dd, *J* = 6.9 Hz and 15.8 Hz, 6H, CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} (C_6D_6): δ 162.2, 136.0, 133.8, 131.2, 129.1, 123.5, 28.3, 24.1, 20.6, 19.9, 18.2. ^{31}P{^{1}H} (C_6D_6): δ 34.0 (br, 4P), -21.0 (br, 2P). IR (KBr, cm^{-1}): 2953, 2866, 1566, 1460, 1433, 1381, 1231, 1157, 1088, 881. UV-Vis-NIR (CD_2Cl_2, nm (M^{-1}cm^{-1})): 314 (20500), 446 (7100), 556 (2800). Anal. Calcd for $C_{48}H_{72}Cu_2P_6$: C, 59.92; H, 7.54. Found: C, 59.61; H, 7.24.

Synthesis of [{(PPP)Cu}$_2$][BPh$_4$] (4). A solution of {(PPP)Cu}$_2$ (0.0541 g, 0.0562 mmol) in 7 mL of CH_2Cl_2 was added to solid ferrocenium tetraphenylborate (0.0284 g, 0.0562 mmol) in one portion at room temperature. The resulting red-purple solution was stirred for 3.5 h and then concentrated *in vacuo* to a red-purple solid. This solid was triturated with petroleum ether and collected on a sintered glass frit. Repeated washes with petroleum ether (5 x 5 mL) yielded analytically-pure [{(PPP)Cu}$_2$][BPh$_4$] as a dark red-purple powder (0.0668 g, 93%). X-ray quality crystals were grown by cooling a saturated CH_3CN solution to -30°C. ^{1}H (CD_2Cl_2): δ 7.31, 7.03, 6.87. IR (KBr, cm^{-1}): 3051, 2960, 2870, 1578, 1459, 1425, 1385, 1238, 1108, 1032, 934, 882. UV-Vis-NIR (CD_2Cl_2, nm (M^{-1}cm^{-1})): 313 (19200), 455 (4200), 553 (3100), 680 (800), 1095 (2800). Anal. Calcd for $C_{72}H_{92}BCu_2P_6$: C, 67.49; H, 7.24. Found: C, 67.03; H, 6.97.

Synthesis of [{(PPP)Cu}$_2$][BAr$^F_4$]$_2$ (5). A solution of {(PPP)Cu}$_2$ (0.0554 g, 0.0576 mmol) in 15 mL of CH_2Cl_2 was added to solid ferrocenium tetrakis(3,5-bis(trifluoromethyl)phenyl)borate (0.121 g, 0.115 mmol) in one portion at room temperature. The resulting blue-purple solution was stirred for 24 h and then concentrated *in vacuo* to a blue-purple solid. This solid was triturated with petroleum ether and collected on a sintered glass frit. Repeated washes with petroleum ether (5 x 10 mL) yielded spectroscopically-pure [{(PPP)Cu}$_2$][BAr$^F_4$]$_2$ as a dark blue-purple powder (0.154 g, 99%). Analytically-pure compound was obtained by layering a CH_2Cl_2 solution with petroleum ether and allowing crystals to grow by standing over 24 h. ^{1}H (CD_2Cl_2): δ 7.90 (m, 4H, Ar-*H*), 7.77 (m, 8H, Ar-*H*), 7.72 (s, 16H, *o*-BAr$^F_4$), 7.56 (dd, *J* = 7.3 Hz, 4H, Ar-*H*), 7.54 (s, 8H, *p*-BAr$^F_4$), 2.47 (m, 4H, C*H*(CH_3)$_2$), 2.44 (sept., *J* = 7.4 Hz, 4H, C*H*(CH_3)$_2$), 1.27 (br d, *J* = 7.2 Hz, 6H, CH(C*H*$_3$)$_2$), 1.12 (br, 6H, CH(C*H*$_3$)$_2$), 1.04 (br, 6H, CH(C*H*$_3$)$_2$), 0.08 (br d, *J* = 6.6 Hz, 6H, CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} (CD_2Cl_2): δ 162.3 (m), 135.3, 133.9 (m), 131.4, 130.5, 129.2 (m), 126.8, 123.2, 119.6, 118.0, 30.2, 27.0, 22.8, 20.9, 19.4, 18.4, 16.9. ^{19}F (CD_2Cl_2): δ -61.4. ^{31}P{^{1}H} (CD_2Cl_2): 266.1 (br, 2P), 37.3 (br, 4P). IR (KBr, cm^{-1}): 3372, 2973, 1611, 1466, 1355, 1278, 1124, 889, 839. UV-Vis-NIR (CD_2Cl_2, nm (M^{-1}cm^{-1})): 447

(2800), 555 (4200), 683 (10600). Anal. Calcd for $C_{112}H_{96}B_2Cu_2F_{48}P_6$: C, 50.04; H, 3.60. Found: C, 48.70; H, 3.13.

Preparation of $[\{(PPP)Cu\}_2][SbF_6]_2$. A solution of $\{(PPP)Cu\}_2$ (6.7 mg, 0.0070 mmol) in 2 mL of CH_2Cl_2 was added in one portion to solid $AgSbF_6$ (4.8 mg, 0.014 mmol) yielding a cloudy, dark red-purple solution. After stirring for 24 h, the solution was filtered through Celite, and the resulting dark blue-purple filtrate was concentrated to 1 mL. After allowing petroleum ether vapors to slowly diffuse into the solution for 18 h, dark purple crystalline plates were recovered and washed with petroleum ether repeatedly. The ^1H and ^{31}P NMR spectra of these crystals in CD_2Cl_2 matched exactly the spectra observed for $[\{(PPP)Cu\}_2][BAr^F{}_4]_2$.

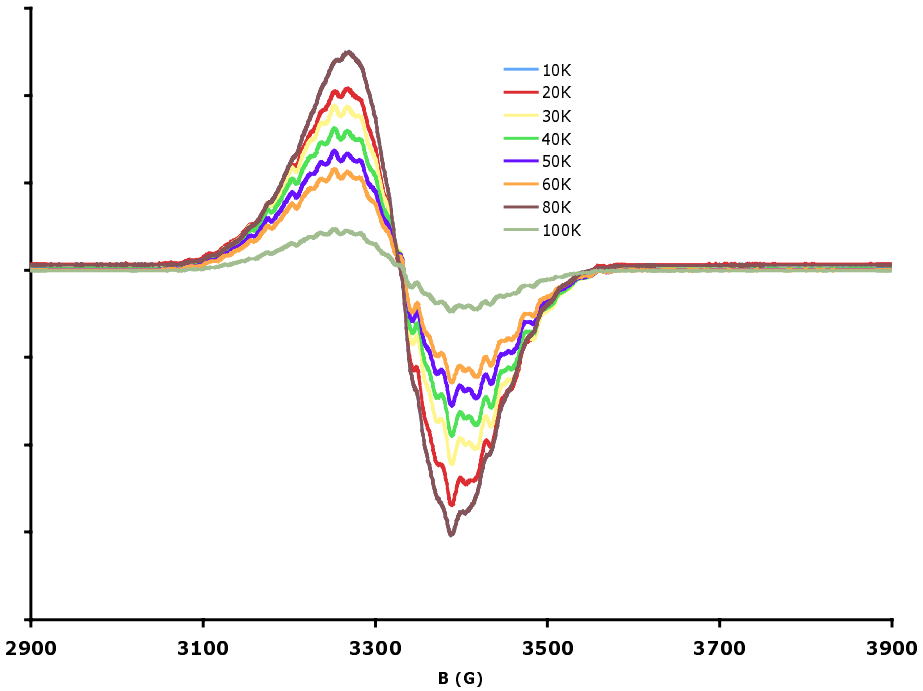

Figure S1. Variable-temperature X-band EPR (9.37 MHz, 2-methyltetrahydrofuran) of **4**.

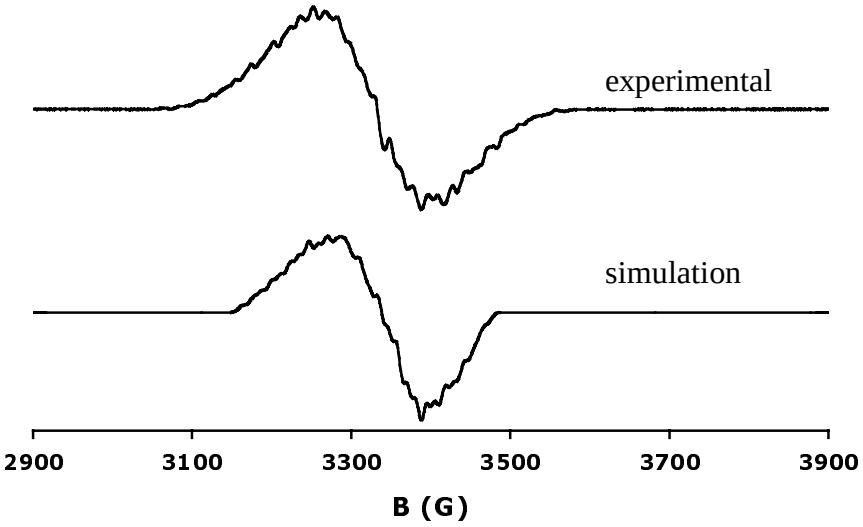

Figure S2. (*top*) Experimental (9.37 MHz, 2-methyltetrahydrofuran, 100 K) and (*bottom*) simulated EPR spectra for **4**.
Simulation parameters: g_1 = 2.072500, g_2 = 2.145500, g_3 = 2.055500; # Cu nuclei (I = 3/2) = 2; $A^{Cu}{}_1 = A^{Cu}{}_2 = A^{Cu}{}_3$ = 23.20 G; # P nuclei (I = 1/2) = 2; $A^{P}{}_1 = A^{P}{}_2 = A^{P}{}_3$ = 13.00 G.

Luminescence experiments.
Luminescence measurements were collected in the Beckman Institute Laser Resource Center at the California Institute of Technology by previously published methods.[4]

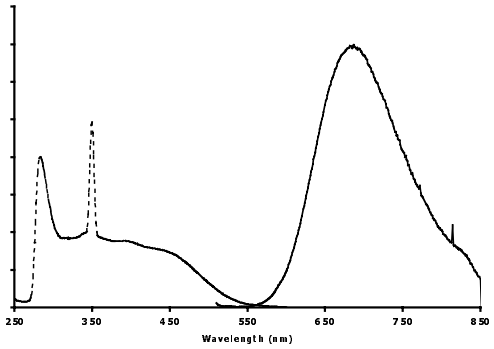

Figure S3. Excitation (λ_{em} = 700 nm; dashed) and emission (λ_{em} = 500 nm; solid) spectra for **3** in THF at 298 K.

Reorganizational energies were calculated according to eq. 1.

$$\Lambda = \frac{(FWHM)^2}{16RT\ln(2)} \qquad (1)$$

Λ:	reorganizational energy
FWHM:	full width at half maximum intensity of the emission band
T:	temperature

Quantum yield experiments.
Solutions of **3** (approx. 40 μM) in tetrahydrofuran (η = 1.407)[5] were prepared in a nitrogen-filled glovebox. Four cuvettes (1-cm path) were charged with these solutions, sparged briefly with argon, and sealed with greased ground-glass stoppers. The absorption spectra were acquired both before and after fluorescence measurements to ensure the samples were not degrading. A solution of tris(2,2'-bipyridyl)ruthenium(II) chloride hexahydrate ($Ru(bpy)_3^{2+}$; Φ = 6.2%)[6] in acetonitrile (η = 1.344)[5] was prepared and sparged with nitrogen, and the concentration was adjusted such that the optical density (OD) at 500 nm was roughly equal to that of the individual solutions of **3**. Fluorescence measurements were performed with λ_{ex} = 500 nm at 298 K and corrected for detector response. The area under the curve of the emission spectrum was determined using standard trapezoidal integration methods. Quantum yields (Table 1) were then calculated by the methods described by Demas and Crosby[7] using eq. 2.

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[4] Wenger, O. S.; Henling, L. M.; Day, M. W.; Winkler, J. R.; Gray, H. B. *Inorg. Chem.* **2004**, *43*, 2043.
[5] Lide, D. R., Ed. *CRC Handbook of Chemistry and Physics, 73rd Edition*; CRC Press: New York, 1996.
[6] Juris, A.; Balzani, V.; Barigelletti, F.; Campagna, S.; Belser, P.; Von Zelewsky, A. *Coord. Chem. Rev.* **1988**, *84*, 85.
[7] Demas, J. N.; Crosby, G. A. *J. Phys. Chem.* **1971**, *75*, 991.

$$\Phi = \Phi_R \frac{I}{I_R} \frac{OD_R}{OD} \frac{\eta^2}{\eta_R^2} \quad (2)$$

Φ: quantum yield of sample
Φ_R: quantum yield of $Ru(bpy)_3^{2+}$
I: integrated intensity of **3**
I_R: integrated intensity of $Ru(bpy)_3^{2+}$
OD_R: optical density of the $Ru(bpy)_3^{2+}$ at λ_{ex} in absorption units
OD: optical density of **3** at λ_{ex} in absorption units
η: index of refraction of the solvent in which **3** was dissolved
η_R: index of refraction of the solvent in which $Ru(bpy)_3^{2+}$ was dissolved

Table 1: Data from Quantum Yield Measurements

Solution	OD @ 500 nm (measured)	*I* (measured)	Φ (calculated)
$Ru(bpy)_3^{2+}$ in CH_3CN	0.344	8.8175E+08	
46.8 μM **3** in THF	0.266	1.6282E+08	0.016
39.0 μM **3** in THF	0.415	1.8066E+08	0.012
41.6 μM **3** in THF	0.594	2.1885E+08	0.0098
36.4 μM **3** in THF	0.287	1.630E+08	0.015
		Average	0.013
		Std. Deviation	0.003

Lifetime measurements.

Solutions of **3** (approx. 100 μM) in tetrahydrofuran were prepared in a nitrogen-filled glovebox. Three cuvettes (1-cm path) were charged with this solution, sparged briefly with argon, and sealed with greased ground-glass stoppers. Absorption spectra were acquired both before and after the fluorescence measurements to ensure the samples were not degrading. Fluorescence measurements were performed with λ_{ex} = 500 nm and λ_{em} = 650 nm at 298 K. A 500-nm low-pass filter was placed in front of the PMT in order to eliminate noise due to scattered laser light. The emission decay was averaged over 50 laser pulses and fit to an exponential function from which k_{obs} was determined (Table 2).

Table 2: Data from Excited State Lifetime Measurements

Entry	Solution	k_{obs} (s^{-1})	$\tau = 1/k_{obs}$ (ns)
1[c]	31.4 μM **3** in THF	1.222E+06	818
2	113 μM **3** in THF	2.442E+06	410
		Average	609
		Std. Deviation	300
	$k_{radiative}$[a] **(avg)**	2.1E+04	
	$k_{non\text{-}radiative}$[b] **(avg)**	1.811E+06	

(a) $k_{radiative} = \Phi/\tau$; (b) $k_{non\text{-}radiative} = k_{obs} - k_{radiative}$; (c) Representative fit shown below.

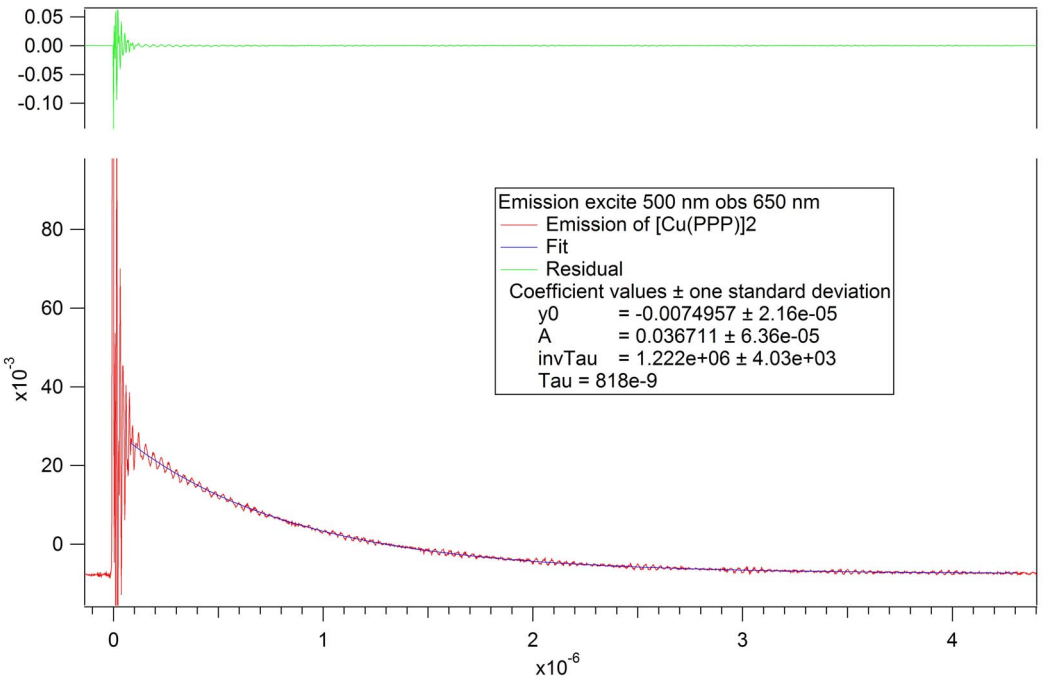

Figure S4. (*top*) Residuals and (*bottom*) fitted excited state decay for Entry 1 (Table 2)

X-ray crystallography

Spatial refinement details.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) 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(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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.

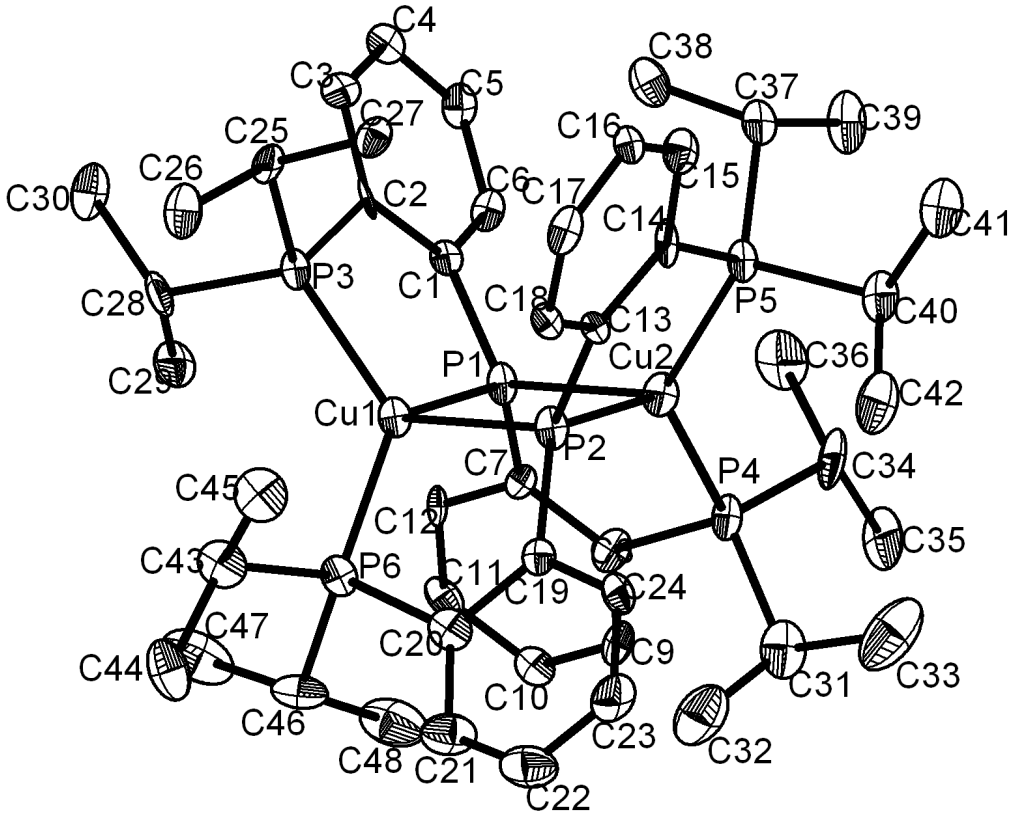

Figure S5. Molecular structure of **3**, fully numbered. Hydrogen atoms have been omitted for clarity.

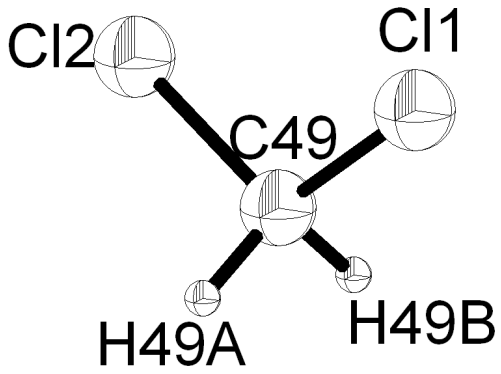

Figure S6. Dichloromethane molecule crystallized with **3**.

Table 3. Crystal data and structure refinement for {(PPP)Cu}$_2$.

Identification code	{(PPP)Cu}$_2$	
Empirical formula	$C_{49}H_{74}Cl_2Cu_2P_6$	
Formula weight	1046.88	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.248(3) Å	α= 90º
	b = 20.021(5) Å	β= 93.695(5)º
	c = 21.114(5)	γ = 90º
Volume	5167(2) Å^3	
Z	4	
Density (calculated)	1.346 Mg/m^3	
Absorption coefficient	1.145 mm^{-1}	
F(000)	2200	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	1.67 to 28.48º	
Index ranges	$-16 \le h \le 15$, $-16 \le k \le 26$, $-27 \le l \le 28$	
Reflections collected	31176	
Independent reflections	11658 [R(int) = 0.1938]	
Completeness to theta = 28.48∞	89.2 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11658 / 0 / 548	
Goodness-of-fit on F^2	0.956	
Final R indices [I>2sigma(I)]	R1 = 0.0760, wR2 = 0.1235	
R indices (all data)	R1 = 0.2219, wR2 = 0.1494	
Largest diff. peak and hole	1.473 and -0.914 Å^{-3}	

Table 4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for {(PPP)Cu}$_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	4578(1)	9544(1)	2574(1)	16(1)
Cu(2)	1891(1)	9495(1)	2649(1)	20(1)
P(1)	3303(2)	8714(1)	2727(1)	16(1)
P(2)	3181(2)	10329(1)	2497(1)	17(1)
P(3)	5537(2)	9193(1)	3443(1)	16(1)
P(4)	1025(2)	8854(1)	1907(1)	18(1)
P(5)	1263(2)	10120(1)	3423(1)	17(1)
P(6)	5183(2)	9938(1)	1676(1)	19(1)
C(1)	3799(6)	8289(4)	3455(3)	14(2)
C(2)	4686(5)	8571(3)	3820(3)	11(2)
C(3)	4928(6)	8340(4)	4446(3)	19(2)
C(4)	4360(6)	7819(3)	4693(3)	17(2)
C(5)	3527(6)	7518(4)	4311(3)	20(2)
C(6)	3261(6)	7737(4)	3707(3)	17(2)
C(7)	2924(6)	8082(4)	2135(3)	13(2)
C(8)	2009(6)	8182(3)	1722(3)	18(2)
C(9)	1817(6)	7781(4)	1173(3)	19(2)
C(10)	2524(6)	7272(4)	1044(3)	20(2)
C(11)	3431(6)	7158(4)	1460(3)	21(2)
C(12)	3628(6)	7548(4)	1999(3)	15(2)
C(13)	2931(6)	10958(3)	3087(3)	10(2)
C(14)	2205(6)	10823(4)	3559(3)	17(2)
C(15)	2194(6)	11226(4)	4098(3)	23(2)
C(16)	2860(6)	11808(4)	4161(3)	14(2)
C(17)	3512(6)	11962(4)	3682(3)	20(2)
C(18)	3562(6)	11547(4)	3151(3)	16(2)
C(19)	3384(6)	10777(4)	1767(3)	16(2)
C(20)	4205(6)	10568(4)	1361(3)	23(2)
C(21)	4259(7)	10860(4)	761(4)	33(2)
C(22)	3559(8)	11348(5)	570(4)	39(3)
C(23)	2783(7)	11571(4)	956(4)	30(2)

C(24)	2696(6)	11294(4)	1551(3)	21(2)
C(25)	5996(6)	9796(4)	4074(3)	19(2)
C(26)	6937(6)	10206(4)	3829(4)	28(2)
C(27)	5056(6)	10251(4)	4217(3)	21(2)
C(28)	6774(6)	8688(4)	3314(3)	25(2)
C(29)	6448(6)	8072(4)	2891(3)	28(2)
C(30)	7450(6)	8461(4)	3915(3)	29(2)
C(31)	493(7)	9166(4)	1139(4)	33(2)
C(32)	1380(7)	9493(5)	786(4)	46(3)
C(33)	-469(8)	9638(5)	1217(4)	60(3)
C(34)	-137(6)	8354(4)	2210(4)	32(2)
C(35)	-783(7)	7915(4)	1728(4)	39(2)
C(36)	299(7)	7940(4)	2786(4)	38(3)
C(37)	1054(6)	9770(4)	4211(3)	19(2)
C(38)	2074(6)	9378(4)	4456(3)	28(2)
C(39)	63(6)	9322(4)	4182(4)	31(2)
C(40)	-24(6)	10571(4)	3199(3)	24(2)
C(41)	-499(7)	11020(4)	3711(3)	31(2)
C(42)	73(7)	10975(4)	2595(4)	39(2)
C(43)	6489(7)	10442(4)	1781(3)	31(2)
C(44)	7044(6)	10653(4)	1186(3)	36(2)
C(45)	6274(7)	11050(4)	2189(3)	32(2)
C(46)	5407(7)	9386(4)	999(3)	26(2)
C(47)	6320(8)	8889(4)	1210(4)	50(3)
C(48)	4366(8)	9026(5)	794(4)	49(3)
Cl(1)	10494(2)	2380(1)	4988(1)	45(1)
Cl(2)	9558(3)	3386(2)	5772(2)	101(1)
C(49)	9568(9)	2544(4)	5508(4)	60(3)

Table 5. Bond lengths [Å] and angles [°] for {(PPP)Cu}$_2$.

Cu(1)-P(6)	2.224(2)
Cu(1)-P(3)	2.226(2)
Cu(1)-P(1)	2.317(2)
Cu(1)-P(2)	2.321(2)
Cu(2)-P(5)	2.232(2)
Cu(2)-P(4)	2.240(2)
Cu(2)-P(1)	2.329(2)
Cu(2)-P(2)	2.336(2)
P(1)-C(7)	1.818(7)
P(1)-C(1)	1.827(7)
P(2)-C(13)	1.812(7)
P(2)-C(19)	1.814(7)
P(3)-C(2)	1.839(7)
P(3)-C(28)	1.856(8)
P(3)-C(25)	1.858(7)
P(4)-C(31)	1.819(8)
P(4)-C(8)	1.864(8)
P(4)-C(34)	1.884(8)
P(5)-C(14)	1.831(7)
P(5)-C(37)	1.838(7)
P(5)-C(40)	1.852(8)
P(6)-C(20)	1.834(8)
P(6)-C(46)	1.840(7)
P(6)-C(43)	1.893(8)
C(1)-C(6)	1.409(9)
C(1)-C(2)	1.409(9)
C(2)-C(3)	1.413(9)
C(3)-C(4)	1.375(9)
C(3)-H(3)	0.9500
C(4)-C(5)	1.395(10)
C(4)-H(4)	0.9500
C(5)-C(6)	1.368(9)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500

C(7)-C(8)	1.389(10)
C(7)-C(12)	1.415(9)
C(8)-C(9)	1.417(9)
C(9)-C(10)	1.377(10)
C(9)-H(9)	0.9500
C(10)-C(11)	1.389(10)
C(10)-H(10)	0.9500
C(11)-C(12)	1.387(9)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(14)	1.404(9)
C(13)-C(18)	1.411(9)
C(14)-C(15)	1.395(9)
C(15)-C(16)	1.425(10)
C(15)-H(15)	0.9500
C(16)-C(17)	1.363(9)
C(16)-H(16)	0.9500
C(17)-C(18)	1.401(9)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(24)	1.393(10)
C(19)-C(20)	1.426(9)
C(20)-C(21)	1.400(9)
C(21)-C(22)	1.345(11)
C(21)-H(21)	0.9500
C(22)-C(23)	1.367(10)
C(22)-H(22)	0.9500
C(23)-C(24)	1.385(9)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-C(27)	1.513(9)
C(25)-C(26)	1.534(9)
C(25)-H(25)	1.0000
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800

C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(30)	1.539(9)
C(28)-C(29)	1.559(10)
C(28)-H(28)	1.0000
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(32)	1.506(10)
C(31)-C(33)	1.528(11)
C(31)-H(31)	1.0000
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.527(10)
C(34)-C(36)	1.539(10)
C(34)-H(34)	1.0000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(39)	1.507(9)
C(37)-C(38)	1.536(10)
C(37)-H(37)	1.0000
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800

C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-C(42)	1.522(10)
C(40)-C(41)	1.549(9)
C(40)-H(40)	1.0000
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-C(45)	1.525(10)
C(43)-C(44)	1.525(9)
C(43)-H(43)	1.0000
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-C(48)	1.504(11)
C(46)-C(47)	1.541(11)
C(46)-H(46)	1.0000
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
Cl(1)-C(49)	1.660(9)
Cl(2)-C(49)	1.778(9)
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900

P(6)-Cu(1)-P(3)	128.82(8)

P(6)-Cu(1)-P(1)	129.58(8)
P(3)-Cu(1)-P(1)	89.09(8)
P(6)-Cu(1)-P(2)	89.11(8)
P(3)-Cu(1)-P(2)	128.21(8)
P(1)-Cu(1)-P(2)	89.71(8)
P(5)-Cu(2)-P(4)	131.57(9)
P(5)-Cu(2)-P(1)	127.89(8)
P(4)-Cu(2)-P(1)	88.88(8)
P(5)-Cu(2)-P(2)	88.16(8)
P(4)-Cu(2)-P(2)	127.39(8)
P(1)-Cu(2)-P(2)	89.03(8)
C(7)-P(1)-C(1)	108.1(3)
C(7)-P(1)-Cu(1)	123.3(2)
C(1)-P(1)-Cu(1)	105.1(2)
C(7)-P(1)-Cu(2)	105.3(3)
C(1)-P(1)-Cu(2)	125.2(2)
Cu(1)-P(1)-Cu(2)	90.77(8)
C(13)-P(2)-C(19)	106.1(3)
C(13)-P(2)-Cu(1)	125.4(2)
C(19)-P(2)-Cu(1)	104.7(3)
C(13)-P(2)-Cu(2)	104.9(2)
C(19)-P(2)-Cu(2)	127.0(2)
Cu(1)-P(2)-Cu(2)	90.49(8)
C(2)-P(3)-C(28)	100.6(3)
C(2)-P(3)-C(25)	106.4(3)
C(28)-P(3)-C(25)	104.3(3)
C(2)-P(3)-Cu(1)	106.7(2)
C(28)-P(3)-Cu(1)	116.3(2)
C(25)-P(3)-Cu(1)	120.4(2)
C(31)-P(4)-C(8)	105.1(3)
C(31)-P(4)-C(34)	104.5(4)
C(8)-P(4)-C(34)	101.6(4)
C(31)-P(4)-Cu(2)	123.6(3)
C(8)-P(4)-Cu(2)	106.1(3)
C(34)-P(4)-Cu(2)	113.6(3)
C(14)-P(5)-C(37)	105.9(3)

C(14)-P(5)-C(40)	100.5(3)
C(37)-P(5)-C(40)	104.5(3)
C(14)-P(5)-Cu(2)	107.6(2)
C(37)-P(5)-Cu(2)	121.6(2)
C(40)-P(5)-Cu(2)	114.5(2)
C(20)-P(6)-C(46)	105.0(4)
C(20)-P(6)-C(43)	101.7(4)
C(46)-P(6)-C(43)	104.0(3)
C(20)-P(6)-Cu(1)	107.9(2)
C(46)-P(6)-Cu(1)	121.6(3)
C(43)-P(6)-Cu(1)	114.5(2)
C(6)-C(1)-C(2)	118.0(6)
C(6)-C(1)-P(1)	123.0(6)
C(2)-C(1)-P(1)	118.5(5)
C(1)-C(2)-C(3)	119.3(7)
C(1)-C(2)-P(3)	118.2(5)
C(3)-C(2)-P(3)	122.5(6)
C(4)-C(3)-C(2)	121.4(7)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	118.6(7)
C(3)-C(4)-H(4)	120.7
C(5)-C(4)-H(4)	120.7
C(6)-C(5)-C(4)	121.4(7)
C(6)-C(5)-H(5)	119.3
C(4)-C(5)-H(5)	119.3
C(5)-C(6)-C(1)	120.9(7)
C(5)-C(6)-H(6)	119.5
C(1)-C(6)-H(6)	119.5
C(8)-C(7)-C(12)	117.3(7)
C(8)-C(7)-P(1)	119.4(6)
C(12)-C(7)-P(1)	122.3(6)
C(7)-C(8)-C(9)	121.1(7)
C(7)-C(8)-P(4)	118.6(6)
C(9)-C(8)-P(4)	120.3(6)
C(10)-C(9)-C(8)	120.5(7)

C(10)-C(9)-H(9)	119.8
C(8)-C(9)-H(9)	119.8
C(9)-C(10)-C(11)	118.9(7)
C(9)-C(10)-H(10)	120.5
C(11)-C(10)-H(10)	120.5
C(12)-C(11)-C(10)	121.1(7)
C(12)-C(11)-H(11)	119.4
C(10)-C(11)-H(11)	119.4
C(11)-C(12)-C(7)	121.0(7)
C(11)-C(12)-H(12)	119.5
C(7)-C(12)-H(12)	119.5
C(14)-C(13)-C(18)	117.5(6)
C(14)-C(13)-P(2)	119.8(5)
C(18)-C(13)-P(2)	122.1(5)
C(15)-C(14)-C(13)	120.4(7)
C(15)-C(14)-P(5)	122.3(6)
C(13)-C(14)-P(5)	117.3(5)
C(14)-C(15)-C(16)	120.9(7)
C(14)-C(15)-H(15)	119.5
C(16)-C(15)-H(15)	119.5
C(17)-C(16)-C(15)	118.4(7)
C(17)-C(16)-H(16)	120.8
C(15)-C(16)-H(16)	120.8
C(16)-C(17)-C(18)	121.1(7)
C(16)-C(17)-H(17)	119.4
C(18)-C(17)-H(17)	119.4
C(17)-C(18)-C(13)	121.4(6)
C(17)-C(18)-H(18)	119.3
C(13)-C(18)-H(18)	119.3
C(24)-C(19)-C(20)	117.2(7)
C(24)-C(19)-P(2)	122.2(6)
C(20)-C(19)-P(2)	120.4(6)
C(21)-C(20)-C(19)	119.8(7)
C(21)-C(20)-P(6)	123.2(6)
C(19)-C(20)-P(6)	117.0(5)
C(22)-C(21)-C(20)	120.6(8)

C(22)-C(21)-H(21)	119.7
C(20)-C(21)-H(21)	119.7
C(21)-C(22)-C(23)	120.9(8)
C(21)-C(22)-H(22)	119.6
C(23)-C(22)-H(22)	119.6
C(22)-C(23)-C(24)	120.5(8)
C(22)-C(23)-H(23)	119.8
C(24)-C(23)-H(23)	119.8
C(23)-C(24)-C(19)	121.0(7)
C(23)-C(24)-H(24)	119.5
C(19)-C(24)-H(24)	119.5
C(27)-C(25)-C(26)	110.1(6)
C(27)-C(25)-P(3)	109.5(5)
C(26)-C(25)-P(3)	107.7(5)
C(27)-C(25)-H(25)	109.8
C(26)-C(25)-H(25)	109.8
P(3)-C(25)-H(25)	109.8
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(30)-C(28)-C(29)	110.1(7)
C(30)-C(28)-P(3)	116.2(5)
C(29)-C(28)-P(3)	109.5(5)
C(30)-C(28)-H(28)	106.9
C(29)-C(28)-H(28)	106.9
P(3)-C(28)-H(28)	106.9
C(28)-C(29)-H(29A)	109.5

C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(33)	111.7(7)
C(32)-C(31)-P(4)	111.2(6)
C(33)-C(31)-P(4)	110.5(6)
C(32)-C(31)-H(31)	107.7
C(33)-C(31)-H(31)	107.7
P(4)-C(31)-H(31)	107.7
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(35)-C(34)-C(36)	110.8(7)
C(35)-C(34)-P(4)	116.7(6)
C(36)-C(34)-P(4)	108.9(5)
C(35)-C(34)-H(34)	106.6
C(36)-C(34)-H(34)	106.6
P(4)-C(34)-H(34)	106.6
C(34)-C(35)-H(35A)	109.5

C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(39)-C(37)-C(38)	110.1(6)
C(39)-C(37)-P(5)	110.4(5)
C(38)-C(37)-P(5)	109.9(5)
C(39)-C(37)-H(37)	108.8
C(38)-C(37)-H(37)	108.8
P(5)-C(37)-H(37)	108.8
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(42)-C(40)-C(41)	109.2(6)
C(42)-C(40)-P(5)	111.2(5)
C(41)-C(40)-P(5)	117.2(5)
C(42)-C(40)-H(40)	106.2
C(41)-C(40)-H(40)	106.2
P(5)-C(40)-H(40)	106.2
C(40)-C(41)-H(41A)	109.5

C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(45)-C(43)-C(44)	110.3(7)
C(45)-C(43)-P(6)	108.4(5)
C(44)-C(43)-P(6)	118.0(5)
C(45)-C(43)-H(43)	106.5
C(44)-C(43)-H(43)	106.5
P(6)-C(43)-H(43)	106.5
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(43)-C(45)-H(45A)	109.5
C(43)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(43)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(48)-C(46)-C(47)	111.1(7)
C(48)-C(46)-P(6)	110.2(6)
C(47)-C(46)-P(6)	107.8(5)
C(48)-C(46)-H(46)	109.3
C(47)-C(46)-H(46)	109.3
P(6)-C(46)-H(46)	109.3
C(46)-C(47)-H(47A)	109.5

C(46)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(46)-C(48)-H(48A)	109.5
C(46)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(46)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
Cl(1)-C(49)-Cl(2)	114.4(6)
Cl(1)-C(49)-H(49A)	108.7
Cl(2)-C(49)-H(49A)	108.7
Cl(1)-C(49)-H(49B)	108.7
Cl(2)-C(49)-H(49B)	108.7
H(49A)-C(49)-H(49B)	107.6

Symmetry transformations used to generate equivalent atoms:

Table 6. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $\{(PPP)Cu\}_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	16(1)	6(1)	25(1)	-1(1)	3(1)	-1(1)
Cu(2)	20(1)	10(1)	30(1)	-4(1)	0(1)	2(1)
P(1)	14(1)	6(1)	27(1)	-1(1)	3(1)	2(1)
P(2)	17(1)	5(1)	29(1)	-1(1)	3(1)	0(1)
P(3)	12(1)	9(1)	25(1)	-2(1)	3(1)	-1(1)
P(4)	13(1)	10(1)	32(1)	-5(1)	-1(1)	1(1)
P(5)	13(1)	10(1)	27(1)	-2(1)	2(1)	0(1)
P(6)	20(1)	12(1)	25(1)	1(1)	5(1)	0(1)
C(1)	16(5)	8(4)	18(4)	-6(3)	2(3)	0(4)
C(2)	5(4)	4(4)	24(4)	-6(3)	8(3)	0(3)
C(3)	26(5)	11(4)	18(4)	-7(4)	1(4)	8(4)
C(4)	24(5)	4(4)	24(4)	1(4)	5(4)	7(4)
C(5)	18(5)	12(4)	31(5)	6(4)	2(4)	1(4)
C(6)	16(5)	9(4)	26(5)	-5(4)	-3(4)	-1(4)
C(7)	15(5)	8(4)	17(4)	3(3)	-2(3)	0(3)
C(8)	21(5)	2(4)	28(5)	-1(3)	-5(4)	-4(4)
C(9)	13(4)	14(4)	29(5)	2(4)	-5(4)	-5(4)
C(10)	23(5)	13(4)	23(5)	-4(4)	5(4)	-6(4)
C(11)	24(5)	17(5)	25(5)	-8(4)	10(4)	1(4)
C(12)	5(4)	15(4)	25(5)	0(4)	1(3)	-1(4)
C(13)	12(4)	2(4)	15(4)	2(3)	4(3)	-2(3)
C(14)	9(4)	5(4)	35(5)	-10(4)	1(4)	4(3)
C(15)	20(5)	17(5)	31(5)	-4(4)	0(4)	5(4)
C(16)	14(4)	9(4)	21(4)	-4(3)	3(4)	0(3)
C(17)	18(5)	6(4)	36(5)	-2(4)	-6(4)	1(4)
C(18)	18(5)	12(4)	20(4)	9(4)	6(4)	9(4)
C(19)	16(4)	12(4)	20(4)	-3(4)	0(4)	-3(4)
C(20)	27(5)	15(5)	27(5)	-2(4)	4(4)	-6(4)
C(21)	51(7)	24(5)	26(5)	4(4)	4(5)	7(5)
C(22)	51(7)	39(6)	27(5)	10(5)	7(5)	-7(6)
C(23)	32(6)	22(5)	35(5)	13(4)	-3(4)	8(4)

C(24)	15(5)	22(5)	26(5)	-1(4)	6(4)	-4(4)
C(25)	15(4)	18(5)	23(4)	14(4)	-2(3)	1(4)
C(26)	19(5)	19(5)	46(5)	-2(4)	-1(4)	-6(4)
C(27)	20(5)	19(5)	24(4)	-7(4)	-5(4)	1(4)
C(28)	12(5)	35(6)	31(5)	-8(4)	10(4)	2(4)
C(29)	29(6)	24(5)	32(5)	-4(4)	6(4)	10(4)
C(30)	24(5)	13(5)	49(6)	6(4)	-3(4)	10(4)
C(31)	32(6)	16(5)	51(6)	-14(4)	1(5)	3(4)
C(32)	45(6)	37(6)	55(6)	17(6)	-12(5)	2(6)
C(33)	64(8)	35(7)	77(7)	-9(6)	-34(6)	14(6)
C(34)	10(5)	30(6)	55(6)	-11(5)	-9(4)	-2(4)
C(35)	18(5)	37(6)	60(6)	-7(5)	3(5)	-18(5)
C(36)	38(6)	24(5)	55(6)	15(5)	11(5)	-12(5)
C(37)	19(5)	7(4)	30(5)	-10(4)	3(4)	3(4)
C(38)	22(5)	27(5)	37(5)	3(4)	10(4)	-10(4)
C(39)	20(5)	14(5)	60(6)	-2(4)	3(4)	-7(4)
C(40)	17(5)	15(5)	39(5)	-9(4)	-1(4)	-7(4)
C(41)	25(5)	15(5)	52(6)	-3(4)	-2(4)	-5(4)
C(42)	30(6)	24(5)	60(6)	-1(5)	-6(5)	13(5)
C(43)	30(5)	28(5)	34(5)	-12(4)	4(4)	-22(5)
C(44)	27(5)	25(6)	58(6)	3(5)	16(5)	-8(4)
C(45)	39(6)	13(5)	44(5)	-6(4)	3(5)	-13(4)
C(46)	47(6)	15(5)	17(4)	0(4)	6(4)	-11(4)
C(47)	84(9)	22(5)	48(6)	-8(5)	28(6)	6(6)
C(48)	61(7)	54(7)	35(6)	-14(5)	12(5)	-29(6)
Cl(1)	45(2)	38(2)	49(2)	-1(1)	-6(1)	9(1)
Cl(2)	89(3)	61(2)	158(3)	-33(2)	48(2)	16(2)
C(49)	116(10)	27(6)	37(6)	3(5)	-2(6)	-3(7)

Table 7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for {(PPP)Cu}$_2$.

	x	y	z	U(eq)
H(3)	5495	8549	4702	22
H(4)	4530	7667	5114	21
H(5)	3136	7153	4474	24
H(6)	2706	7513	3453	21
H(9)	1196	7865	891	23
H(10)	2394	7002	677	23
H(11)	3924	6808	1374	26
H(12)	4246	7455	2280	18
H(15)	1735	11110	4427	27
H(16)	2850	12082	4528	17
H(17)	3941	12358	3710	24
H(18)	4029	11664	2826	20
H(21)	4794	10712	487	40
H(22)	3604	11540	161	47
H(23)	2299	11920	815	36
H(24)	2159	11459	1817	25
H(25)	6256	9549	4467	22
H(26A)	6732	10365	3398	42
H(26B)	7593	9926	3822	42
H(26C)	7089	10590	4109	42
H(27A)	5320	10601	4513	32
H(27B)	4485	9990	4408	32
H(27C)	4754	10456	3822	32
H(28)	7264	8972	3066	31
H(29A)	7111	7848	2763	42
H(29B)	6010	8220	2513	42
H(29C)	6020	7759	3132	42
H(30A)	7028	8138	4147	43
H(30B)	7624	8849	4186	43
H(30C)	8131	8253	3795	43

H(31)	215	8775	882	40
H(32A)	1074	9652	373	70
H(32B)	1963	9169	723	70
H(32C)	1682	9872	1034	70
H(33A)	-223	10021	1478	91
H(33B)	-1048	9400	1424	91
H(33C)	-753	9795	799	91
H(34)	-667	8683	2371	39
H(35A)	-287	7596	1543	58
H(35B)	-1125	8196	1390	58
H(35C)	-1350	7672	1939	58
H(36A)	-317	7752	3000	58
H(36B)	733	8227	3082	58
H(36C)	760	7577	2643	58
H(37)	933	10146	4510	22
H(38A)	1932	9161	4858	42
H(38B)	2694	9685	4522	42
H(38C)	2245	9038	4143	42
H(39A)	71	9034	3807	47
H(39B)	-602	9596	4155	47
H(39C)	76	9045	4565	47
H(40)	-588	10220	3094	29
H(41A)	-11	11402	3799	46
H(41B)	-562	10762	4101	46
H(41C)	-1224	11182	3557	46
H(42A)	-648	11149	2449	58
H(42B)	352	10689	2265	58
H(42C)	578	11349	2681	58
H(43)	7029	10158	2034	37
H(44A)	6565	10961	937	54
H(44B)	7183	10257	930	54
H(44C)	7738	10875	1308	54
H(45A)	6972	11238	2357	48
H(45B)	5838	10917	2541	48
H(45C)	5873	11387	1930	48
H(46)	5649	9660	638	31

H(47A)	6160	8690	1618	75
H(47B)	7023	9124	1255	75
H(47C)	6359	8536	890	75
H(48A)	4496	8733	435	74
H(48B)	3799	9353	665	74
H(48C)	4125	8759	1148	74
H(49A)	9705	2249	5881	72
H(49B)	8834	2433	5311	72

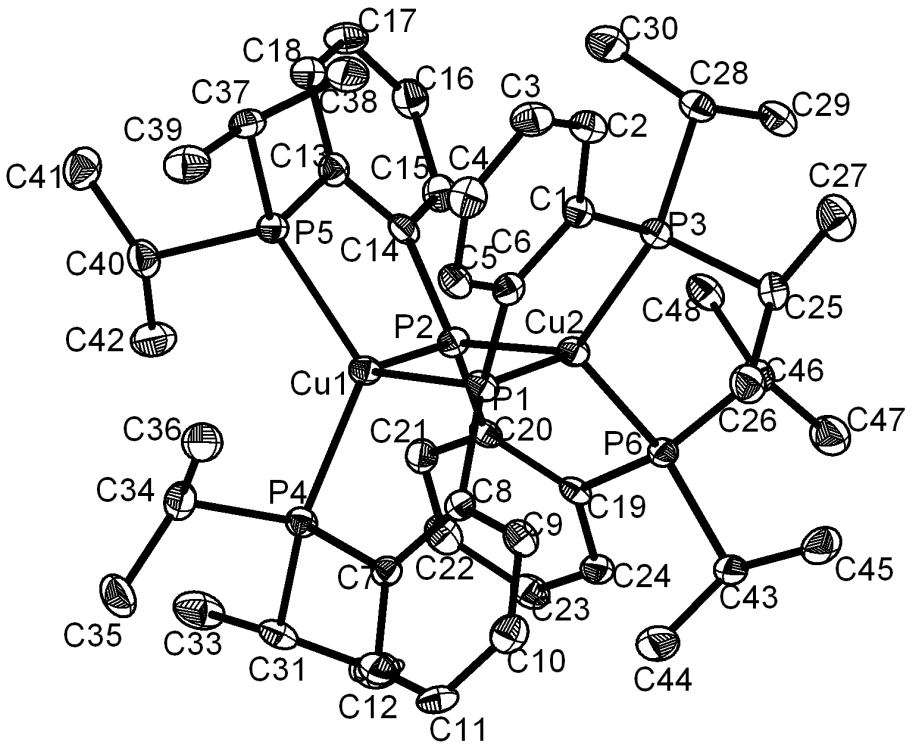

Figure S7. Molecular structure of $[(PPP)Cu]_2^+$. Hydrogen atoms have been omitted for clarity.

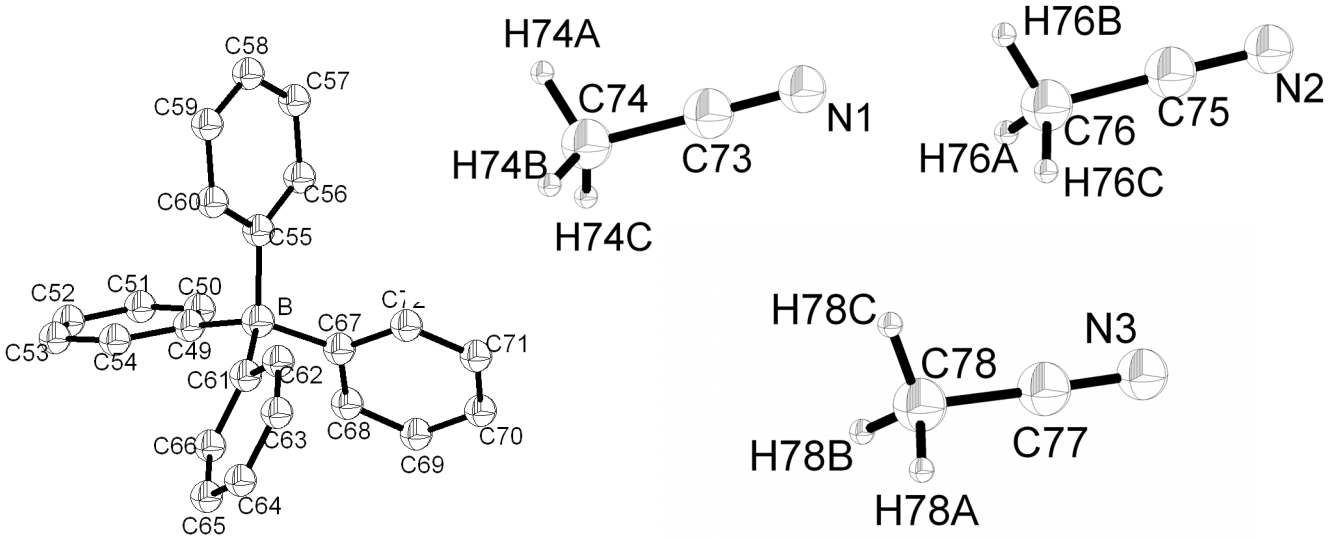

Figure S8. Tetraphenylborate anion and acetonitrile molecules in the crystal structure of **4**. Hydrogen atoms on the anion have been omitted for clarity.

Table 8. Crystal data and structure refinement for {(PPP)Cu}$_2$BPh$_4$.

Identification code	{(PPP)Cu}$_2$BPh$_4$	
Empirical formula	$C_{39}H_{50.5}B_{0.5}CuN_{1.5}P_3$	
Formula weight	702.16	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.3063(11) Å	a= 82.727(2)°
	b = 17.3023(16) Å	b= 81.199(2)°
	c = 19.9594(19)	g = 79.000(2)°
Volume	3768.6(6) Å^3	
Z	4	
Density (calculated)	1.238 Mg/m^3	
Absorption coefficient	0.735 mm^{-1}	
F(000)	1486	
Crystal size	0.596 x 0.426 x 0.078 mm^3	
Theta range for data collection	1.85 to 28.44º	
Index ranges	$-15 \le h \le 14$, $-22 \le k \le 21$, $-26 \le l \le 26$	
Reflections collected	40943	
Independent reflections	16740 [R(int) = 0.0654]	
Completeness to theta = 28.44∞	88.1 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16740 / 0 / 830	
Goodness-of-fit on F^2	1.327	
Final R indices [I>2sigma(I)]	R1 = 0.0463, wR2 = 0.0783	
R indices (all data)	R1 = 0.0814, wR2 = 0.0841	
Largest diff. peak and hole	0.948 and -0.751 Å^{-3}	

Table 9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for {(PPP)Cu}$_2$BPh$_4$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	5742(1)	2437(1)	1167(1)	16(1)
Cu(2)	5992(1)	2064(1)	2534(1)	16(1)
P(1)	6581(1)	1258(1)	1676(1)	16(1)
P(2)	5212(1)	3260(1)	1994(1)	15(1)
P(3)	5147(1)	1039(1)	3126(1)	16(1)
P(4)	7456(1)	2353(1)	401(1)	16(1)
P(5)	3787(1)	2793(1)	921(1)	17(1)
P(6)	7035(1)	2752(1)	3068(1)	16(1)
C(1)	5042(2)	363(2)	2507(1)	16(1)
C(2)	4296(2)	-211(2)	2630(1)	22(1)
C(3)	4333(3)	-741(2)	2158(2)	25(1)
C(4)	5141(3)	-716(2)	1560(1)	24(1)
C(5)	5871(2)	-143(2)	1421(1)	19(1)
C(6)	5824(2)	407(2)	1884(1)	17(1)
C(7)	8513(2)	1474(2)	686(1)	16(1)
C(8)	8068(2)	946(2)	1209(1)	15(1)
C(9)	8832(3)	235(2)	1402(1)	21(1)
C(10)	10007(3)	54(2)	1084(1)	24(1)
C(11)	10450(2)	588(2)	572(1)	22(1)
C(12)	9715(2)	1285(2)	374(1)	21(1)
C(13)	2951(2)	3409(2)	1585(1)	17(1)
C(14)	3632(2)	3711(2)	1994(1)	17(1)
C(15)	3036(3)	4284(2)	2431(1)	21(1)
C(16)	1789(3)	4529(2)	2485(1)	24(1)
C(17)	1115(3)	4196(2)	2110(1)	27(1)
C(18)	1686(2)	3641(2)	1666(1)	23(1)
C(19)	6950(2)	3747(2)	2607(1)	15(1)
C(20)	6042(2)	3993(2)	2178(1)	15(1)
C(21)	5900(2)	4758(2)	1854(1)	19(1)
C(22)	6648(3)	5273(2)	1943(1)	23(1)
C(23)	7544(3)	5033(2)	2361(1)	23(1)

C(24)	7689(2)	4273(2)	2699(1)	19(1)
C(25)	6253(2)	409(2)	3660(1)	20(1)
C(26)	7435(2)	88(2)	3224(1)	25(1)
C(27)	5767(3)	-278(2)	4092(2)	30(1)
C(28)	3679(2)	1139(2)	3693(1)	20(1)
C(29)	3770(3)	1580(2)	4299(1)	24(1)
C(30)	2639(3)	1570(2)	3307(2)	31(1)
C(31)	8425(2)	3121(2)	170(1)	20(1)
C(32)	8933(3)	3281(2)	792(2)	31(1)
C(33)	7712(3)	3891(2)	-152(2)	34(1)
C(34)	7124(3)	2098(2)	-424(1)	22(1)
C(35)	8114(3)	2159(2)	-1029(1)	30(1)
C(36)	6804(3)	1269(2)	-326(1)	29(1)
C(37)	2814(2)	2078(2)	822(1)	20(1)
C(38)	2606(3)	1544(2)	1484(1)	29(1)
C(39)	3394(3)	1592(2)	227(2)	29(1)
C(40)	3666(2)	3498(2)	138(1)	23(1)
C(41)	2372(3)	3853(2)	-12(2)	29(1)
C(42)	4356(3)	4165(2)	172(2)	35(1)
C(43)	8639(2)	2438(2)	3209(1)	20(1)
C(44)	9444(3)	2298(2)	2535(1)	32(1)
C(45)	8794(3)	1689(2)	3712(2)	29(1)
C(46)	6189(2)	2968(2)	3922(1)	18(1)
C(47)	6847(3)	3367(2)	4357(1)	29(1)
C(48)	4932(2)	3465(2)	3842(1)	23(1)
B	185(3)	2695(2)	6768(2)	18(1)
C(49)	-33(2)	1843(2)	6558(1)	20(1)
C(50)	157(3)	1658(2)	5882(2)	27(1)
C(51)	-141(3)	979(2)	5695(2)	34(1)
C(52)	-638(3)	455(2)	6178(2)	38(1)
C(53)	-841(3)	607(2)	6845(2)	32(1)
C(54)	-547(2)	1295(2)	7029(2)	24(1)
C(55)	-1098(2)	3305(2)	6645(1)	18(1)
C(56)	-1284(3)	3723(2)	6006(2)	24(1)
C(57)	-2396(3)	4165(2)	5874(2)	32(1)
C(58)	-3382(3)	4212(2)	6380(2)	33(1)

C(59)	-3235(3)	3819(2)	7014(2)	26(1)
C(60)	-2109(2)	3371(2)	7140(1)	19(1)
C(61)	497(2)	2639(2)	7550(1)	16(1)
C(62)	271(2)	3304(2)	7920(1)	19(1)
C(63)	680(2)	3292(2)	8546(1)	21(1)
C(64)	1311(3)	2600(2)	8836(1)	24(1)
C(65)	1542(2)	1929(2)	8494(1)	24(1)
C(66)	1158(2)	1951(2)	7866(1)	20(1)
C(67)	1380(3)	3010(2)	6318(1)	20(1)
C(68)	2417(3)	2510(2)	6049(1)	23(1)
C(69)	3478(3)	2774(2)	5748(1)	31(1)
C(70)	3539(3)	3568(2)	5717(1)	35(1)
C(71)	2542(3)	4093(2)	5969(1)	32(1)
C(72)	1481(3)	3813(2)	6263(1)	25(1)
N(1)	5138(2)	7317(1)	1458(1)	34(1)
N(2)	3433(2)	8755(2)	4789(1)	39(1)
N(3)	-450(3)	4057(2)	3970(2)	55(1)
C(73)	5573(3)	7279(2)	1939(2)	24(1)
C(74)	6152(3)	7220(2)	2559(1)	31(1)
C(75)	3301(3)	8380(2)	4386(2)	24(1)
C(76)	3154(3)	7888(2)	3882(2)	32(1)
C(77)	463(3)	3933(2)	4157(2)	29(1)
C(78)	1635(3)	3784(2)	4381(2)	50(1)

Table 10. Bond lengths [Å] and angles [°] for $\{(PPP)Cu\}_2BPh_4$.

Cu(1)-P(2)	2.2547(8)
Cu(1)-P(1)	2.2643(8)
Cu(1)-P(4)	2.2705(8)
Cu(1)-P(5)	2.2898(8)
Cu(2)-P(6)	2.2763(7)
Cu(2)-P(3)	2.2849(8)
Cu(2)-P(1)	2.2852(8)
Cu(2)-P(2)	2.2918(8)
P(1)-C(8)	1.813(3)
P(1)-C(6)	1.814(3)
P(2)-C(14)	1.808(3)
P(2)-C(20)	1.815(3)
P(3)-C(1)	1.837(3)
P(3)-C(28)	1.853(3)
P(3)-C(25)	1.866(3)
P(4)-C(7)	1.833(3)
P(4)-C(31)	1.850(3)
P(4)-C(34)	1.866(3)
P(5)-C(13)	1.836(3)
P(5)-C(37)	1.852(3)
P(5)-C(40)	1.863(3)
P(6)-C(19)	1.838(3)
P(6)-C(43)	1.846(3)
P(6)-C(46)	1.868(3)
C(1)-C(2)	1.398(3)
C(1)-C(6)	1.414(4)
C(2)-C(3)	1.386(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.389(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.383(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.396(3)
C(5)-H(5)	0.9500

C(7)-C(8)	1.397(3)
C(7)-C(12)	1.401(4)
C(8)-C(9)	1.408(3)
C(9)-C(10)	1.378(4)
C(9)-H(9)	0.9500
C(10)-C(11)	1.389(4)
C(10)-H(10)	0.9500
C(11)-C(12)	1.378(4)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(18)	1.399(4)
C(13)-C(14)	1.411(3)
C(14)-C(15)	1.408(4)
C(15)-C(16)	1.384(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.387(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.388(4)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(24)	1.394(3)
C(19)-C(20)	1.407(3)
C(20)-C(21)	1.390(3)
C(21)-C(22)	1.383(4)
C(21)-H(21)	0.9500
C(22)-C(23)	1.381(4)
C(22)-H(22)	0.9500
C(23)-C(24)	1.391(3)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-C(27)	1.518(4)
C(25)-C(26)	1.529(4)
C(25)-H(25)	1.0000
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800

C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(30)	1.526(4)
C(28)-C(29)	1.535(4)
C(28)-H(28)	1.0000
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(32)	1.521(4)
C(31)-C(33)	1.540(4)
C(31)-H(31)	1.0000
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.524(4)
C(34)-C(36)	1.528(4)
C(34)-H(34)	1.0000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(38)	1.528(4)
C(37)-C(39)	1.532(4)
C(37)-H(37)	1.0000
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800

C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-C(42)	1.525(4)
C(40)-C(41)	1.534(4)
C(40)-H(40)	1.0000
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-C(44)	1.524(4)
C(43)-C(45)	1.535(3)
C(43)-H(43)	1.0000
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-C(47)	1.526(3)
C(46)-C(48)	1.534(4)
C(46)-H(46)	1.0000
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
B-C(61)	1.639(4)
B-C(67)	1.648(4)
B-C(49)	1.654(4)
B-C(55)	1.654(4)
C(49)-C(54)	1.391(4)
C(49)-C(50)	1.403(4)

C(50)-C(51)	1.391(4)
C(50)-H(50)	0.9500
C(51)-C(52)	1.368(4)
C(51)-H(51)	0.9500
C(52)-C(53)	1.367(4)
C(52)-H(52)	0.9500
C(53)-C(54)	1.400(4)
C(53)-H(53)	0.9500
C(54)-H(54)	0.9500
C(55)-C(60)	1.389(4)
C(55)-C(56)	1.408(4)
C(56)-C(57)	1.385(4)
C(56)-H(56)	0.9500
C(57)-C(58)	1.383(4)
C(57)-H(57)	0.9500
C(58)-C(59)	1.377(4)
C(58)-H(58)	0.9500
C(59)-C(60)	1.399(4)
C(59)-H(59)	0.9500
C(60)-H(60)	0.9500
C(61)-C(62)	1.407(3)
C(61)-C(66)	1.409(3)
C(62)-C(63)	1.393(3)
C(62)-H(62)	0.9500
C(63)-C(64)	1.379(4)
C(63)-H(63)	0.9500
C(64)-C(65)	1.383(4)
C(64)-H(64)	0.9500
C(65)-C(66)	1.383(4)
C(65)-H(65)	0.9500
C(66)-H(66)	0.9500
C(67)-C(68)	1.397(4)
C(67)-C(72)	1.404(4)
C(68)-C(69)	1.388(4)
C(68)-H(68)	0.9500
C(69)-C(70)	1.382(4)

C(69)-H(69)	0.9500
C(70)-C(71)	1.380(4)
C(70)-H(70)	0.9500
C(71)-C(72)	1.398(4)
C(71)-H(71)	0.9500
C(72)-H(72)	0.9500
N(1)-C(73)	1.134(3)
N(2)-C(75)	1.139(4)
N(3)-C(77)	1.124(4)
C(73)-C(74)	1.470(4)
C(74)-H(74A)	0.9800
C(74)-H(74B)	0.9800
C(74)-H(74C)	0.9800
C(75)-C(76)	1.445(4)
C(76)-H(76A)	0.9800
C(76)-H(76B)	0.9800
C(76)-H(76C)	0.9800
C(77)-C(78)	1.429(4)
C(78)-H(78A)	0.9800
C(78)-H(78B)	0.9800
C(78)-H(78C)	0.9800

P(2)-Cu(1)-P(1)	105.90(3)
P(2)-Cu(1)-P(4)	126.22(3)
P(1)-Cu(1)-P(4)	87.17(3)
P(2)-Cu(1)-P(5)	87.22(3)
P(1)-Cu(1)-P(5)	126.60(3)
P(4)-Cu(1)-P(5)	126.26(3)
P(6)-Cu(2)-P(3)	120.01(3)
P(6)-Cu(2)-P(1)	132.37(3)
P(3)-Cu(2)-P(1)	85.70(3)
P(6)-Cu(2)-P(2)	86.47(3)
P(3)-Cu(2)-P(2)	133.90(3)
P(1)-Cu(2)-P(2)	103.99(3)
C(8)-P(1)-C(6)	108.44(12)
C(8)-P(1)-Cu(1)	108.34(9)

C(6)-P(1)-Cu(1)	124.19(9)
C(8)-P(1)-Cu(2)	130.66(8)
C(6)-P(1)-Cu(2)	108.69(9)
Cu(1)-P(1)-Cu(2)	75.00(3)
C(14)-P(2)-C(20)	108.53(12)
C(14)-P(2)-Cu(1)	108.87(9)
C(20)-P(2)-Cu(1)	127.51(9)
C(14)-P(2)-Cu(2)	127.83(9)
C(20)-P(2)-Cu(2)	107.87(9)
Cu(1)-P(2)-Cu(2)	75.05(3)
C(1)-P(3)-C(28)	106.00(12)
C(1)-P(3)-C(25)	101.61(12)
C(28)-P(3)-C(25)	104.35(12)
C(1)-P(3)-Cu(2)	107.26(9)
C(28)-P(3)-Cu(2)	125.38(9)
C(25)-P(3)-Cu(2)	109.77(9)
C(7)-P(4)-C(31)	103.54(12)
C(7)-P(4)-C(34)	102.72(12)
C(31)-P(4)-C(34)	105.58(12)
C(7)-P(4)-Cu(1)	107.40(9)
C(31)-P(4)-Cu(1)	125.74(9)
C(34)-P(4)-Cu(1)	109.50(9)
C(13)-P(5)-C(37)	106.60(12)
C(13)-P(5)-C(40)	101.80(12)
C(37)-P(5)-C(40)	103.23(12)
C(13)-P(5)-Cu(1)	106.57(8)
C(37)-P(5)-Cu(1)	123.95(9)
C(40)-P(5)-Cu(1)	112.47(9)
C(19)-P(6)-C(43)	105.36(12)
C(19)-P(6)-C(46)	102.04(12)
C(43)-P(6)-C(46)	105.12(12)
C(19)-P(6)-Cu(2)	107.16(8)
C(43)-P(6)-Cu(2)	124.79(10)
C(46)-P(6)-Cu(2)	110.06(9)
C(2)-C(1)-C(6)	118.9(2)
C(2)-C(1)-P(3)	124.2(2)

C(6)-C(1)-P(3)	116.79(19)
C(3)-C(2)-C(1)	120.9(3)
C(3)-C(2)-H(2)	119.5
C(1)-C(2)-H(2)	119.5
C(2)-C(3)-C(4)	119.9(3)
C(2)-C(3)-H(3)	120.1
C(4)-C(3)-H(3)	120.1
C(5)-C(4)-C(3)	120.2(3)
C(5)-C(4)-H(4)	119.9
C(3)-C(4)-H(4)	119.9
C(4)-C(5)-C(6)	120.7(3)
C(4)-C(5)-H(5)	119.6
C(6)-C(5)-H(5)	119.6
C(5)-C(6)-C(1)	119.4(2)
C(5)-C(6)-P(1)	122.5(2)
C(1)-C(6)-P(1)	117.63(19)
C(8)-C(7)-C(12)	118.9(2)
C(8)-C(7)-P(4)	117.9(2)
C(12)-C(7)-P(4)	123.1(2)
C(7)-C(8)-C(9)	119.2(3)
C(7)-C(8)-P(1)	118.1(2)
C(9)-C(8)-P(1)	122.4(2)
C(10)-C(9)-C(8)	121.2(3)
C(10)-C(9)-H(9)	119.4
C(8)-C(9)-H(9)	119.4
C(9)-C(10)-C(11)	119.4(3)
C(9)-C(10)-H(10)	120.3
C(11)-C(10)-H(10)	120.3
C(12)-C(11)-C(10)	120.3(3)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(11)-C(12)-C(7)	121.1(3)
C(11)-C(12)-H(12)	119.5
C(7)-C(12)-H(12)	119.5
C(18)-C(13)-C(14)	118.7(2)
C(18)-C(13)-P(5)	123.3(2)

C(14)-C(13)-P(5)	117.8(2)
C(15)-C(14)-C(13)	119.2(2)
C(15)-C(14)-P(2)	123.0(2)
C(13)-C(14)-P(2)	117.4(2)
C(16)-C(15)-C(14)	121.0(3)
C(16)-C(15)-H(15)	119.5
C(14)-C(15)-H(15)	119.5
C(15)-C(16)-C(17)	119.5(3)
C(15)-C(16)-H(16)	120.3
C(17)-C(16)-H(16)	120.3
C(16)-C(17)-C(18)	120.5(3)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(17)-C(18)-C(13)	120.9(3)
C(17)-C(18)-H(18)	119.5
C(13)-C(18)-H(18)	119.5
C(24)-C(19)-C(20)	119.5(2)
C(24)-C(19)-P(6)	122.9(2)
C(20)-C(19)-P(6)	117.53(19)
C(21)-C(20)-C(19)	119.2(2)
C(21)-C(20)-P(2)	122.24(19)
C(19)-C(20)-P(2)	118.22(19)
C(22)-C(21)-C(20)	120.8(2)
C(22)-C(21)-H(21)	119.6
C(20)-C(21)-H(21)	119.6
C(23)-C(22)-C(21)	120.2(3)
C(23)-C(22)-H(22)	119.9
C(21)-C(22)-H(22)	119.9
C(22)-C(23)-C(24)	119.9(3)
C(22)-C(23)-H(23)	120.0
C(24)-C(23)-H(23)	120.0
C(23)-C(24)-C(19)	120.4(2)
C(23)-C(24)-H(24)	119.8
C(19)-C(24)-H(24)	119.8
C(27)-C(25)-C(26)	108.8(2)
C(27)-C(25)-P(3)	114.10(19)

C(26)-C(25)-P(3)	111.28(18)
C(27)-C(25)-H(25)	107.5
C(26)-C(25)-H(25)	107.5
P(3)-C(25)-H(25)	107.5
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(30)-C(28)-C(29)	110.7(2)
C(30)-C(28)-P(3)	111.05(19)
C(29)-C(28)-P(3)	109.25(18)
C(30)-C(28)-H(28)	108.6
C(29)-C(28)-H(28)	108.6
P(3)-C(28)-H(28)	108.6
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(33)	110.2(2)
C(32)-C(31)-P(4)	110.56(19)

C(33)-C(31)-P(4)	111.02(18)
C(32)-C(31)-H(31)	108.3
C(33)-C(31)-H(31)	108.3
P(4)-C(31)-H(31)	108.3
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(35)-C(34)-C(36)	109.7(2)
C(35)-C(34)-P(4)	116.13(19)
C(36)-C(34)-P(4)	109.50(18)
C(35)-C(34)-H(34)	107.0
C(36)-C(34)-H(34)	107.0
P(4)-C(34)-H(34)	107.0
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-C(39)	111.3(2)
C(38)-C(37)-P(5)	110.46(18)

C(39)-C(37)-P(5)	109.85(18)
C(38)-C(37)-H(37)	108.4
C(39)-C(37)-H(37)	108.4
P(5)-C(37)-H(37)	108.4
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(42)-C(40)-C(41)	109.3(2)
C(42)-C(40)-P(5)	109.27(19)
C(41)-C(40)-P(5)	115.9(2)
C(42)-C(40)-H(40)	107.3
C(41)-C(40)-H(40)	107.3
P(5)-C(40)-H(40)	107.3
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(44)-C(43)-C(45)	110.5(2)
C(44)-C(43)-P(6)	110.23(19)

C(45)-C(43)-P(6)	110.86(18)
C(44)-C(43)-H(43)	108.4
C(45)-C(43)-H(43)	108.4
P(6)-C(43)-H(43)	108.4
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(43)-C(45)-H(45A)	109.5
C(43)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(43)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(47)-C(46)-C(48)	109.8(2)
C(47)-C(46)-P(6)	115.13(19)
C(48)-C(46)-P(6)	110.01(18)
C(47)-C(46)-H(46)	107.2
C(48)-C(46)-H(46)	107.2
P(6)-C(46)-H(46)	107.2
C(46)-C(47)-H(47A)	109.5
C(46)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(46)-C(48)-H(48A)	109.5
C(46)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(46)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(61)-B-C(67)	102.2(2)
C(61)-B-C(49)	113.0(2)

C(67)-B-C(49)	113.4(2)
C(61)-B-C(55)	112.8(2)
C(67)-B-C(55)	112.2(2)
C(49)-B-C(55)	103.6(2)
C(54)-C(49)-C(50)	114.8(3)
C(54)-C(49)-B	122.4(2)
C(50)-C(49)-B	122.4(3)
C(51)-C(50)-C(49)	122.6(3)
C(51)-C(50)-H(50)	118.7
C(49)-C(50)-H(50)	118.7
C(52)-C(51)-C(50)	120.4(3)
C(52)-C(51)-H(51)	119.8
C(50)-C(51)-H(51)	119.8
C(53)-C(52)-C(51)	119.3(3)
C(53)-C(52)-H(52)	120.3
C(51)-C(52)-H(52)	120.3
C(52)-C(53)-C(54)	120.0(3)
C(52)-C(53)-H(53)	120.0
C(54)-C(53)-H(53)	120.0
C(49)-C(54)-C(53)	122.8(3)
C(49)-C(54)-H(54)	118.6
C(53)-C(54)-H(54)	118.6
C(60)-C(55)-C(56)	115.2(2)
C(60)-C(55)-B	122.2(2)
C(56)-C(55)-B	122.2(3)
C(57)-C(56)-C(55)	122.9(3)
C(57)-C(56)-H(56)	118.6
C(55)-C(56)-H(56)	118.6
C(58)-C(57)-C(56)	120.0(3)
C(58)-C(57)-H(57)	120.0
C(56)-C(57)-H(57)	120.0
C(59)-C(58)-C(57)	119.0(3)
C(59)-C(58)-H(58)	120.5
C(57)-C(58)-H(58)	120.5
C(58)-C(59)-C(60)	120.3(3)
C(58)-C(59)-H(59)	119.8

C(60)-C(59)-H(59)	119.8
C(55)-C(60)-C(59)	122.5(3)
C(55)-C(60)-H(60)	118.7
C(59)-C(60)-H(60)	118.7
C(62)-C(61)-C(66)	114.8(2)
C(62)-C(61)-B	122.2(2)
C(66)-C(61)-B	122.4(2)
C(63)-C(62)-C(61)	123.0(3)
C(63)-C(62)-H(62)	118.5
C(61)-C(62)-H(62)	118.5
C(64)-C(63)-C(62)	119.8(3)
C(64)-C(63)-H(63)	120.1
C(62)-C(63)-H(63)	120.1
C(63)-C(64)-C(65)	119.2(3)
C(63)-C(64)-H(64)	120.4
C(65)-C(64)-H(64)	120.4
C(66)-C(65)-C(64)	120.6(3)
C(66)-C(65)-H(65)	119.7
C(64)-C(65)-H(65)	119.7
C(65)-C(66)-C(61)	122.5(3)
C(65)-C(66)-H(66)	118.7
C(61)-C(66)-H(66)	118.7
C(68)-C(67)-C(72)	115.0(3)
C(68)-C(67)-B	123.8(3)
C(72)-C(67)-B	120.6(3)
C(69)-C(68)-C(67)	123.3(3)
C(69)-C(68)-H(68)	118.3
C(67)-C(68)-H(68)	118.3
C(70)-C(69)-C(68)	119.4(3)
C(70)-C(69)-H(69)	120.3
C(68)-C(69)-H(69)	120.3
C(71)-C(70)-C(69)	120.0(3)
C(71)-C(70)-H(70)	120.0
C(69)-C(70)-H(70)	120.0
C(70)-C(71)-C(72)	119.4(3)
C(70)-C(71)-H(71)	120.3

C(72)-C(71)-H(71)	120.3
C(71)-C(72)-C(67)	122.8(3)
C(71)-C(72)-H(72)	118.6
C(67)-C(72)-H(72)	118.6
N(1)-C(73)-C(74)	179.1(4)
C(73)-C(74)-H(74A)	109.5
C(73)-C(74)-H(74B)	109.5
H(74A)-C(74)-H(74B)	109.5
C(73)-C(74)-H(74C)	109.5
H(74A)-C(74)-H(74C)	109.5
H(74B)-C(74)-H(74C)	109.5
N(2)-C(75)-C(76)	178.7(3)
C(75)-C(76)-H(76A)	109.5
C(75)-C(76)-H(76B)	109.5
H(76A)-C(76)-H(76B)	109.5
C(75)-C(76)-H(76C)	109.5
H(76A)-C(76)-H(76C)	109.5
H(76B)-C(76)-H(76C)	109.5
N(3)-C(77)-C(78)	178.8(4)
C(77)-C(78)-H(78A)	109.5
C(77)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
C(77)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $\{(PPP)Cu\}_2BPh_4$. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	14(1)	15(1)	18(1)	-2(1)	-1(1)	-2(1)
Cu(2)	16(1)	14(1)	17(1)	-1(1)	-1(1)	-3(1)
P(1)	17(1)	13(1)	18(1)	-1(1)	1(1)	-3(1)
P(2)	14(1)	14(1)	18(1)	-2(1)	-3(1)	-2(1)
P(3)	16(1)	16(1)	16(1)	-1(1)	0(1)	-4(1)
P(4)	15(1)	16(1)	17(1)	-1(1)	-1(1)	-2(1)
P(5)	15(1)	18(1)	17(1)	-2(1)	-1(1)	-3(1)
P(6)	15(1)	16(1)	17(1)	1(1)	-3(1)	-4(1)
C(1)	17(2)	12(1)	18(2)	1(1)	-2(1)	-1(1)
C(2)	19(2)	23(2)	24(2)	-1(1)	0(1)	-6(1)
C(3)	24(2)	21(2)	33(2)	-2(1)	-3(2)	-11(1)
C(4)	30(2)	18(2)	27(2)	-6(1)	-6(2)	-5(1)
C(5)	20(2)	19(2)	17(2)	-4(1)	1(1)	-2(1)
C(6)	17(2)	12(1)	21(2)	2(1)	-5(1)	-1(1)
C(7)	14(2)	17(2)	16(2)	-3(1)	-2(1)	-2(1)
C(8)	14(2)	16(2)	15(1)	-6(1)	-2(1)	-1(1)
C(9)	25(2)	16(2)	20(2)	1(1)	-1(1)	-4(1)
C(10)	22(2)	20(2)	28(2)	-3(1)	-5(1)	4(1)
C(11)	11(2)	23(2)	31(2)	-4(1)	-1(1)	-1(1)
C(12)	21(2)	20(2)	21(2)	-1(1)	1(1)	-8(1)
C(13)	18(2)	16(2)	17(2)	0(1)	-3(1)	-1(1)
C(14)	16(2)	17(2)	15(2)	3(1)	2(1)	-2(1)
C(15)	24(2)	20(2)	19(2)	-3(1)	-3(1)	-4(1)
C(16)	24(2)	23(2)	20(2)	-3(1)	0(1)	3(1)
C(17)	12(2)	34(2)	31(2)	-6(2)	3(1)	3(1)
C(18)	18(2)	30(2)	21(2)	-3(1)	-2(1)	-6(1)
C(19)	14(2)	14(1)	14(1)	-2(1)	4(1)	-2(1)
C(20)	14(2)	16(2)	14(1)	-4(1)	4(1)	-2(1)
C(21)	18(2)	22(2)	17(2)	-3(1)	-2(1)	1(1)
C(22)	28(2)	15(2)	24(2)	1(1)	0(1)	-2(1)
C(23)	25(2)	20(2)	23(2)	-2(1)	1(1)	-9(1)

C(24)	15(2)	22(2)	18(2)	-3(1)	0(1)	-4(1)
C(25)	24(2)	18(2)	16(2)	0(1)	-3(1)	-3(1)
C(26)	25(2)	23(2)	24(2)	2(1)	-3(1)	-1(1)
C(27)	36(2)	22(2)	28(2)	5(1)	-4(2)	1(2)
C(28)	20(2)	20(2)	20(2)	-1(1)	2(1)	-8(1)
C(29)	23(2)	25(2)	20(2)	-1(1)	5(1)	-4(1)
C(30)	22(2)	43(2)	27(2)	-7(2)	3(2)	-5(2)
C(31)	17(2)	18(2)	23(2)	-1(1)	6(1)	-3(1)
C(32)	25(2)	34(2)	36(2)	-5(2)	-3(2)	-12(2)
C(33)	29(2)	22(2)	46(2)	6(2)	3(2)	-8(2)
C(34)	23(2)	25(2)	19(2)	-3(1)	-6(1)	-1(1)
C(35)	36(2)	39(2)	16(2)	-4(1)	2(2)	-10(2)
C(36)	27(2)	37(2)	26(2)	-8(2)	-2(1)	-9(2)
C(37)	14(2)	22(2)	24(2)	-2(1)	-3(1)	-5(1)
C(38)	27(2)	31(2)	34(2)	2(2)	-4(2)	-15(2)
C(39)	27(2)	26(2)	36(2)	-10(2)	-3(2)	-10(2)
C(40)	23(2)	23(2)	18(2)	2(1)	-1(1)	2(1)
C(41)	32(2)	25(2)	30(2)	4(1)	-11(2)	-7(2)
C(42)	21(2)	34(2)	47(2)	17(2)	-8(2)	-7(2)
C(43)	16(2)	22(2)	21(2)	2(1)	-3(1)	-6(1)
C(44)	18(2)	39(2)	34(2)	2(2)	-1(2)	0(2)
C(45)	21(2)	26(2)	37(2)	8(2)	-10(2)	-1(1)
C(46)	21(2)	17(2)	15(2)	1(1)	0(1)	-5(1)
C(47)	30(2)	36(2)	24(2)	-6(1)	0(1)	-9(2)
C(48)	24(2)	22(2)	19(2)	-3(1)	5(1)	-2(1)
B	16(2)	18(2)	20(2)	-4(1)	-1(1)	-2(1)
C(49)	13(2)	18(2)	26(2)	-4(1)	-8(1)	5(1)
C(50)	24(2)	25(2)	32(2)	-7(1)	-10(2)	3(1)
C(51)	34(2)	31(2)	39(2)	-20(2)	-17(2)	9(2)
C(52)	33(2)	21(2)	65(3)	-11(2)	-24(2)	2(2)
C(53)	23(2)	19(2)	54(2)	-2(2)	-13(2)	-3(1)
C(54)	19(2)	22(2)	32(2)	-5(1)	-6(1)	0(1)
C(55)	21(2)	9(1)	24(2)	-3(1)	-5(1)	-3(1)
C(56)	27(2)	21(2)	24(2)	-2(1)	-3(1)	-4(1)
C(57)	45(2)	21(2)	34(2)	0(2)	-21(2)	-3(2)
C(58)	27(2)	17(2)	56(2)	-12(2)	-22(2)	8(1)

C(59)	19(2)	23(2)	37(2)	-13(2)	0(2)	-4(1)
C(60)	23(2)	14(2)	22(2)	-3(1)	-2(1)	-6(1)
C(61)	9(1)	19(2)	19(2)	1(1)	3(1)	-6(1)
C(62)	17(2)	17(2)	22(2)	-1(1)	-1(1)	-3(1)
C(63)	22(2)	23(2)	19(2)	-4(1)	3(1)	-8(1)
C(64)	24(2)	33(2)	16(2)	0(1)	-4(1)	-11(2)
C(65)	21(2)	23(2)	25(2)	6(1)	-3(1)	-4(1)
C(66)	18(2)	20(2)	20(2)	-3(1)	2(1)	-4(1)
C(67)	21(2)	28(2)	11(1)	-2(1)	-2(1)	-5(1)
C(68)	20(2)	32(2)	17(2)	-3(1)	-3(1)	-2(1)
C(69)	19(2)	55(2)	19(2)	-12(2)	-2(1)	2(2)
C(70)	26(2)	69(3)	15(2)	-4(2)	3(1)	-23(2)
C(71)	42(2)	42(2)	19(2)	-3(2)	-1(2)	-23(2)
C(72)	23(2)	35(2)	19(2)	-7(1)	0(1)	-8(2)
N(1)	43(2)	27(2)	32(2)	-3(1)	-14(1)	-1(1)
N(2)	38(2)	48(2)	36(2)	-3(2)	-7(1)	-17(2)
N(3)	44(2)	76(2)	51(2)	11(2)	-19(2)	-26(2)
C(73)	27(2)	15(2)	28(2)	1(1)	0(2)	-5(1)
C(74)	31(2)	36(2)	27(2)	0(2)	-7(2)	-9(2)
C(75)	17(2)	28(2)	26(2)	7(1)	-4(1)	-7(1)
C(76)	27(2)	28(2)	41(2)	-3(2)	-9(2)	-4(2)
C(77)	33(2)	33(2)	23(2)	3(1)	-5(2)	-13(2)
C(78)	33(2)	67(3)	47(2)	15(2)	-11(2)	-12(2)

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $\{(PPP)Cu\}_2BPh_4$.

	x	y	z	U(eq)
H(2)	3756	-239	3043	26
H(3)	3806	-1120	2242	30
H(4)	5193	-1094	1245	29
H(5)	6411	-124	1007	23
H(9)	8532	-126	1757	25
H(10)	10509	-431	1214	29
H(11)	11264	471	357	26
H(12)	10028	1643	21	25
H(15)	3496	4506	2693	25
H(16)	1398	4921	2777	28
H(17)	256	4348	2158	32
H(18)	1212	3417	1414	27
H(21)	5282	4930	1568	23
H(22)	6544	5793	1716	28
H(23)	8062	5386	2418	27
H(24)	8295	4113	2994	22
H(25)	6456	753	3977	23
H(26A)	8041	-170	3521	37
H(26B)	7740	525	2930	37
H(26C)	7283	-298	2942	37
H(27A)	5532	-618	3796	45
H(27B)	5056	-74	4408	45
H(27C)	6399	-586	4352	45
H(28)	3514	598	3870	24
H(29A)	3904	2119	4134	36
H(29B)	4452	1300	4534	36
H(29C)	3014	1603	4615	36
H(30A)	1891	1669	3628	47
H(30B)	2522	1243	2964	47
H(30C)	2837	2075	3082	47

H(31)	9122	2921	-173	24
H(32A)	9409	3707	665	46
H(32B)	9455	2800	963	46
H(32C)	8261	3439	1147	46
H(33A)	7108	4142	198	50
H(33B)	7298	3770	-513	50
H(33C)	8275	4252	-346	50
H(34)	6382	2475	-544	27
H(35A)	8870	1814	-922	45
H(35B)	8248	2707	-1125	45
H(35C)	7862	1994	-1429	45
H(36A)	6473	1176	-729	44
H(36B)	6196	1223	76	44
H(36C)	7537	875	-264	44
H(37)	2009	2381	714	24
H(38A)	2088	1170	1423	44
H(38B)	2207	1869	1850	44
H(38C)	3389	1250	1603	44
H(39A)	4125	1233	352	43
H(39B)	3614	1950	-175	43
H(39C)	2813	1284	124	43
H(40)	4083	3204	-258	27
H(41A)	1967	4196	341	43
H(41B)	1915	3426	-14	43
H(41C)	2407	4164	-458	43
H(42A)	4440	4473	-274	52
H(42B)	5165	3940	299	52
H(42C)	3908	4509	514	52
H(43)	8896	2872	3409	24
H(44A)	10291	2123	2617	48
H(44B)	9377	2791	2231	48
H(44C)	9181	1890	2322	48
H(45A)	8584	1250	3515	43
H(45B)	8256	1784	4139	43
H(45C)	9640	1554	3804	43
H(46)	6055	2450	4178	22

H(47A)	6997	3878	4120	44
H(47B)	7624	3028	4434	44
H(47C)	6344	3451	4796	44
H(48A)	4428	3474	4287	34
H(48B)	4544	3232	3529	34
H(48C)	5022	4007	3658	34
H(50)	502	2012	5537	32
H(51)	3	877	5230	40
H(52)	-842	-9	6050	46
H(53)	-1180	245	7185	38
H(54)	-706	1392	7495	29
H(56)	-619	3701	5651	29
H(57)	-2482	4436	5434	39
H(58)	-4149	4510	6292	39
H(59)	-3902	3852	7369	31
H(60)	-2032	3101	7580	23
H(62)	-181	3782	7735	22
H(63)	524	3759	8773	25
H(64)	1584	2585	9266	29
H(65)	1969	1449	8693	28
H(66)	1347	1484	7638	24
H(68)	2394	1961	6072	28
H(69)	4156	2411	5565	38
H(70)	4268	3751	5522	42
H(71)	2577	4641	5944	39
H(72)	798	4181	6432	30
H(74A)	7029	7038	2453	46
H(74B)	5807	6841	2906	46
H(74C)	6004	7740	2732	46
H(76A)	3897	7811	3555	47
H(76B)	2467	8146	3641	47
H(76C)	2997	7374	4107	47
H(78A)	2059	3256	4275	75
H(78B)	1541	3813	4874	75
H(78C)	2109	4182	4147	75

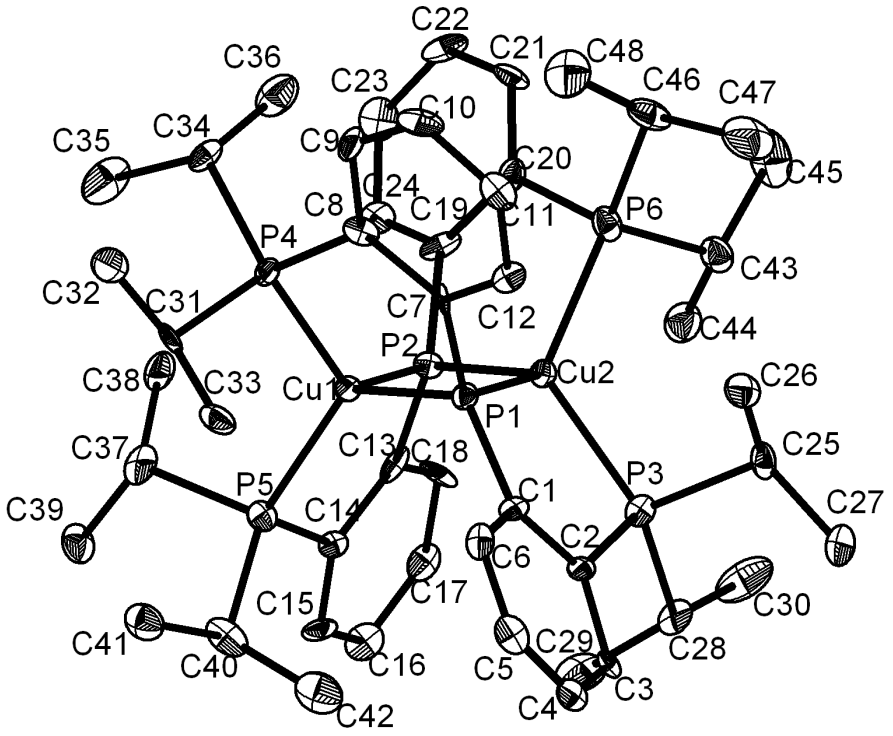

Figure S9. Molecular structure of $[\{(PPP)Cu\}_2]^{2+}$, fully numbered. Hydrogen atoms omitted for clarity.

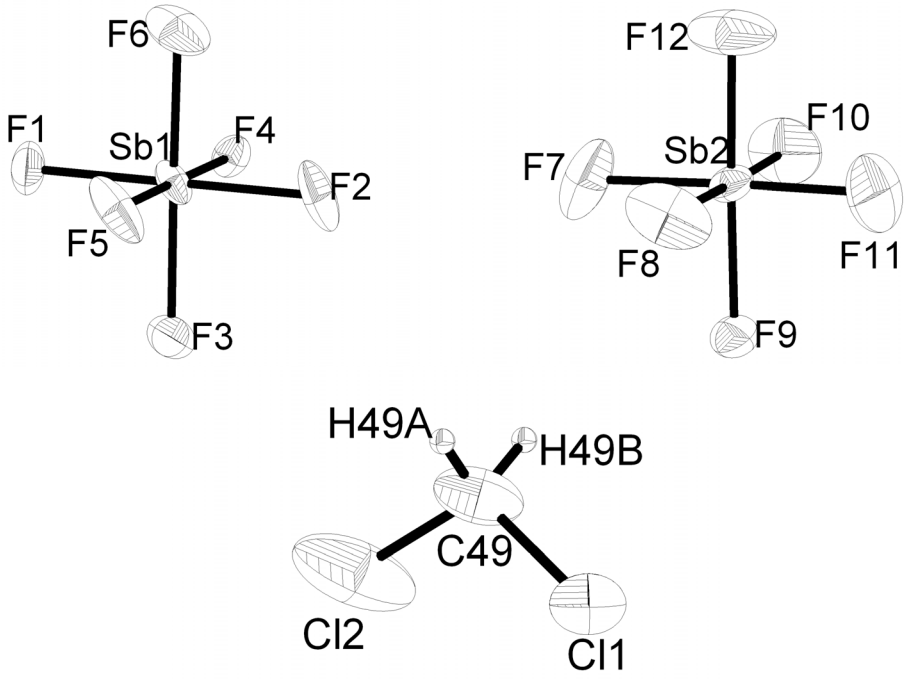

Figure S10. Anions and a CH_2Cl_2 molecule from the crystal structure of $[\{(PPP)Cu)\}_2][SbF_6]_2$.

Table 13. Crystal data and structure refinement for [{(PPP)Cu}$_2$][SbF$_6$]$_2$.

Identification code	[{(PPP)Cu}$_2$][SbF$_6$]$_2$	
Empirical formula	$C_{49}H_{74}Cl_2Cu_2F_{12}P_6Sb_2$	
Formula weight	1518.38	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.8917(16) Å	α= 90°
	b = 12.1007(17) Å	β= 91.634(3) °
	c = 42.690(6) Å	γ = 90°
Volume	6140.5(15) Å^3	
Z	5	
Density (calculated)	2.053 Mg/m^3	
Absorption coefficient	2.332 mm^{-1}	
F(000)	3800	
Crystal size	0.148 x 0.056 x 0.056 mm^3	
Theta range for data collection	1.75 to 25.03°	
Index ranges	$-14 \le h \le 13$, $-14 \le k \le 14$, $-49 \le l \le 50$	
Reflections collected	41692	
Independent reflections	9807 [R(int) = 0.1547]	
Completeness to theta = 25.03∞	90.3 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9807 / 0 / 675	
Goodness-of-fit on F^2	0.958	
Final R indices [I>2sigma(I)]	R1 = 0.0550, wR2 = 0.1087	
R indices (all data)	R1 = 0.1388, wR2 = 0.1381	
Largest diff. peak and hole	0.917 and -1.016 e.Å^{-3}	

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for [{(PPP)Cu}$_2$][SbF_6]$_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	2762(1)	8773(1)	3763(1)	11(1)
Cu(2)	1329(1)	7351(1)	3532(1)	12(1)
P(1)	881(2)	8902(2)	3786(1)	12(1)
P(2)	3192(2)	7199(2)	3508(1)	13(1)
P(3)	120(2)	7946(2)	3144(1)	15(1)
P(4)	2779(2)	9113(2)	4291(1)	14(1)
P(5)	3979(2)	9614(2)	3434(1)	15(1)
P(6)	1348(2)	5594(2)	3731(1)	18(1)
C(1)	-58(7)	9746(8)	3546(2)	12(2)
C(2)	-235(7)	9376(8)	3234(2)	14(2)
C(3)	-804(7)	10079(7)	3023(2)	14(2)
C(4)	-1195(7)	11085(8)	3129(2)	19(2)
C(5)	-1068(7)	11403(8)	3430(2)	18(2)
C(6)	-482(7)	10755(8)	3643(2)	16(2)
C(7)	460(7)	8968(7)	4182(2)	10(2)
C(8)	1339(7)	8879(7)	4417(2)	13(2)
C(9)	1056(8)	8731(7)	4727(2)	19(2)
C(10)	-78(8)	8674(8)	4812(2)	24(2)
C(11)	-926(8)	8791(7)	4582(2)	18(2)
C(12)	-659(7)	8940(7)	4277(2)	15(2)
C(13)	4031(7)	7521(8)	3178(2)	13(2)
C(14)	4210(7)	8649(7)	3112(2)	12(2)
C(15)	4697(7)	8924(8)	2834(2)	17(2)
C(16)	4995(7)	8149(8)	2615(2)	18(2)
C(17)	4838(7)	7028(8)	2682(2)	19(2)
C(18)	4354(7)	6720(8)	2963(2)	18(2)
C(19)	3652(7)	5926(8)	3687(2)	16(2)
C(20)	2814(7)	5282(7)	3833(2)	16(2)
C(21)	3159(8)	4400(7)	4020(2)	19(2)
C(22)	4292(8)	4126(8)	4054(2)	21(2)
C(23)	5105(8)	4723(8)	3898(2)	23(2)

C(24)	4772(8)	5620(8)	3715(2)	18(2)
C(25)	-1243(7)	7210(8)	3196(2)	18(2)
C(26)	-1681(7)	7440(8)	3524(2)	22(2)
C(27)	-2144(8)	7488(8)	2940(2)	28(3)
C(28)	369(8)	7917(7)	2721(2)	20(2)
C(29)	1403(8)	8594(9)	2640(2)	34(3)
C(30)	448(9)	6716(9)	2604(2)	41(3)
C(31)	2958(8)	10630(7)	4359(2)	19(2)
C(32)	3011(9)	10938(9)	4711(2)	34(3)
C(33)	2022(8)	11307(7)	4204(2)	20(2)
C(34)	3715(7)	8415(8)	4578(2)	17(2)
C(35)	4936(8)	8817(10)	4552(2)	39(3)
C(36)	3642(8)	7178(8)	4544(2)	31(3)
C(37)	5400(7)	9672(8)	3627(2)	22(2)
C(38)	5774(7)	8534(8)	3740(2)	23(2)
C(39)	6287(7)	10199(8)	3424(2)	23(2)
C(40)	3772(8)	10982(8)	3265(2)	22(2)
C(41)	3883(8)	11878(8)	3517(2)	24(2)
C(42)	2655(8)	11076(8)	3084(2)	31(3)
C(43)	1035(8)	4611(8)	3402(2)	21(2)
C(44)	1917(8)	4701(8)	3147(2)	28(3)
C(45)	970(9)	3382(8)	3510(3)	39(3)
C(46)	531(8)	5090(8)	4057(2)	24(2)
C(47)	-752(8)	5046(10)	3971(3)	42(3)
C(48)	737(9)	5738(9)	4353(2)	34(3)
Sb(1)	8231(1)	8975(1)	1940(1)	23(1)
F(1)	6654(4)	8888(5)	1927(1)	36(2)
F(2)	9814(5)	9050(5)	1959(2)	46(2)
F(3)	8298(5)	8149(5)	1571(1)	34(2)
F(4)	8152(4)	10285(4)	1712(1)	23(1)
F(5)	8322(5)	7655(5)	2168(1)	47(2)
F(6)	8198(6)	9770(5)	2310(1)	53(2)
Sb(2)	7188(1)	1842(1)	4390(1)	26(1)
F(7)	7348(5)	794(6)	4080(1)	66(2)
F(8)	5637(5)	1827(6)	4299(2)	64(2)
F(9)	7011(5)	695(5)	4674(1)	39(2)

F(10)	8746(5)	1795(6)	4462(2)	67(2)
F(11)	7033(8)	2838(6)	4705(2)	88(3)
F(12)	7348(6)	3014(7)	4117(2)	90(3)
C(49)	3525(12)	4584(11)	5298(3)	61(5)
Cl(1)	3651(4)	4206(3)	4903(1)	75(2)
Cl(2)	2890(4)	3559(4)	5520(1)	104(2)

Table 15. Bond lengths [Å] and angles [°] for [{(PPP)Cu}$_2$][SbF$_6$]$_2$.

Cu(1)-P(1)	2.247(3)
Cu(1)-P(2)	2.259(3)
Cu(1)-P(5)	2.283(3)
Cu(1)-P(4)	2.291(2)
Cu(1)-Cu(2)	2.5963(15)
Cu(2)-P(2)	2.229(3)
Cu(2)-P(1)	2.239(3)
Cu(2)-P(3)	2.278(3)
Cu(2)-P(6)	2.290(3)
P(1)-C(7)	1.779(8)
P(1)-C(1)	1.810(9)
P(2)-C(13)	1.793(9)
P(2)-C(19)	1.799(9)
P(3)-C(2)	1.825(10)
P(3)-C(28)	1.837(9)
P(3)-C(25)	1.869(9)
P(4)-C(8)	1.831(9)
P(4)-C(34)	1.838(8)
P(4)-C(31)	1.870(9)
P(5)-C(40)	1.820(10)
P(5)-C(14)	1.832(9)
P(5)-C(37)	1.860(9)
P(6)-C(46)	1.824(9)
P(6)-C(20)	1.824(9)
P(6)-C(43)	1.870(9)
C(1)-C(6)	1.388(12)
C(1)-C(2)	1.412(11)
C(2)-C(3)	1.400(11)
C(3)-C(4)	1.384(12)
C(3)-H(3)	0.9500
C(4)-C(5)	1.346(12)
C(4)-H(4)	0.9500
C(5)-C(6)	1.374(12)
C(5)-H(5)	0.9500

C(6)-H(6)	0.9500
C(7)-C(12)	1.404(11)
C(7)-C(8)	1.432(11)
C(8)-C(9)	1.387(12)
C(9)-C(10)	1.408(12)
C(9)-H(9)	0.9500
C(10)-C(11)	1.395(12)
C(10)-H(10)	0.9500
C(11)-C(12)	1.360(11)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(18)	1.396(12)
C(13)-C(14)	1.411(12)
C(14)-C(15)	1.376(12)
C(15)-C(16)	1.377(12)
C(15)-H(15)	0.9500
C(16)-C(17)	1.399(13)
C(16)-H(16)	0.9500
C(17)-C(18)	1.395(12)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(24)	1.384(12)
C(19)-C(20)	1.421(12)
C(20)-C(21)	1.387(12)
C(21)-C(22)	1.391(12)
C(21)-H(21)	0.9500
C(22)-C(23)	1.391(13)
C(22)-H(22)	0.9500
C(23)-C(24)	1.389(12)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-C(26)	1.535(12)
C(25)-C(27)	1.544(12)
C(25)-H(25)	1.0000
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800

C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(29)	1.526(13)
C(28)-C(30)	1.540(13)
C(28)-H(28)	1.0000
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(33)	1.520(12)
C(31)-C(32)	1.544(12)
C(31)-H(31)	1.0000
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(36)	1.506(13)
C(34)-C(35)	1.539(12)
C(34)-H(34)	1.0000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(38)	1.521(12)
C(37)-C(39)	1.523(12)
C(37)-H(37)	1.0000
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800

C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-C(42)	1.521(13)
C(40)-C(41)	1.531(12)
C(40)-H(40)	1.0000
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-C(44)	1.537(12)
C(43)-C(45)	1.558(13)
C(43)-H(43)	1.0000
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-C(48)	1.500(13)
C(46)-C(47)	1.560(13)
C(46)-H(46)	1.0000
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
Sb(1)-F(6)	1.850(6)
Sb(1)-F(4)	1.862(5)
Sb(1)-F(3)	1.870(5)
Sb(1)-F(5)	1.873(6)
Sb(1)-F(1)	1.878(5)

Sb(1)-F(2)	1.884(5)
Sb(2)-F(11)	1.821(7)
Sb(2)-F(7)	1.846(7)
Sb(2)-F(12)	1.848(7)
Sb(2)-F(9)	1.859(5)
Sb(2)-F(10)	1.870(6)
Sb(2)-F(8)	1.874(6)
C(49)-Cl(2)	1.744(14)
C(49)-Cl(1)	1.759(14)
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900

P(1)-Cu(1)-P(2)	108.59(10)
P(1)-Cu(1)-P(5)	130.17(10)
P(2)-Cu(1)-P(5)	85.61(9)
P(1)-Cu(1)-P(4)	85.73(9)
P(2)-Cu(1)-P(4)	129.01(10)
P(5)-Cu(1)-P(4)	122.45(10)
P(1)-Cu(1)-Cu(2)	54.48(7)
P(2)-Cu(1)-Cu(2)	54.10(7)
P(5)-Cu(1)-Cu(2)	118.87(8)
P(4)-Cu(1)-Cu(2)	118.67(8)
P(2)-Cu(2)-P(1)	109.99(10)
P(2)-Cu(2)-P(3)	126.85(10)
P(1)-Cu(2)-P(3)	86.17(9)
P(2)-Cu(2)-P(6)	86.61(9)
P(1)-Cu(2)-P(6)	126.77(10)
P(3)-Cu(2)-P(6)	124.26(10)
P(2)-Cu(2)-Cu(1)	55.20(7)
P(1)-Cu(2)-Cu(1)	54.79(7)
P(3)-Cu(2)-Cu(1)	117.40(8)
P(6)-Cu(2)-Cu(1)	118.34(8)
C(7)-P(1)-C(1)	109.1(4)
C(7)-P(1)-Cu(2)	125.1(3)
C(1)-P(1)-Cu(2)	110.5(3)
C(7)-P(1)-Cu(1)	110.6(3)

C(1)-P(1)-Cu(1)	127.8(3)
Cu(2)-P(1)-Cu(1)	70.73(8)
C(13)-P(2)-C(19)	110.6(4)
C(13)-P(2)-Cu(2)	126.5(3)
C(19)-P(2)-Cu(2)	110.0(3)
C(13)-P(2)-Cu(1)	109.5(3)
C(19)-P(2)-Cu(1)	125.9(3)
Cu(2)-P(2)-Cu(1)	70.69(8)
C(2)-P(3)-C(28)	105.7(4)
C(2)-P(3)-C(25)	102.7(4)
C(28)-P(3)-C(25)	105.8(4)
C(2)-P(3)-Cu(2)	106.9(3)
C(28)-P(3)-Cu(2)	126.3(3)
C(25)-P(3)-Cu(2)	107.1(3)
C(8)-P(4)-C(34)	106.7(4)
C(8)-P(4)-C(31)	102.1(4)
C(34)-P(4)-C(31)	106.4(4)
C(8)-P(4)-Cu(1)	106.2(3)
C(34)-P(4)-Cu(1)	124.2(3)
C(31)-P(4)-Cu(1)	109.1(3)
C(40)-P(5)-C(14)	107.6(4)
C(40)-P(5)-C(37)	104.6(5)
C(14)-P(5)-C(37)	101.7(4)
C(40)-P(5)-Cu(1)	124.6(3)
C(14)-P(5)-Cu(1)	106.8(3)
C(37)-P(5)-Cu(1)	109.2(3)
C(46)-P(6)-C(20)	106.0(4)
C(46)-P(6)-C(43)	105.1(4)
C(20)-P(6)-C(43)	102.5(4)
C(46)-P(6)-Cu(2)	126.4(3)
C(20)-P(6)-Cu(2)	106.3(3)
C(43)-P(6)-Cu(2)	108.2(3)
C(6)-C(1)-C(2)	120.9(8)
C(6)-C(1)-P(1)	123.4(7)
C(2)-C(1)-P(1)	115.2(7)
C(3)-C(2)-C(1)	118.0(8)

C(3)-C(2)-P(3)	123.4(7)
C(1)-C(2)-P(3)	118.1(7)
C(4)-C(3)-C(2)	119.0(8)
C(4)-C(3)-H(3)	120.5
C(2)-C(3)-H(3)	120.5
C(5)-C(4)-C(3)	122.3(9)
C(5)-C(4)-H(4)	118.9
C(3)-C(4)-H(4)	118.9
C(4)-C(5)-C(6)	120.6(9)
C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7
C(5)-C(6)-C(1)	119.1(8)
C(5)-C(6)-H(6)	120.5
C(1)-C(6)-H(6)	120.5
C(12)-C(7)-C(8)	118.3(7)
C(12)-C(7)-P(1)	124.7(6)
C(8)-C(7)-P(1)	116.3(6)
C(9)-C(8)-C(7)	119.1(8)
C(9)-C(8)-P(4)	123.7(7)
C(7)-C(8)-P(4)	116.9(6)
C(8)-C(9)-C(10)	120.9(8)
C(8)-C(9)-H(9)	119.5
C(10)-C(9)-H(9)	119.5
C(11)-C(10)-C(9)	119.4(8)
C(11)-C(10)-H(10)	120.3
C(9)-C(10)-H(10)	120.3
C(12)-C(11)-C(10)	120.3(9)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(11)-C(12)-C(7)	122.0(8)
C(11)-C(12)-H(12)	119.0
C(7)-C(12)-H(12)	119.0
C(18)-C(13)-C(14)	119.6(8)
C(18)-C(13)-P(2)	122.4(7)
C(14)-C(13)-P(2)	117.2(6)
C(15)-C(14)-C(13)	118.4(8)

C(15)-C(14)-P(5)	124.8(7)
C(13)-C(14)-P(5)	116.1(6)
C(14)-C(15)-C(16)	122.9(9)
C(14)-C(15)-H(15)	118.6
C(16)-C(15)-H(15)	118.6
C(15)-C(16)-C(17)	119.0(9)
C(15)-C(16)-H(16)	120.5
C(17)-C(16)-H(16)	120.5
C(18)-C(17)-C(16)	119.6(9)
C(18)-C(17)-H(17)	120.2
C(16)-C(17)-H(17)	120.2
C(17)-C(18)-C(13)	120.5(9)
C(17)-C(18)-H(18)	119.8
C(13)-C(18)-H(18)	119.8
C(24)-C(19)-C(20)	120.0(8)
C(24)-C(19)-P(2)	123.1(7)
C(20)-C(19)-P(2)	116.6(6)
C(21)-C(20)-C(19)	118.3(8)
C(21)-C(20)-P(6)	124.1(7)
C(19)-C(20)-P(6)	117.3(7)
C(20)-C(21)-C(22)	121.0(9)
C(20)-C(21)-H(21)	119.5
C(22)-C(21)-H(21)	119.5
C(23)-C(22)-C(21)	120.6(9)
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(24)-C(23)-C(22)	119.0(9)
C(24)-C(23)-H(23)	120.5
C(22)-C(23)-H(23)	120.5
C(19)-C(24)-C(23)	121.0(9)
C(19)-C(24)-H(24)	119.5
C(23)-C(24)-H(24)	119.5
C(26)-C(25)-C(27)	111.1(7)
C(26)-C(25)-P(3)	109.9(6)
C(27)-C(25)-P(3)	113.5(7)
C(26)-C(25)-H(25)	107.4

C(27)-C(25)-H(25)	107.3
P(3)-C(25)-H(25)	107.4
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(29)-C(28)-C(30)	112.2(8)
C(29)-C(28)-P(3)	111.4(6)
C(30)-C(28)-P(3)	110.4(6)
C(29)-C(28)-H(28)	107.5
C(30)-C(28)-H(28)	107.5
P(3)-C(28)-H(28)	107.5
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(33)-C(31)-C(32)	107.7(8)
C(33)-C(31)-P(4)	112.5(6)
C(32)-C(31)-P(4)	113.0(6)
C(33)-C(31)-H(31)	107.8

C(32)-C(31)-H(31)	107.8
P(4)-C(31)-H(31)	107.8
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(36)-C(34)-C(35)	111.0(8)
C(36)-C(34)-P(4)	111.0(6)
C(35)-C(34)-P(4)	111.1(6)
C(36)-C(34)-H(34)	107.8
C(35)-C(34)-H(34)	107.8
P(4)-C(34)-H(34)	107.8
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-C(39)	111.0(8)
C(38)-C(37)-P(5)	111.1(6)
C(39)-C(37)-P(5)	113.5(6)
C(38)-C(37)-H(37)	107.0

C(39)-C(37)-H(37)	107.0
P(5)-C(37)-H(37)	107.0
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(42)-C(40)-C(41)	111.1(8)
C(42)-C(40)-P(5)	112.1(7)
C(41)-C(40)-P(5)	110.9(6)
C(42)-C(40)-H(40)	107.5
C(41)-C(40)-H(40)	107.5
P(5)-C(40)-H(40)	107.5
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(44)-C(43)-C(45)	108.5(8)
C(44)-C(43)-P(6)	111.2(6)
C(45)-C(43)-P(6)	113.3(7)
C(44)-C(43)-H(43)	107.9

C(45)-C(43)-H(43)	107.9
P(6)-C(43)-H(43)	107.9
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(43)-C(45)-H(45A)	109.5
C(43)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(43)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(48)-C(46)-C(47)	110.4(8)
C(48)-C(46)-P(6)	112.9(7)
C(47)-C(46)-P(6)	111.8(7)
C(48)-C(46)-H(46)	107.1
C(47)-C(46)-H(46)	107.1
P(6)-C(46)-H(46)	107.1
C(46)-C(47)-H(47A)	109.5
C(46)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(46)-C(48)-H(48A)	109.5
C(46)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(46)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
F(6)-Sb(1)-F(4)	90.2(2)
F(6)-Sb(1)-F(3)	178.4(3)
F(4)-Sb(1)-F(3)	90.9(2)
F(6)-Sb(1)-F(5)	90.1(3)

F(4)-Sb(1)-F(5)	179.5(3)
F(3)-Sb(1)-F(5)	88.8(3)
F(6)-Sb(1)-F(1)	90.5(3)
F(4)-Sb(1)-F(1)	89.9(2)
F(3)-Sb(1)-F(1)	90.7(2)
F(5)-Sb(1)-F(1)	90.6(3)
F(6)-Sb(1)-F(2)	89.0(3)
F(4)-Sb(1)-F(2)	91.0(2)
F(3)-Sb(1)-F(2)	89.8(3)
F(5)-Sb(1)-F(2)	88.6(3)
F(1)-Sb(1)-F(2)	179.1(3)
F(11)-Sb(2)-F(7)	178.0(3)
F(11)-Sb(2)-F(12)	88.4(4)
F(7)-Sb(2)-F(12)	93.5(4)
F(11)-Sb(2)-F(9)	89.7(3)
F(7)-Sb(2)-F(9)	88.3(3)
F(12)-Sb(2)-F(9)	178.1(4)
F(11)-Sb(2)-F(10)	91.1(4)
F(7)-Sb(2)-F(10)	88.6(3)
F(12)-Sb(2)-F(10)	90.5(3)
F(9)-Sb(2)-F(10)	90.0(3)
F(11)-Sb(2)-F(8)	92.2(4)
F(7)-Sb(2)-F(8)	88.1(3)
F(12)-Sb(2)-F(8)	89.8(3)
F(9)-Sb(2)-F(8)	89.9(3)
F(10)-Sb(2)-F(8)	176.7(3)
Cl(2)-C(49)-Cl(1)	112.7(8)
Cl(2)-C(49)-H(49A)	109.1
Cl(1)-C(49)-H(49A)	109.1
Cl(2)-C(49)-H(49B)	109.1
Cl(1)-C(49)-H(49B)	109.1
H(49A)-C(49)-H(49B)	107.8

Symmetry transformations used to generate equivalent atoms:

Table 16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[\{(PPP)Cu\}_2][SbF_6]_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	9(1)	14(1)	11(1)	0(1)	1(1)	0(1)
Cu(2)	11(1)	13(1)	13(1)	-1(1)	0(1)	1(1)
P(1)	12(1)	15(2)	10(1)	-1(1)	1(1)	-1(1)
P(2)	13(1)	13(1)	13(1)	1(1)	2(1)	1(1)
P(3)	13(1)	18(2)	14(1)	-2(1)	1(1)	2(1)
P(4)	13(1)	19(2)	9(1)	0(1)	-2(1)	-3(1)
P(5)	14(1)	15(2)	15(1)	-1(1)	3(1)	0(1)
P(6)	12(1)	16(2)	26(2)	1(1)	1(1)	-1(1)
C(1)	7(5)	22(6)	8(5)	4(4)	4(4)	0(4)
C(2)	10(5)	22(6)	11(5)	6(4)	2(4)	-4(4)
C(3)	14(5)	13(6)	16(5)	3(4)	1(4)	-7(4)
C(4)	7(5)	18(6)	30(6)	8(5)	-2(4)	0(4)
C(5)	11(5)	15(6)	29(6)	-3(5)	7(4)	4(4)
C(6)	14(5)	24(6)	10(5)	-8(5)	6(4)	-4(5)
C(7)	5(5)	12(5)	12(5)	-5(4)	3(4)	-6(4)
C(8)	12(5)	11(5)	16(5)	0(4)	9(4)	7(4)
C(9)	22(6)	19(6)	16(5)	-3(5)	-9(4)	-3(5)
C(10)	34(7)	24(6)	14(5)	6(5)	14(5)	2(5)
C(11)	17(5)	15(6)	21(6)	-6(5)	12(4)	2(4)
C(12)	19(5)	14(6)	12(5)	-4(4)	0(4)	5(4)
C(13)	5(5)	26(7)	9(5)	-8(4)	-1(4)	7(4)
C(14)	11(5)	15(6)	11(5)	0(4)	2(4)	2(4)
C(15)	13(5)	23(6)	16(5)	11(5)	-3(4)	4(5)
C(16)	12(5)	26(6)	16(5)	-4(5)	7(4)	9(5)
C(17)	10(5)	30(7)	18(5)	-3(5)	1(4)	4(5)
C(18)	11(5)	9(6)	34(6)	14(5)	5(4)	4(4)
C(19)	17(6)	22(6)	10(5)	0(4)	1(4)	15(5)
C(20)	16(5)	12(6)	19(5)	-4(5)	-5(4)	2(4)
C(21)	15(6)	13(6)	29(6)	12(5)	2(4)	0(4)
C(22)	28(6)	20(6)	16(5)	3(5)	-3(5)	18(5)
C(23)	19(6)	21(6)	27(6)	-8(5)	5(5)	8(5)

C(24)	25(6)	20(6)	9(5)	-5(4)	5(4)	-1(5)
C(25)	16(5)	9(5)	28(6)	-4(5)	-5(4)	0(4)
C(26)	13(5)	26(6)	26(6)	6(5)	2(4)	0(5)
C(27)	20(6)	32(7)	32(6)	2(5)	-9(5)	-8(5)
C(28)	33(6)	13(6)	12(5)	-10(4)	-5(4)	3(5)
C(29)	31(7)	53(8)	17(6)	5(5)	10(5)	3(6)
C(30)	54(8)	52(8)	16(6)	-9(6)	-3(5)	19(6)
C(31)	29(6)	10(6)	18(5)	0(4)	-1(4)	-15(5)
C(32)	52(8)	29(7)	21(6)	3(5)	-7(5)	-18(6)
C(33)	31(6)	10(6)	19(5)	1(4)	4(5)	-4(5)
C(34)	8(5)	31(7)	11(5)	1(4)	0(4)	5(4)
C(35)	13(6)	79(10)	26(6)	7(6)	4(5)	2(6)
C(36)	32(7)	31(7)	30(6)	-2(5)	-10(5)	9(5)
C(37)	24(6)	33(7)	8(5)	-11(5)	3(4)	-4(5)
C(38)	13(5)	28(7)	27(6)	-1(5)	-6(4)	1(5)
C(39)	20(6)	31(7)	20(6)	-3(5)	7(4)	-9(5)
C(40)	26(6)	16(6)	24(5)	-4(5)	17(5)	0(5)
C(41)	33(6)	16(6)	24(6)	-2(5)	3(5)	-1(5)
C(42)	40(7)	18(6)	35(6)	-1(5)	6(5)	5(5)
C(43)	20(6)	14(6)	30(6)	2(5)	-2(5)	0(5)
C(44)	32(7)	23(7)	27(6)	-3(5)	-6(5)	-1(5)
C(45)	33(7)	18(7)	67(8)	-12(6)	0(6)	5(5)
C(46)	20(6)	25(6)	29(6)	11(5)	11(5)	1(5)
C(47)	25(7)	52(9)	51(7)	20(7)	12(5)	-2(6)
C(48)	36(7)	45(8)	22(6)	-9(5)	10(5)	-2(6)
Sb(1)	26(1)	25(1)	18(1)	6(1)	-9(1)	-10(1)
F(1)	20(3)	50(4)	38(3)	0(3)	5(3)	-10(3)
F(2)	25(4)	38(4)	73(5)	12(4)	-22(3)	-13(3)
F(3)	39(4)	31(4)	32(3)	-5(3)	0(3)	-6(3)
F(4)	21(3)	21(3)	27(3)	4(3)	4(2)	5(3)
F(5)	61(4)	37(4)	42(4)	18(3)	-27(3)	-27(3)
F(6)	88(5)	51(5)	17(3)	-1(3)	-3(3)	-28(4)
Sb(2)	26(1)	33(1)	20(1)	7(1)	-3(1)	-2(1)
F(7)	53(5)	109(7)	36(4)	-24(4)	2(3)	8(4)
F(8)	25(4)	52(5)	116(6)	25(5)	-10(4)	17(3)
F(9)	46(4)	42(4)	28(3)	9(3)	-9(3)	-11(3)

F(10)	35(4)	87(6)	77(5)	17(5)	-22(4)	-14(4)
F(11)	148(8)	38(5)	79(6)	-31(4)	15(5)	9(5)
F(12)	75(6)	112(7)	81(6)	67(5)	-47(5)	-55(5)
C(49)	56(10)	38(10)	90(12)	-19(9)	15(9)	3(8)
Cl(1)	105(4)	52(3)	67(3)	-7(2)	-16(2)	-14(2)
Cl(2)	107(4)	53(3)	155(5)	-28(3)	83(4)	-16(3)

Table 17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[\{(PPP)Cu\}_2][SbF_6]_2$.

	x	y	z	U(eq)
H(3)	-921	9868	2810	17
H(4)	-1565	11568	2984	22
H(5)	-1387	12081	3496	22
H(6)	-369	10994	3853	19
H(9)	1635	8668	4884	23
H(10)	-263	8556	5025	28
H(11)	-1692	8767	4639	21
H(12)	-1248	9027	4124	18
H(15)	4833	9682	2791	21
H(16)	5302	8371	2422	22
H(17)	5061	6480	2537	23
H(18)	4242	5960	3008	21
H(21)	2614	3977	4125	22
H(22)	4513	3527	4186	26
H(23)	5876	4520	3917	27
H(24)	5321	6029	3607	21
H(25)	-1088	6399	3182	21
H(26A)	-1921	8212	3538	33
H(26B)	-1080	7299	3681	33
H(26C)	-2321	6954	3563	33
H(27A)	-2830	7064	2978	43
H(27B)	-1860	7296	2734	43
H(27C)	-2315	8280	2946	43
H(28)	-297	8265	2612	24
H(29A)	2045	8362	2774	50
H(29B)	1251	9380	2675	50
H(29C)	1579	8476	2420	50
H(30A)	501	6712	2376	61
H(30B)	-225	6308	2664	61
H(30C)	1117	6364	2699	61

H(31)	3684	10859	4266	23
H(32A)	3007	11744	4732	51
H(32B)	3702	10639	4808	51
H(32C)	2357	10627	4814	51
H(33A)	1329	11216	4320	30
H(33B)	1896	11054	3987	30
H(33C)	2237	12089	4203	30
H(34)	3458	8610	4792	20
H(35A)	5393	8526	4728	59
H(35B)	4953	9627	4556	59
H(35C)	5241	8555	4354	59
H(36A)	3865	6966	4333	47
H(36B)	2867	6937	4576	47
H(36C)	4146	6826	4699	47
H(37)	5335	10147	3818	26
H(38A)	5912	8061	3559	34
H(38B)	5184	8205	3865	34
H(38C)	6468	8603	3868	34
H(39A)	7005	10235	3542	35
H(39B)	6048	10948	3365	35
H(39C)	6378	9754	3235	35
H(40)	4384	11105	3113	26
H(41A)	3718	12601	3423	37
H(41B)	4652	11878	3606	37
H(41C)	3351	11729	3683	37
H(42A)	2039	10905	3224	47
H(42B)	2643	10554	2909	47
H(42C)	2565	11830	3004	47
H(43)	288	4816	3306	26
H(44A)	2620	4354	3222	41
H(44B)	2054	5482	3101	41
H(44C)	1640	4325	2957	41
H(45A)	767	2914	3330	59
H(45B)	399	3308	3670	59
H(45C)	1703	3152	3598	59
H(46)	780	4314	4100	29

H(47A)	-1129	4555	4118	63
H(47B)	-862	4766	3757	63
H(47C)	-1072	5791	3985	63
H(48A)	510	6508	4318	51
H(48B)	1539	5710	4412	51
H(48C)	297	5419	4521	51
H(49A)	4283	4741	5390	73
H(49B)	3075	5270	5310	73