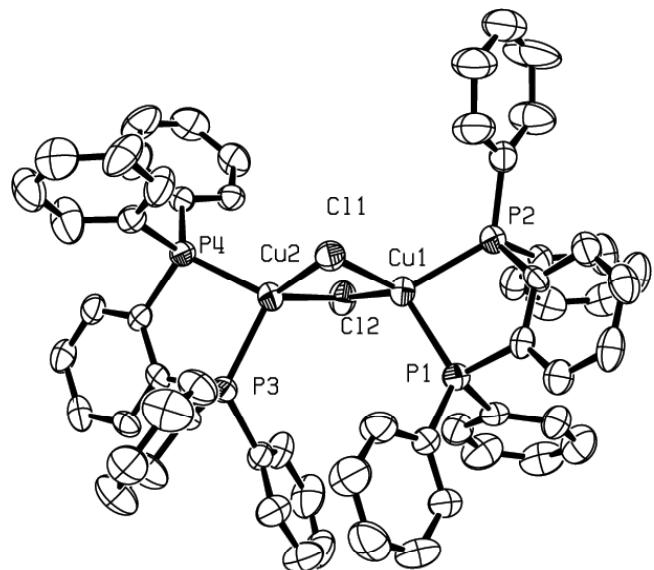


(A)



(B)

Figure S1. ORTEP diagram of (2) (A) and (3) (B).

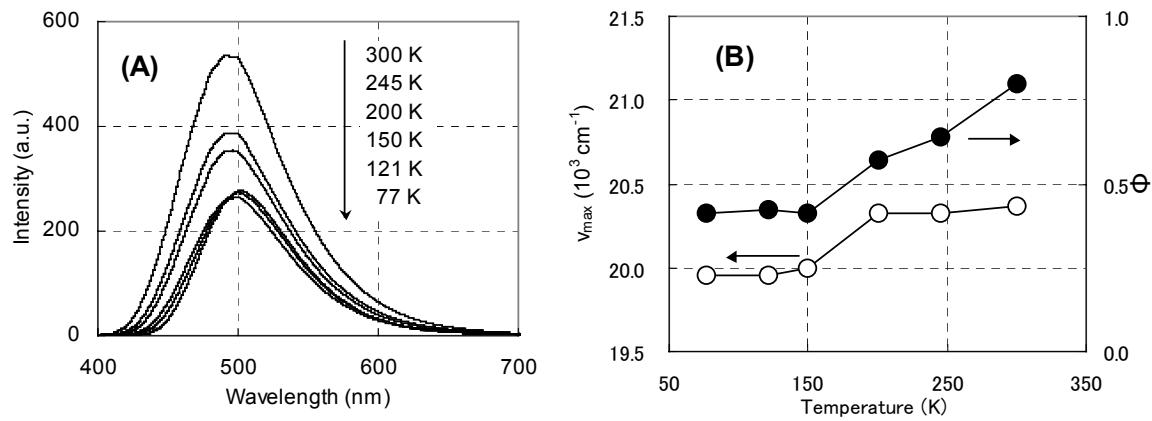


Figure S2. Temperature-dependent emission spectra of the complex (**4**) in the range of 77 – 300 K in solid states (**A**) and plots of emission peak energy and quantum yield (Φ) vs temperature (**B**), obtained with the excitation wavelength at 350 nm.

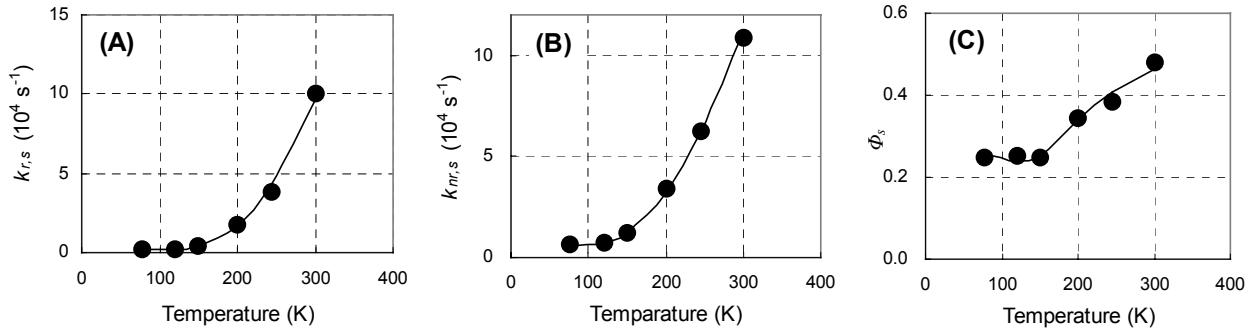


Figure S3. Radiative constant, $k_{r,s}$ **(A)**, non-radiative constant, $k_{nr,s}$ **(B)**, and emission quantum yield, Φ_s **(C)**, for the slower decay component of the complex **(4)** in the solid state, represented as a function of T. The closed circles are observed data at the temperatures and the solid lines are the calculated ones with the use of Equation (10)–(16) and parameters listed in Table 3.

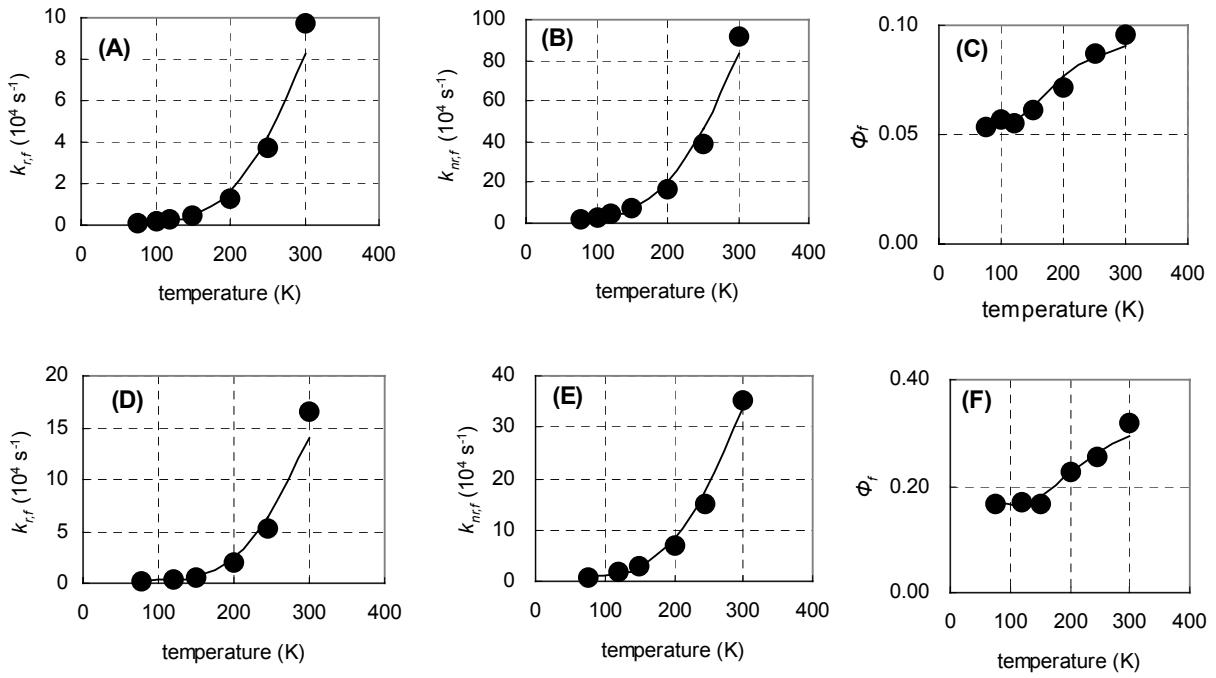


Figure S4. Radiative constant, $k_{r,f}$ [(A) and (D)], non-radiative constant, $k_{nr,f}$ [(B) and (E)], and emission quantum yield, Φ_f [(C) and (F)], for the faster decay component of the complex (1) and (4) in the solid state, represented as a function of T: (A), (B) and (C) are for the complex (1) and (C), (D) and (E) are for the complex (4). The closed circles are observed data at the temperatures and the solid lines are the calculated ones with the use of Equation (10)–(16) and parameters listed in Table S2.

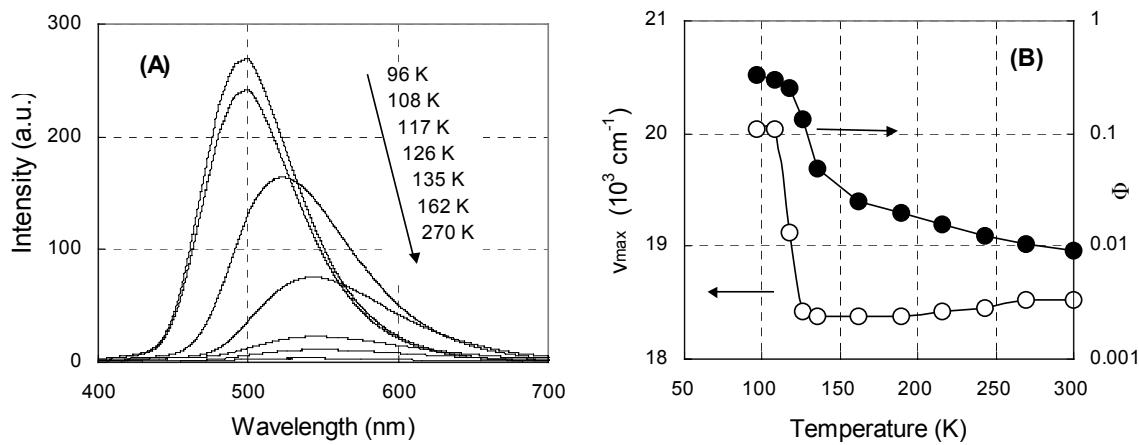


Figure S5. Temperature-dependent emission spectra of the complex **(4)** **(A)** in the range of 96–300 K in the 2mTHF solutions, and plots of emission peak energy (ν_{\max}) and quantum yield (Φ) vs temperature of **(4)** **(B)**.

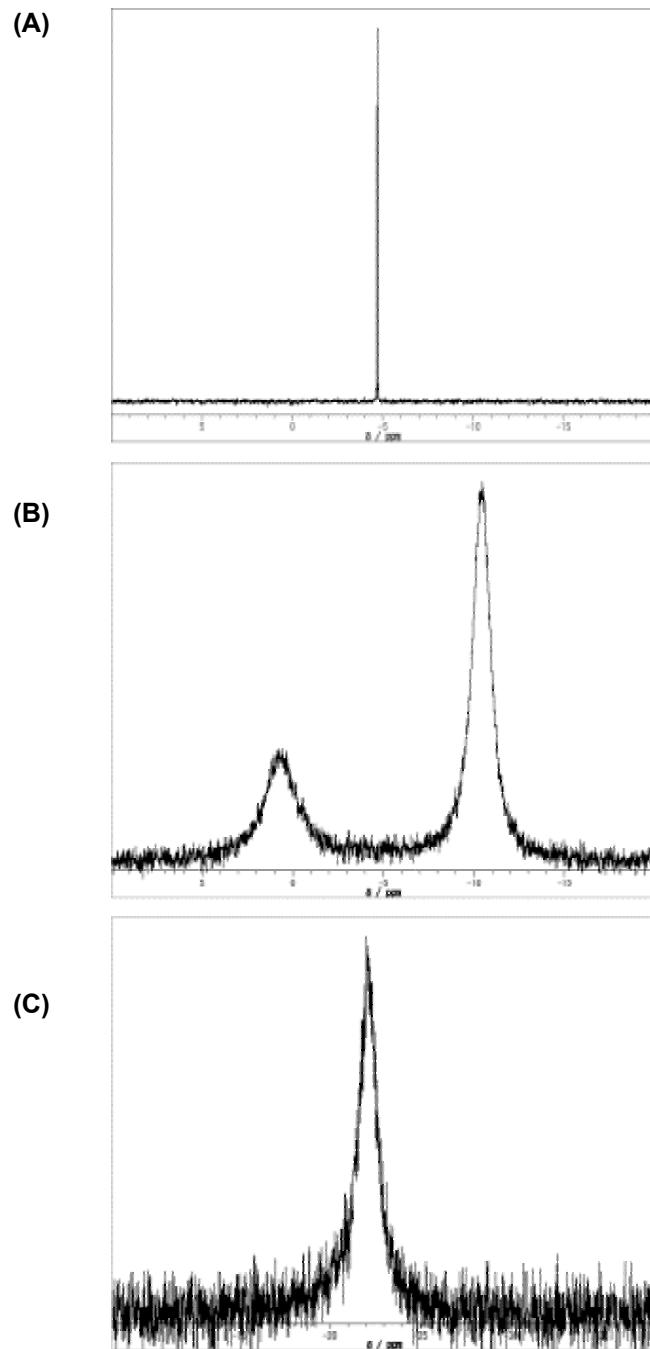


Figure S6. ^{31}P -NMR spectra of PPh_3 (A), (4) (B) and (1) (C).

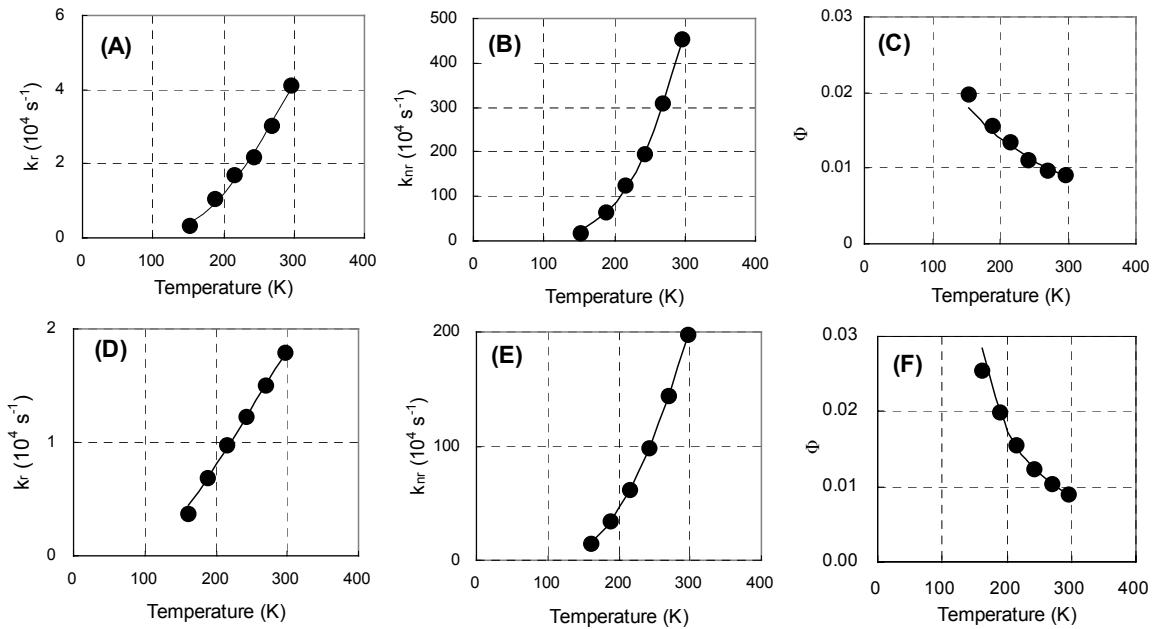


Figure S7. Radiative constant, k_r [(A) and (D)], non-radiative constant, k_{nr} [(B) and (E)], and emission quantum yield, Φ [(C) and (F)], for the complex (1) and (4) in 2mTHF solutions, represented as a function of T: (A), (B) and (C) are for the complex (1) and (C), (D) and (E) are for the complex (4). The closed circles are observed data at the temperatures and the solid lines are the calculated ones with the use of Equation (10)–(16) and parameters listed in Table 4.

Table S1. Selected Crystallographic Data for the Complex (1)–(4).

	(1)	(2)	(3)	(4)
formula	C ₆₀ H ₄₈ Cu ₂ I ₂ P ₄	C ₆₀ H ₄₈ Br ₂ Cu ₂ P ₄	C ₆₀ H ₄₈ Cl ₂ Cu ₂ P ₄	C ₄₈ H ₄₀ CuIP ₃
mol wt	1273.84	1179.83	1090.93	900.22
cryst syst	monoclinic	monoclinic	monoclinic	monoclinic
space group	<i>P</i> 2 ₁ (No. 4)	<i>P</i> 2 ₁ (No. 4)	<i>P</i> 2 ₁ (No. 4)	<i>P</i> 2 ₁ (No. 4)
<i>a</i> , Å	11.61(1)	11.20(1)	11.137(8)	15.11(1)
<i>b</i> , Å	11.61(1)	18.73(2)	18.74(2)	14.67(1)
<i>c</i> , Å	24.36(2)	12.12(1)	12.303(8)	18.33(2)
β, deg	98.29(4)	97.59(4)	97.45(3)	99.60(4)
<i>V</i> , Å ³	5346(10)	2520(4)	2545(3)	4004(5)
<i>Z</i>	4	2	2	4
<i>D</i> _{calcd.} , g/cm ³	1.583	1.554	1.423	1.493
total no. of reflns	46171	24210	23769	35524
no. of unique reflns	21811	24182	11026	35498
<i>R</i>	0.0320	0.0450	0.042	0.037
<i>R</i> _w	0.0670	0.1090	0.052	0.082
temp (°C)	23	-173	20	-173

Table S2. Kinetics parameters of the faster decay component for the complex **(1)** and **(4)** in solid state*.

complex	(1)	(4)
ΔH_f	2.0	2.2
$k_{L,r,f}$	1.6×10^3	2.2×10^3
$k_{H,r,f}$	1.0×10^8	1.0×10^8
A	0.024	0.053
ΔE_L	1.8	1.8
ΔE_H	0	0
$k_{L,nr,f}$	1.7×10^7	0.7×10^7
$k_{L,nr,f}(0)$	2.7×10^4	1.1×10^4
$k_{H,nr,f}$	0	0
$k_{H,nr,f}(0)$	0	0

* Energy separation, ΔE and ΔH , are in kcal/mol and rate constants are in s^{-1} .

Table S3.

[Cu(μl)dppb]₂ (**1**)

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	C ₆₀ H ₄₈ Cu ₂ I ₂ P ₄
Formula Weight	1273.84
Crystal Color, Habit	yellow, block
Crystal Dimensions	0.30 X 0.20 X 0.10 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 90.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 11.61(1) Å b = 19.11(3) Å c = 24.36(2) Å β = 98.29(4) ° V = 5346(10) Å ³
Space Group	P2 ₁ (#4)
Z value	4
D _{calc}	1.583 g/cm ³
F ₀₀₀	2528.00
μ(MoKα)	21.09 cm ⁻¹

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Detector Aperture	280 mm x 256 mm
Data Images	73 exposures
ω oscillation Range (χ =45.0, ϕ =30.0)	130.0 - 190.0°
Exposure Rate	40.2 sec./°
ω oscillation Range (χ =45.0, ϕ =180.0)	0.0 - 159.0°
Exposure Rate	40.2 sec./°
Detector Position	127.40 mm
Pixel Size	0.100 mm
2θ _{max}	54.9°
No. of Reflections Measured	Total: 46171

Corrections

Unique: 21811 ($R_{\text{int}} = 0.047$)
 Lorentz-polarization
 Absorption
 (trans. factors: 0.5615 - 1.0000)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF99 PATTY)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma w (Fo^2 - Fc^2)^2$
Least Squares Weights	$1/[0.0001Fo^2 + 0.3000\sigma(Fo^2)]/(4Fo^2)$
$2\theta_{\text{max}}$ cutoff	54.9°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	21811
No. Variables	1321
Reflection/Parameter Ratio	16.51
Residuals: R (All reflections)	0.075
Residuals: R1 ($I > 2.00\sigma(I)$)	0.032
Residuals: wR2 (All reflections)	0.067
Goodness of Fit Indicator	1.004
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	$1.56 \text{ e}^-/\text{\AA}^3$
Minimum peak in Final Diff. Map	$-1.41 \text{ e}^-/\text{\AA}^3$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
I(1)	Cu(1)	2.6155(8)	I(1)	Cu(2)	2.6528(8)
I(2)	Cu(1)	2.6729(9)	I(2)	Cu(2)	2.5960(8)
I(3)	Cu(3)	2.6198(6)	I(3)	Cu(4)	2.6587(8)
I(4)	Cu(3)	2.6806(8)	I(4)	Cu(4)	2.5787(9)
Cu(1)	P(1)	2.283(2)	Cu(1)	P(2)	2.274(2)
Cu(2)	P(3)	2.289(2)	Cu(2)	P(4)	2.279(2)
Cu(3)	P(5)	2.286(2)	Cu(3)	P(6)	2.272(2)
Cu(4)	P(7)	2.282(2)	Cu(4)	P(8)	2.272(2)
P(1)	C(6)	1.836(6)	P(1)	C(7)	1.826(6)
P(1)	C(13)	1.824(7)	P(2)	C(1)	1.852(6)
P(2)	C(19)	1.810(6)	P(2)	C(25)	1.816(7)
P(3)	C(31)	1.827(7)	P(3)	C(37)	1.795(8)
P(3)	C(43)	1.832(7)	P(4)	C(36)	1.830(6)
P(4)	C(49)	1.809(7)	P(4)	C(55)	1.815(7)
P(5)	C(61)	1.827(6)	P(5)	C(67)	1.819(6)
P(5)	C(73)	1.820(6)	P(6)	C(66)	1.847(5)
P(6)	C(79)	1.806(6)	P(6)	C(85)	1.831(7)
P(7)	C(91)	1.830(6)	P(7)	C(97)	1.812(7)
P(7)	C(103)	1.810(6)	P(8)	C(96)	1.839(6)
P(8)	C(109)	1.800(6)	P(8)	C(115)	1.813(7)
C(1)	C(2)	1.389(9)	C(1)	C(6)	1.395(9)
C(2)	C(3)	1.390(9)	C(3)	C(4)	1.37(1)

C(4)	C(5)	1.36(1)	C(5)	C(6)	1.400(8)
C(7)	C(8)	1.35(1)	C(7)	C(12)	1.338(9)
C(8)	C(9)	1.39(1)	C(9)	C(10)	1.37(1)
C(10)	C(11)	1.32(1)	C(11)	C(12)	1.38(1)
C(13)	C(14)	1.382(8)	C(13)	C(18)	1.381(9)
C(14)	C(15)	1.38(1)	C(15)	C(16)	1.35(1)
C(16)	C(17)	1.37(1)	C(17)	C(18)	1.36(1)
C(19)	C(20)	1.34(1)	C(19)	C(24)	1.37(1)
C(20)	C(21)	1.39(1)	C(21)	C(22)	1.33(1)
C(22)	C(23)	1.35(1)	C(23)	C(24)	1.36(1)
C(25)	C(26)	1.37(1)	C(25)	C(30)	1.40(1)
C(26)	C(27)	1.39(1)	C(27)	C(28)	1.38(1)
C(28)	C(29)	1.34(1)	C(29)	C(30)	1.36(1)
C(31)	C(32)	1.380(8)	C(31)	C(36)	1.40(1)
C(32)	C(33)	1.388(9)	C(33)	C(34)	1.38(1)

Table 4. Bond lengths (Å) -- continued

atom	atom	distance	atom	atom	distance
C(34)	C(35)	1.393(9)	C(35)	C(36)	1.392(9)
C(37)	C(38)	1.38(1)	C(37)	C(42)	1.39(1)
C(38)	C(39)	1.39(2)	C(39)	C(40)	1.33(2)
C(40)	C(41)	1.36(2)	C(41)	C(42)	1.37(1)
C(43)	C(44)	1.35(1)	C(43)	C(48)	1.400(9)
C(44)	C(45)	1.38(1)	C(45)	C(46)	1.38(1)
C(46)	C(47)	1.36(1)	C(47)	C(48)	1.37(1)
C(49)	C(50)	1.38(1)	C(49)	C(54)	1.39(1)
C(50)	C(51)	1.36(1)	C(51)	C(52)	1.36(2)
C(52)	C(53)	1.35(2)	C(53)	C(54)	1.37(1)
C(55)	C(56)	1.382(9)	C(55)	C(60)	1.38(1)
C(56)	C(57)	1.38(1)	C(57)	C(58)	1.34(1)
C(58)	C(59)	1.36(1)	C(59)	C(60)	1.39(1)
C(61)	C(62)	1.405(8)	C(61)	C(66)	1.400(8)
C(62)	C(63)	1.38(1)	C(63)	C(64)	1.38(1)
C(64)	C(65)	1.375(8)	C(65)	C(66)	1.399(8)
C(67)	C(68)	1.389(8)	C(67)	C(72)	1.360(9)
C(68)	C(69)	1.378(9)	C(69)	C(70)	1.37(1)
C(70)	C(71)	1.35(1)	C(71)	C(72)	1.40(1)
C(73)	C(74)	1.35(1)	C(73)	C(78)	1.35(1)
C(74)	C(75)	1.38(1)	C(75)	C(76)	1.35(2)
C(76)	C(77)	1.33(1)	C(77)	C(78)	1.37(1)
C(79)	C(80)	1.381(9)	C(79)	C(84)	1.37(1)
C(80)	C(81)	1.38(1)	C(81)	C(82)	1.35(1)
C(82)	C(83)	1.34(1)	C(83)	C(84)	1.37(1)
C(85)	C(86)	1.39(1)	C(85)	C(90)	1.39(1)
C(86)	C(87)	1.39(1)	C(87)	C(88)	1.37(1)
C(88)	C(89)	1.38(1)	C(89)	C(90)	1.37(1)
C(91)	C(92)	1.390(8)	C(91)	C(96)	1.407(9)
C(92)	C(93)	1.38(1)	C(93)	C(94)	1.37(1)
C(94)	C(95)	1.373(9)	C(95)	C(96)	1.382(9)
C(97)	C(98)	1.38(1)	C(97)	C(102)	1.40(1)

C(98)	C(99)	1.37(1)	C(99)	C(100)	1.36(1)
C(100)	C(101)	1.37(1)	C(101)	C(102)	1.37(1)
C(103)	C(104)	1.387(9)	C(103)	C(108)	1.365(9)
C(104)	C(105)	1.38(1)	C(105)	C(106)	1.34(1)
C(106)	C(107)	1.36(1)	C(107)	C(108)	1.40(1)

Table 4. Bond lengths (Å) -- continued

atom	atom	distance	atom	atom	distance
C(109)	C(110)	1.378(8)	C(109)	C(114)	1.38(1)
C(110)	C(111)	1.39(1)	C(111)	C(112)	1.34(1)
C(112)	C(113)	1.35(1)	C(113)	C(114)	1.39(1)
C(115)	C(116)	1.37(1)	C(115)	C(120)	1.371(9)
C(116)	C(117)	1.37(1)	C(117)	C(118)	1.36(1)
C(118)	C(119)	1.35(1)	C(119)	C(120)	1.38(1)

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cu(2)	I(1)	Cu(1)	66.74(2)	I(1)	Cu(1)	I(2)	108.69(3)
I(1)	Cu(1)	P(1)	117.70(5)	I(1)	Cu(1)	P(2)	123.56(6)
I(1)	Cu(2)	I(2)	109.91(3)	I(1)	Cu(2)	P(3)	107.62(6)
I(1)	Cu(2)	P(4)	111.76(6)	Cu(2)	I(2)	Cu(1)	66.71(2)
I(2)	Cu(1)	P(1)	109.55(5)	I(2)	Cu(1)	P(2)	107.08(5)
I(2)	Cu(2)	P(3)	121.09(6)	I(2)	Cu(2)	P(4)	117.98(5)
Cu(4)	I(3)	Cu(3)	65.66(2)	I(3)	Cu(3)	I(4)	109.56(3)
I(3)	Cu(3)	P(5)	121.11(5)	I(3)	Cu(3)	P(6)	119.86(5)
I(3)	Cu(4)	I(4)	111.54(3)	I(3)	Cu(4)	P(7)	104.13(5)
I(3)	Cu(4)	P(8)	110.38(6)	Cu(4)	I(4)	Cu(3)	65.90(2)
I(4)	Cu(3)	P(5)	105.46(5)	I(4)	Cu(3)	P(6)	109.79(5)
I(4)	Cu(4)	P(7)	118.91(6)	I(4)	Cu(4)	P(8)	121.92(6)
P(2)	Cu(1)	P(1)	88.46(6)	Cu(1)	P(1)	C(6)	102.4(2)
Cu(1)	P(1)	C(7)	114.6(2)	Cu(1)	P(1)	C(13)	125.1(2)
Cu(1)	P(2)	C(1)	102.2(2)	Cu(1)	P(2)	C(19)	118.8(2)
Cu(1)	P(2)	C(25)	121.5(2)	P(4)	Cu(2)	P(3)	86.47(6)
Cu(2)	P(3)	C(31)	100.5(2)	Cu(2)	P(3)	C(43)	116.9(2)
Cu(2)	P(3)	C(37)	123.6(2)	Cu(2)	P(4)	C(36)	101.0(2)
Cu(2)	P(4)	C(55)	113.7(2)	Cu(2)	P(4)	C(49)	125.5(2)
P(6)	Cu(3)	P(5)	88.96(6)	Cu(3)	P(5)	C(61)	102.4(2)
Cu(3)	P(5)	C(67)	116.0(2)	Cu(3)	P(5)	C(73)	124.5(2)
Cu(3)	P(6)	C(66)	102.5(2)	Cu(3)	P(6)	C(79)	120.1(2)
Cu(3)	P(6)	C(85)	119.6(2)	P(8)	Cu(4)	P(7)	86.68(6)
Cu(4)	P(7)	C(91)	101.1(2)	Cu(4)	P(7)	C(103)	116.4(2)
Cu(4)	P(7)	C(97)	124.3(2)	Cu(4)	P(8)	C(96)	101.3(2)
Cu(4)	P(8)	C(109)	115.4(2)	Cu(4)	P(8)	C(115)	125.5(2)
P(1)	C(6)	C(1)	118.9(4)	C(7)	P(1)	C(6)	105.2(3)
P(1)	C(6)	C(5)	122.9(5)	C(13)	P(1)	C(6)	104.4(3)
P(1)	C(7)	C(8)	123.5(5)	P(1)	C(7)	C(12)	118.5(4)
C(13)	P(1)	C(7)	103.2(3)	P(1)	C(13)	C(14)	125.0(5)
P(1)	C(13)	C(18)	117.6(4)	P(2)	C(1)	C(6)	118.9(4)

C(19)	P(2)	C(1)	102.6(3)	C(25)	P(2)	C(1)	103.6(3)
P(2)	C(1)	C(2)	121.3(5)	C(25)	P(2)	C(19)	105.3(3)
P(2)	C(19)	C(20)	120.3(5)	P(2)	C(19)	C(24)	123.1(6)
P(2)	C(25)	C(26)	120.3(5)	P(2)	C(25)	C(30)	121.7(5)
P(3)	C(31)	C(36)	117.7(4)	C(43)	P(3)	C(31)	102.3(3)
P(3)	C(31)	C(32)	123.6(6)	C(37)	P(3)	C(31)	104.8(3)

Table 6. Bond angles ($^{\circ}$) -- continued

atom	atom	atom	angle	atom	atom	atom	angle
C(43)	P(3)	C(37)	105.7(4)	P(3)	C(37)	C(38)	123.3(7)
P(3)	C(37)	C(42)	120.1(6)	P(3)	C(43)	C(44)	119.7(5)
P(3)	C(43)	C(48)	122.6(6)	P(4)	C(36)	C(31)	118.8(4)
C(55)	P(4)	C(36)	104.4(3)	P(4)	C(36)	C(35)	121.0(5)
C(49)	P(4)	C(36)	104.5(3)	C(55)	P(4)	C(49)	105.3(3)
P(4)	C(49)	C(50)	126.6(6)	P(4)	C(49)	C(54)	117.4(6)
P(4)	C(55)	C(56)	124.2(5)	P(4)	C(55)	C(60)	118.1(5)
P(5)	C(61)	C(66)	119.4(4)	C(67)	P(5)	C(61)	104.5(3)
P(5)	C(61)	C(62)	122.0(5)	C(73)	P(5)	C(61)	103.8(3)
P(5)	C(67)	C(68)	124.2(5)	P(5)	C(67)	C(72)	118.1(4)
C(73)	P(5)	C(67)	103.3(3)	P(5)	C(73)	C(74)	124.7(6)
P(5)	C(73)	C(78)	119.8(5)	P(6)	C(66)	C(61)	119.1(4)
C(79)	P(6)	C(66)	103.2(3)	C(85)	P(6)	C(66)	104.5(3)
P(6)	C(66)	C(65)	121.6(4)	C(85)	P(6)	C(79)	104.5(3)
P(6)	C(79)	C(80)	124.6(5)	P(6)	C(79)	C(84)	120.3(5)
P(6)	C(85)	C(86)	117.5(5)	P(6)	C(85)	C(90)	123.6(5)
P(7)	C(91)	C(96)	117.9(4)	C(103)	P(7)	C(91)	101.7(3)
P(7)	C(91)	C(92)	123.5(5)	C(97)	P(7)	C(91)	105.8(3)
C(103)	P(7)	C(97)	104.7(3)	P(7)	C(97)	C(98)	121.7(5)
P(7)	C(97)	C(102)	121.0(5)	P(7)	C(103)	C(104)	123.3(5)
P(7)	C(103)	C(108)	119.1(4)	P(8)	C(96)	C(91)	118.0(4)
C(109)	P(8)	C(96)	103.2(3)	P(8)	C(96)	C(95)	123.1(5)
C(115)	P(8)	C(96)	104.6(3)	P(8)	C(109)	C(110)	125.4(5)
P(8)	C(109)	C(114)	118.1(5)	C(115)	P(8)	C(109)	104.2(3)
P(8)	C(115)	C(116)	124.4(5)	P(8)	C(115)	C(120)	118.3(5)
C(6)	C(1)	C(2)	119.8(5)	C(1)	C(2)	C(3)	120.7(6)
C(1)	C(6)	C(5)	118.2(6)	C(2)	C(3)	C(4)	119.3(7)
C(3)	C(4)	C(5)	120.5(6)	C(4)	C(5)	C(6)	121.5(7)
C(12)	C(7)	C(8)	118.0(6)	C(7)	C(8)	C(9)	120.0(9)
C(7)	C(12)	C(11)	122.7(6)	C(8)	C(9)	C(10)	119.6(9)
C(9)	C(10)	C(11)	120.1(8)	C(10)	C(11)	C(12)	119.3(7)
C(18)	C(13)	C(14)	117.3(6)	C(13)	C(14)	C(15)	120.8(6)
C(13)	C(18)	C(17)	121.8(6)	C(14)	C(15)	C(16)	120.2(7)
C(15)	C(16)	C(17)	120.3(7)	C(16)	C(17)	C(18)	119.5(7)
C(24)	C(19)	C(20)	116.5(7)	C(19)	C(20)	C(21)	120.7(8)
C(19)	C(24)	C(23)	121.8(8)	C(20)	C(21)	C(22)	122(1)
C(21)	C(22)	C(23)	117.1(9)	C(22)	C(23)	C(24)	121.4(8)

Table 6. Bond angles ($^{\circ}$) -- continued

atom	atom	atom	angle	atom	atom	atom	angle
C(30)	C(25)	C(26)	117.9(6)	C(25)	C(26)	C(27)	121.5(7)
C(25)	C(30)	C(29)	119.8(7)	C(26)	C(27)	C(28)	119.0(7)
C(27)	C(28)	C(29)	119.7(8)	C(28)	C(29)	C(30)	122.0(8)
C(36)	C(31)	C(32)	118.6(6)	C(31)	C(32)	C(33)	121.7(7)
C(31)	C(36)	C(35)	120.2(5)	C(32)	C(33)	C(34)	119.5(6)
C(33)	C(34)	C(35)	119.7(6)	C(34)	C(35)	C(36)	120.2(7)
C(42)	C(37)	C(38)	116.4(8)	C(37)	C(38)	C(39)	120(1)
C(37)	C(42)	C(41)	122.4(9)	C(38)	C(39)	C(40)	121(1)
C(39)	C(40)	C(41)	119(1)	C(40)	C(41)	C(42)	119(1)
C(48)	C(43)	C(44)	117.7(6)	C(43)	C(44)	C(45)	122.4(7)
C(43)	C(48)	C(47)	119.7(7)	C(44)	C(45)	C(46)	119.7(8)
C(45)	C(46)	C(47)	118.4(8)	C(46)	C(47)	C(48)	122.0(8)
C(54)	C(49)	C(50)	116.0(7)	C(49)	C(50)	C(51)	122.7(8)
C(49)	C(54)	C(53)	121.2(8)	C(50)	C(51)	C(52)	119.9(9)
C(51)	C(52)	C(53)	119(1)	C(52)	C(53)	C(54)	120(1)
C(60)	C(55)	C(56)	117.4(6)	C(55)	C(56)	C(57)	121.5(7)
C(55)	C(60)	C(59)	119.9(6)	C(56)	C(57)	C(58)	120.8(7)
C(57)	C(58)	C(59)	119.4(8)	C(58)	C(59)	C(60)	120.9(9)
C(66)	C(61)	C(62)	118.7(5)	C(61)	C(62)	C(63)	120.5(6)
C(61)	C(66)	C(65)	119.3(5)	C(62)	C(63)	C(64)	120.8(6)
C(63)	C(64)	C(65)	119.4(6)	C(64)	C(65)	C(66)	121.3(6)
C(72)	C(67)	C(68)	117.7(5)	C(67)	C(68)	C(69)	120.8(6)
C(67)	C(72)	C(71)	121.7(6)	C(68)	C(69)	C(70)	119.9(6)
C(69)	C(70)	C(71)	120.4(7)	C(70)	C(71)	C(72)	119.4(7)
C(78)	C(73)	C(74)	115.4(7)	C(73)	C(74)	C(75)	122.2(8)
C(73)	C(78)	C(77)	122.8(7)	C(74)	C(75)	C(76)	120.3(9)
C(75)	C(76)	C(77)	118.4(9)	C(76)	C(77)	C(78)	120.8(9)
C(84)	C(79)	C(80)	115.1(6)	C(79)	C(80)	C(81)	122.9(7)
C(79)	C(84)	C(83)	121.6(8)	C(80)	C(81)	C(82)	119.7(8)
C(81)	C(82)	C(83)	118.9(9)	C(82)	C(83)	C(84)	121.7(9)
C(90)	C(85)	C(86)	118.5(6)	C(85)	C(86)	C(87)	121.2(7)
C(85)	C(90)	C(89)	120.4(7)	C(86)	C(87)	C(88)	118.8(7)
C(87)	C(88)	C(89)	121.2(8)	C(88)	C(89)	C(90)	120.0(8)
C(96)	C(91)	C(92)	118.6(6)	C(91)	C(92)	C(93)	120.9(7)
C(91)	C(96)	C(95)	118.9(5)	C(92)	C(93)	C(94)	120.2(6)
C(93)	C(94)	C(95)	119.7(7)	C(94)	C(95)	C(96)	121.6(7)
C(102)	C(97)	C(98)	116.6(6)	C(97)	C(98)	C(99)	122.0(7)

Table 6. Bond angles ($^{\circ}$) -- continued

atom	atom	atom	angle	atom	atom	atom	angle
C(97)	C(102)	C(101)	120.9(7)	C(98)	C(99)	C(100)	120.5(8)
C(99)	C(100)	C(101)	119.1(8)	C(100)	C(101)	C(102)	120.9(8)
C(108)	C(103)	C(104)	117.3(6)	C(103)	C(104)	C(105)	120.4(7)
C(103)	C(108)	C(107)	122.3(6)	C(104)	C(105)	C(106)	120.8(7)
C(105)	C(106)	C(107)	120.6(7)	C(106)	C(107)	C(108)	118.4(7)
C(114)	C(109)	C(110)	116.4(6)	C(109)	C(110)	C(111)	121.8(7)
C(109)	C(114)	C(113)	121.6(7)	C(110)	C(111)	C(112)	119.5(8)
C(111)	C(112)	C(113)	120.9(8)	C(112)	C(113)	C(114)	119.6(9)
C(120)	C(115)	C(116)	117.3(6)	C(115)	C(116)	C(117)	122.0(7)

C(115)	C(120)	C(119)	120.3(7)	C(116)	C(117)	C(118)	119.7(8)
C(117)	C(118)	C(119)	119.3(9)	C(118)	C(119)	C(120)	121.3(8)

Table 8. Torsion Angles($^{\circ}$)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cu(2)	I(1)	Cu(1)	I(2)	21.43(3)	Cu(2)	I(1)	Cu(1)	P(1)	146.64(7)
Cu(2)	I(1)	Cu(1)	P(2)	-105.18(6)	Cu(1)	I(1)	Cu(2)	I(2)	-22.27(4)
Cu(1)	I(1)	Cu(2)	P(3)	-156.00(6)	Cu(1)	I(1)	Cu(2)	P(4)	110.71(6)
Cu(2)	I(2)	Cu(1)	I(1)	-21.93(3)	Cu(2)	I(2)	Cu(1)	P(1)	-151.78(6)
Cu(2)	I(2)	Cu(1)	P(2)	113.66(5)	Cu(1)	I(2)	Cu(2)	I(1)	21.77(4)
Cu(1)	I(2)	Cu(2)	P(3)	148.24(7)	Cu(1)	I(2)	Cu(2)	P(4)	-107.93(6)
Cu(4)	I(3)	Cu(3)	I(4)	20.50(3)	Cu(4)	I(3)	Cu(3)	P(5)	143.51(7)
Cu(4)	I(3)	Cu(3)	P(6)	-107.70(5)	Cu(3)	I(3)	Cu(4)	I(4)	-21.64(4)
Cu(3)	I(3)	Cu(4)	P(7)	-151.08(6)	Cu(3)	I(3)	Cu(4)	P(8)	117.22(6)
Cu(4)	I(4)	Cu(3)	I(3)	-21.12(3)	Cu(4)	I(4)	Cu(3)	P(5)	-152.98(6)
Cu(4)	I(4)	Cu(3)	P(6)	112.46(5)	Cu(3)	I(4)	Cu(4)	I(3)	21.08(4)
Cu(3)	I(4)	Cu(4)	P(7)	142.26(6)	Cu(3)	I(4)	Cu(4)	P(8)	-112.31(7)
I(1)	Cu(1)	P(1)	C(6)	153.1(2)	I(1)	Cu(1)	P(1)	C(7)	39.8(2)
I(1)	Cu(1)	P(1)	C(13)	-89.1(3)	I(2)	Cu(1)	P(1)	C(6)	-82.1(2)
I(2)	Cu(1)	P(1)	C(7)	164.6(2)	I(2)	Cu(1)	P(1)	C(13)	35.7(3)
P(2)	Cu(1)	P(1)	C(6)	25.5(2)	P(2)	Cu(1)	P(1)	C(7)	-87.8(2)
P(2)	Cu(1)	P(1)	C(13)	143.3(3)	I(1)	Cu(1)	P(2)	C(1)	-148.1(2)
I(1)	Cu(1)	P(2)	C(19)	-36.2(2)	I(1)	Cu(1)	P(2)	C(25)	97.5(2)
I(2)	Cu(1)	P(2)	C(1)	84.6(2)	I(2)	Cu(1)	P(2)	C(19)	-163.5(2)
I(2)	Cu(1)	P(2)	C(25)	-29.9(2)	P(1)	Cu(1)	P(2)	C(1)	-25.4(2)
P(1)	Cu(1)	P(2)	C(19)	86.5(2)	P(1)	Cu(1)	P(2)	C(25)	-139.9(2)
I(1)	Cu(2)	P(3)	C(31)	-78.0(2)	I(1)	Cu(2)	P(3)	C(37)	37.8(3)
I(1)	Cu(2)	P(3)	C(43)	172.3(2)	I(2)	Cu(2)	P(3)	C(31)	154.5(2)
I(2)	Cu(2)	P(3)	C(37)	-89.7(3)	I(2)	Cu(2)	P(3)	C(43)	44.8(3)
P(4)	Cu(2)	P(3)	C(31)	33.7(2)	P(4)	Cu(2)	P(3)	C(37)	149.5(3)
P(4)	Cu(2)	P(3)	C(43)	-75.9(3)	I(1)	Cu(2)	P(4)	C(36)	75.8(2)
I(1)	Cu(2)	P(4)	C(49)	-41.1(3)	I(1)	Cu(2)	P(4)	C(55)	-173.0(2)
I(2)	Cu(2)	P(4)	C(36)	-155.4(2)	I(2)	Cu(2)	P(4)	C(49)	87.8(3)
I(2)	Cu(2)	P(4)	C(55)	-44.1(2)	P(3)	Cu(2)	P(4)	C(36)	-31.8(2)
P(3)	Cu(2)	P(4)	C(49)	-148.6(3)	P(3)	Cu(2)	P(4)	C(55)	79.4(2)
I(3)	Cu(3)	P(5)	C(61)	148.7(2)	I(3)	Cu(3)	P(5)	C(67)	35.6(2)
I(3)	Cu(3)	P(5)	C(73)	-94.7(3)	I(4)	Cu(3)	P(5)	C(61)	-86.4(2)
I(4)	Cu(3)	P(5)	C(67)	160.5(2)	I(4)	Cu(3)	P(5)	C(73)	30.2(3)
P(6)	Cu(3)	P(5)	C(61)	23.9(2)	P(6)	Cu(3)	P(5)	C(67)	-89.2(2)
P(6)	Cu(3)	P(5)	C(73)	140.5(3)	I(3)	Cu(3)	P(6)	C(66)	-148.7(2)
I(3)	Cu(3)	P(6)	C(79)	-35.2(2)	I(3)	Cu(3)	P(6)	C(85)	96.4(2)
I(4)	Cu(3)	P(6)	C(66)	83.2(2)	I(4)	Cu(3)	P(6)	C(79)	-163.2(2)

Table 8. Torsion angles ($^{\circ}$) -- continued

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
I(4)	Cu(3)	P(6)	C(85)	-31.7(2)	P(5)	Cu(3)	P(6)	C(66)	-22.9(2)
P(5)	Cu(3)	P(6)	C(79)	90.7(2)	P(5)	Cu(3)	P(6)	C(85)	-137.8(2)
I(3)	Cu(4)	P(7)	C(91)	-77.3(2)	I(3)	Cu(4)	P(7)	C(97)	40.7(3)
I(3)	Cu(4)	P(7)	C(103)	173.6(2)	I(4)	Cu(4)	P(7)	C(91)	157.9(2)
I(4)	Cu(4)	P(7)	C(97)	-84.2(3)	I(4)	Cu(4)	P(7)	C(103)	48.8(2)

P(8)	Cu(4)	P(7)	C(91)	32.9(2)	P(8)	Cu(4)	P(7)	C(97)	150.9(3)
P(8)	Cu(4)	P(7)	C(103)	-76.2(2)	I(3)	Cu(4)	P(8)	C(96)	71.7(2)
I(3)	Cu(4)	P(8)	C(109)	-177.6(2)	I(3)	Cu(4)	P(8)	C(115)	-45.5(3)
I(4)	Cu(4)	P(8)	C(96)	-154.4(2)	I(4)	Cu(4)	P(8)	C(109)	-43.7(2)
I(4)	Cu(4)	P(8)	C(115)	88.4(3)	P(7)	Cu(4)	P(8)	C(96)	-32.1(2)
P(7)	Cu(4)	P(8)	C(109)	78.6(2)	P(7)	Cu(4)	P(8)	C(115)	-149.3(3)
Cu(1)	P(1)	C(6)	C(1)	-20.5(5)	Cu(1)	P(1)	C(6)	C(5)	160.6(5)
C(7)	P(1)	C(6)	C(1)	99.5(5)	C(7)	P(1)	C(6)	C(5)	-79.3(5)
C(13)	P(1)	C(6)	C(1)	-152.1(4)	C(13)	P(1)	C(6)	C(5)	29.0(5)
Cu(1)	P(1)	C(7)	C(8)	121.6(6)	Cu(1)	P(1)	C(7)	C(12)	-57.6(6)
C(6)	P(1)	C(7)	C(8)	9.9(7)	C(6)	P(1)	C(7)	C(12)	-169.3(5)
C(13)	P(1)	C(7)	C(8)	-99.3(7)	C(13)	P(1)	C(7)	C(12)	81.5(5)
Cu(1)	P(1)	C(13)	C(14)	164.8(5)	Cu(1)	P(1)	C(13)	C(18)	-12.5(6)
C(6)	P(1)	C(13)	C(14)	-78.4(6)	C(6)	P(1)	C(13)	C(18)	104.4(5)
C(7)	P(1)	C(13)	C(14)	31.4(6)	C(7)	P(1)	C(13)	C(18)	-145.8(5)
Cu(1)	P(2)	C(1)	C(2)	-158.3(5)	Cu(1)	P(2)	C(1)	C(6)	20.7(5)
C(19)	P(2)	C(1)	C(2)	78.1(5)	C(19)	P(2)	C(1)	C(6)	-102.9(5)
C(25)	P(2)	C(1)	C(2)	-31.2(5)	C(25)	P(2)	C(1)	C(6)	147.7(4)
Cu(1)	P(2)	C(19)	C(20)	23.8(6)	Cu(1)	P(2)	C(19)	C(24)	-159.1(5)
C(1)	P(2)	C(19)	C(20)	135.5(5)	C(1)	P(2)	C(19)	C(24)	-47.4(6)
C(25)	P(2)	C(19)	C(20)	-116.5(5)	C(25)	P(2)	C(19)	C(24)	60.7(6)
Cu(1)	P(2)	C(25)	C(26)	56.4(5)	Cu(1)	P(2)	C(25)	C(30)	-119.4(5)
C(1)	P(2)	C(25)	C(26)	-57.4(5)	C(1)	P(2)	C(25)	C(30)	126.9(5)
C(19)	P(2)	C(25)	C(26)	-164.7(5)	C(19)	P(2)	C(25)	C(30)	19.5(6)
Cu(2)	P(3)	C(31)	C(32)	152.9(4)	Cu(2)	P(3)	C(31)	C(36)	-29.9(5)
C(37)	P(3)	C(31)	C(32)	23.8(5)	C(37)	P(3)	C(31)	C(36)	-159.1(4)
C(43)	P(3)	C(31)	C(32)	-86.3(5)	C(43)	P(3)	C(31)	C(36)	90.8(4)
Cu(2)	P(3)	C(37)	C(38)	118.7(6)	Cu(2)	P(3)	C(37)	C(42)	-57.0(6)
C(31)	P(3)	C(37)	C(38)	-127.6(6)	C(31)	P(3)	C(37)	C(42)	56.7(6)
C(43)	P(3)	C(37)	C(38)	-20.0(6)	C(43)	P(3)	C(37)	C(42)	164.4(5)
Cu(2)	P(3)	C(43)	C(44)	-21.9(7)	Cu(2)	P(3)	C(43)	C(48)	156.6(6)
C(31)	P(3)	C(43)	C(44)	-130.6(6)	C(31)	P(3)	C(43)	C(48)	48.0(7)

Table 8. Torsion angles ($^{\circ}$) -- continued

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(37)	P(3)	C(43)	C(44)	120.0(6)	C(37)	P(3)	C(43)	C(48)	-61.5(6)
Cu(2)	P(4)	C(36)	C(31)	23.3(5)	Cu(2)	P(4)	C(36)	C(35)	-156.6(4)
C(49)	P(4)	C(36)	C(31)	154.6(4)	C(49)	P(4)	C(36)	C(35)	-25.2(5)
C(55)	P(4)	C(36)	C(31)	-95.0(5)	C(55)	P(4)	C(36)	C(35)	85.2(5)
Cu(2)	P(4)	C(49)	C(50)	-142.8(5)	Cu(2)	P(4)	C(49)	C(54)	34.7(6)
C(36)	P(4)	C(49)	C(50)	101.9(6)	C(36)	P(4)	C(49)	C(54)	-80.5(5)
C(55)	P(4)	C(49)	C(50)	-7.8(6)	C(55)	P(4)	C(49)	C(54)	169.8(5)
Cu(2)	P(4)	C(55)	C(56)	-117.0(6)	Cu(2)	P(4)	C(55)	C(60)	56.5(6)
C(36)	P(4)	C(55)	C(56)	-7.9(7)	C(36)	P(4)	C(55)	C(60)	165.7(5)
C(49)	P(4)	C(55)	C(56)	101.9(6)	C(49)	P(4)	C(55)	C(60)	-84.5(6)
Cu(3)	P(5)	C(61)	C(62)	160.2(4)	Cu(3)	P(5)	C(61)	C(66)	-20.6(5)
C(67)	P(5)	C(61)	C(62)	-78.4(5)	C(67)	P(5)	C(61)	C(66)	100.8(4)
C(73)	P(5)	C(61)	C(62)	29.6(5)	C(73)	P(5)	C(61)	C(66)	-151.2(4)
Cu(3)	P(5)	C(67)	C(68)	137.9(5)	Cu(3)	P(5)	C(67)	C(72)	-41.6(6)
C(61)	P(5)	C(67)	C(68)	26.0(6)	C(61)	P(5)	C(67)	C(72)	-153.5(5)

C(73)	P(5)	C(67)	C(68)	-82.3(6)	C(73)	P(5)	C(67)	C(72)	98.2(5)
Cu(3)	P(5)	C(73)	C(74)	131.9(6)	Cu(3)	P(5)	C(73)	C(78)	-44.4(7)
C(61)	P(5)	C(73)	C(74)	-112.2(6)	C(61)	P(5)	C(73)	C(78)	71.4(6)
C(67)	P(5)	C(73)	C(74)	-3.3(7)	C(67)	P(5)	C(73)	C(78)	-179.7(5)
Cu(3)	P(6)	C(66)	C(61)	17.3(5)	Cu(3)	P(6)	C(66)	C(65)	-161.2(4)
C(79)	P(6)	C(66)	C(61)	-108.2(4)	C(79)	P(6)	C(66)	C(65)	73.4(5)
C(85)	P(6)	C(66)	C(61)	142.8(4)	C(85)	P(6)	C(66)	C(65)	-35.7(5)
Cu(3)	P(6)	C(79)	C(80)	-169.3(5)	Cu(3)	P(6)	C(79)	C(84)	12.6(6)
C(66)	P(6)	C(79)	C(80)	-56.1(6)	C(66)	P(6)	C(79)	C(84)	125.8(5)
C(85)	P(6)	C(79)	C(80)	52.9(6)	C(85)	P(6)	C(79)	C(84)	-125.2(5)
Cu(3)	P(6)	C(85)	C(86)	52.2(5)	Cu(3)	P(6)	C(85)	C(90)	-120.2(5)
C(66)	P(6)	C(85)	C(86)	-61.6(5)	C(66)	P(6)	C(85)	C(90)	125.9(5)
C(79)	P(6)	C(85)	C(86)	-169.8(4)	C(79)	P(6)	C(85)	C(90)	17.8(6)
Cu(4)	P(7)	C(91)	C(92)	153.9(4)	Cu(4)	P(7)	C(91)	C(96)	-27.5(4)
C(97)	P(7)	C(91)	C(92)	23.2(5)	C(97)	P(7)	C(91)	C(96)	-158.2(4)
C(103)	P(7)	C(91)	C(92)	-85.9(5)	C(103)	P(7)	C(91)	C(96)	92.6(4)
Cu(4)	P(7)	C(97)	C(98)	-63.7(5)	Cu(4)	P(7)	C(97)	C(102)	106.7(5)
C(91)	P(7)	C(97)	C(98)	52.0(5)	C(91)	P(7)	C(97)	C(102)	-137.6(4)
C(103)	P(7)	C(97)	C(98)	159.0(4)	C(103)	P(7)	C(97)	C(102)	-30.6(5)
Cu(4)	P(7)	C(103)	C(104)	156.2(5)	Cu(4)	P(7)	C(103)	C(108)	-17.8(6)
C(91)	P(7)	C(103)	C(104)	47.5(6)	C(91)	P(7)	C(103)	C(108)	-126.6(5)
C(97)	P(7)	C(103)	C(104)	-62.5(6)	C(97)	P(7)	C(103)	C(108)	123.4(5)

Table 8. Torsion angles ($^{\circ}$) -- continued

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cu(4)	P(8)	C(96)	C(91)	25.0(5)	Cu(4)	P(8)	C(96)	C(95)	-156.4(5)
C(109)	P(8)	C(96)	C(91)	-94.7(4)	C(109)	P(8)	C(96)	C(95)	83.9(5)
C(115)	P(8)	C(96)	C(91)	156.6(4)	C(115)	P(8)	C(96)	C(95)	-24.8(5)
Cu(4)	P(8)	C(109)	C(110)	-119.4(6)	Cu(4)	P(8)	C(109)	C(114)	57.6(6)
C(96)	P(8)	C(109)	C(110)	-9.9(6)	C(96)	P(8)	C(109)	C(114)	167.1(5)
C(115)	P(8)	C(109)	C(110)	99.1(6)	C(115)	P(8)	C(109)	C(114)	-83.8(5)
Cu(4)	P(8)	C(115)	C(116)	-156.9(5)	Cu(4)	P(8)	C(115)	C(120)	22.2(7)
C(96)	P(8)	C(115)	C(116)	87.4(6)	C(96)	P(8)	C(115)	C(120)	-93.5(5)
C(109)	P(8)	C(115)	C(116)	-20.7(7)	C(109)	P(8)	C(115)	C(120)	158.5(5)
P(2)	C(1)	C(2)	C(3)	-179.5(5)	C(6)	C(1)	C(2)	C(3)	1.6(9)
P(2)	C(1)	C(6)	P(1)	-0.1(6)	P(2)	C(1)	C(6)	C(5)	178.8(5)
C(2)	C(1)	C(6)	P(1)	178.9(4)	C(2)	C(1)	C(6)	C(5)	-2.2(8)
C(1)	C(2)	C(3)	C(4)	-0.4(9)	C(2)	C(3)	C(4)	C(5)	-0.2(8)
C(3)	C(4)	C(5)	C(6)	0(1)	C(4)	C(5)	C(6)	P(1)	-179.5(5)
C(4)	C(5)	C(6)	C(1)	1.7(9)	P(1)	C(7)	C(8)	C(9)	177.7(8)
C(12)	C(7)	C(8)	C(9)	-3(1)	P(1)	C(7)	C(12)	C(11)	179.5(6)
C(8)	C(7)	C(12)	C(11)	0.2(8)	C(7)	C(8)	C(9)	C(10)	4(1)
C(8)	C(9)	C(10)	C(11)	-3(1)	C(9)	C(10)	C(11)	C(12)	0(1)
C(10)	C(11)	C(12)	C(7)	0(1)	P(1)	C(13)	C(14)	C(15)	179.4(6)
C(18)	C(13)	C(14)	C(15)	-3(1)	P(1)	C(13)	C(18)	C(17)	-179.4(6)
C(14)	C(13)	C(18)	C(17)	3(1)	C(13)	C(14)	C(15)	C(16)	2(1)
C(14)	C(15)	C(16)	C(17)	0(1)	C(15)	C(16)	C(17)	C(18)	0(1)
C(16)	C(17)	C(18)	C(13)	-1(1)	P(2)	C(19)	C(20)	C(21)	178.1(7)
C(24)	C(19)	C(20)	C(21)	0(1)	P(2)	C(19)	C(24)	C(23)	-176.5(7)
C(20)	C(19)	C(24)	C(23)	0(1)	C(19)	C(20)	C(21)	C(22)	-1(1)

C(20)	C(21)	C(22)	C(23)	0(1)	C(21)	C(22)	C(23)	C(24)	1(1)
C(22)	C(23)	C(24)	C(19)	-1(1)	P(2)	C(25)	C(26)	C(27)	-175.5(6)
C(30)	C(25)	C(26)	C(27)	0.4(8)	P(2)	C(25)	C(30)	C(29)	176.3(6)
C(26)	C(25)	C(30)	C(29)	0.5(9)	C(25)	C(26)	C(27)	C(28)	-1(1)
C(26)	C(27)	C(28)	C(29)	0(1)	C(27)	C(28)	C(29)	C(30)	0(1)
C(28)	C(29)	C(30)	C(25)	0(1)	P(3)	C(31)	C(32)	C(33)	178.4(5)
C(36)	C(31)	C(32)	C(33)	1.3(8)	P(3)	C(31)	C(36)	P(4)	4.7(7)
P(3)	C(31)	C(36)	C(35)	-175.5(5)	C(32)	C(31)	C(36)	P(4)	-178.0(4)
C(32)	C(31)	C(36)	C(35)	1.8(8)	C(31)	C(32)	C(33)	C(34)	-3.6(8)
C(32)	C(33)	C(34)	C(35)	2.8(9)	C(33)	C(34)	C(35)	C(36)	0.2(6)
C(34)	C(35)	C(36)	P(4)	177.3(4)	C(34)	C(35)	C(36)	C(31)	-2.6(8)
P(3)	C(37)	C(38)	C(39)	-175.3(7)	C(42)	C(37)	C(38)	C(39)	0(1)

Table 8. Torsion angles ($^{\circ}$) -- continued

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
P(3)	C(37)	C(42)	C(41)	174.3(6)	C(38)	C(37)	C(42)	C(41)	-1(1)
C(37)	C(38)	C(39)	C(40)	1(1)	C(38)	C(39)	C(40)	C(41)	-2(1)
C(39)	C(40)	C(41)	C(42)	1(1)	C(40)	C(41)	C(42)	C(37)	0(1)
P(3)	C(43)	C(44)	C(45)	178.2(7)	C(48)	C(43)	C(44)	C(45)	-0.4(9)
P(3)	C(43)	C(48)	C(47)	-177.1(7)	C(44)	C(43)	C(48)	C(47)	1(1)
C(43)	C(44)	C(45)	C(46)	0(1)	C(44)	C(45)	C(46)	C(47)	0(1)
C(45)	C(46)	C(47)	C(48)	1(1)	C(46)	C(47)	C(48)	C(43)	-2(1)
P(4)	C(49)	C(50)	C(51)	177.5(6)	C(54)	C(49)	C(50)	C(51)	-0.0(9)
P(4)	C(49)	C(54)	C(53)	-177.8(6)	C(50)	C(49)	C(54)	C(53)	0(1)
C(49)	C(50)	C(51)	C(52)	0.2(9)	C(50)	C(51)	C(52)	C(53)	0(1)
C(51)	C(52)	C(53)	C(54)	0.4(9)	C(52)	C(53)	C(54)	C(49)	0(1)
P(4)	C(55)	C(56)	C(57)	173.1(6)	C(60)	C(55)	C(56)	C(57)	0(1)
P(4)	C(55)	C(60)	C(59)	-174.2(7)	C(56)	C(55)	C(60)	C(59)	-0.1(9)
C(55)	C(56)	C(57)	C(58)	-0.3(9)	C(56)	C(57)	C(58)	C(59)	1(1)
C(57)	C(58)	C(59)	C(60)	-2(1)	C(58)	C(59)	C(60)	C(55)	1(1)
P(5)	C(61)	C(62)	C(63)	178.5(5)	C(66)	C(61)	C(62)	C(63)	-0.7(9)
P(5)	C(61)	C(66)	P(6)	2.4(7)	P(5)	C(61)	C(66)	C(65)	-179.1(5)
C(62)	C(61)	C(66)	P(6)	-178.4(4)	C(62)	C(61)	C(66)	C(65)	0.1(7)
C(61)	C(62)	C(63)	C(64)	-0.0(9)	C(62)	C(63)	C(64)	C(65)	1(1)
C(63)	C(64)	C(65)	C(66)	-2.0(9)	C(64)	C(65)	C(66)	P(6)	179.7(4)
C(64)	C(65)	C(66)	C(61)	1.3(8)	P(5)	C(67)	C(68)	C(69)	-179.7(6)
C(72)	C(67)	C(68)	C(69)	-0.2(8)	P(5)	C(67)	C(72)	C(71)	179.3(7)
C(68)	C(67)	C(72)	C(71)	-0.2(8)	C(67)	C(68)	C(69)	C(70)	0(1)
C(68)	C(69)	C(70)	C(71)	2(1)	C(69)	C(70)	C(71)	C(72)	-2(1)
C(70)	C(71)	C(72)	C(67)	1(1)	P(5)	C(73)	C(74)	C(75)	-176.7(7)
C(78)	C(73)	C(74)	C(75)	-0.2(9)	P(5)	C(73)	C(78)	C(77)	173.2(7)
C(74)	C(73)	C(78)	C(77)	-3(1)	C(73)	C(74)	C(75)	C(76)	2(1)
C(74)	C(75)	C(76)	C(77)	0(1)	C(75)	C(76)	C(77)	C(78)	-2(1)
C(76)	C(77)	C(78)	C(73)	5(1)	P(6)	C(79)	C(80)	C(81)	-178.6(6)
C(84)	C(79)	C(80)	C(81)	-0.4(9)	P(6)	C(79)	C(84)	C(83)	179.3(7)
C(80)	C(79)	C(84)	C(83)	1(1)	C(79)	C(80)	C(81)	C(82)	1(1)
C(80)	C(81)	C(82)	C(83)	-2(1)	C(81)	C(82)	C(83)	C(84)	3(1)
C(82)	C(83)	C(84)	C(79)	-2(1)	P(6)	C(85)	C(86)	C(87)	-174.4(6)
C(90)	C(85)	C(86)	C(87)	-1.5(9)	P(6)	C(85)	C(90)	C(89)	172.7(6)
C(86)	C(85)	C(90)	C(89)	0.3(8)	C(85)	C(86)	C(87)	C(88)	2(1)

C(86)	C(87)	C(88)	C(89)	-1(1)		C(87)	C(88)	C(89)	C(90)	0.3(9)
C(88)	C(89)	C(90)	C(85)	0.3(9)		P(7)	C(91)	C(92)	C(93)	177.1(5)

Table 8. Torsion angles ($^{\circ}$) -- continued

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(96)	C(91)	C(92)	C(93)	-1.4(9)	P(7)	C(91)	C(96)	P(8)	1.8(6)
P(7)	C(91)	C(96)	C(95)	-176.9(5)	C(92)	C(91)	C(96)	P(8)	-179.5(4)
C(92)	C(91)	C(96)	C(95)	1.7(8)	C(91)	C(92)	C(93)	C(94)	0.0(9)
C(92)	C(93)	C(94)	C(95)	1(1)	C(93)	C(94)	C(95)	C(96)	-0.7(9)
C(94)	C(95)	C(96)	P(8)	-179.3(4)	C(94)	C(95)	C(96)	C(91)	-0.7(8)
P(7)	C(97)	C(98)	C(99)	171.2(5)	C(102)	C(97)	C(98)	C(99)	0.4(7)
P(7)	C(97)	C(102)	C(101)	-170.0(6)	C(98)	C(97)	C(102)	C(101)	0.9(9)
C(97)	C(98)	C(99)	C(100)	0(1)	C(98)	C(99)	C(100)	C(101)	0(1)
C(99)	C(100)	C(101)	C(102)	1(1)	C(100)	C(101)	C(102)	C(97)	-1(1)
P(7)	C(103)	C(104)	C(105)	-173.4(7)	C(108)	C(103)	C(104)	C(105)	0(1)
P(7)	C(103)	C(108)	C(107)	172.9(6)	C(104)	C(103)	C(108)	C(107)	-1(1)
C(103)	C(104)	C(105)	C(106)	0(1)	C(104)	C(105)	C(106)	C(107)	0(1)
C(105)	C(106)	C(107)	C(108)	-1(1)	C(106)	C(107)	C(108)	C(103)	1(1)
P(8)	C(109)	C(110)	C(111)	179.3(7)	C(114)	C(109)	C(110)	C(111)	2(1)
P(8)	C(109)	C(114)	C(113)	-178.1(6)	C(110)	C(109)	C(114)	C(113)	0(1)
C(109)	C(110)	C(111)	C(112)	-3(1)	C(110)	C(111)	C(112)	C(113)	3(1)
C(111)	C(112)	C(113)	C(114)	-2(1)	C(112)	C(113)	C(114)	C(109)	0(1)
P(8)	C(115)	C(116)	C(117)	178.5(7)	C(120)	C(115)	C(116)	C(117)	0(1)
P(8)	C(115)	C(120)	C(119)	-178.0(6)	C(116)	C(115)	C(120)	C(119)	1(1)
C(115)	C(116)	C(117)	C(118)	1(1)	C(116)	C(117)	C(118)	C(119)	-2(1)
C(117)	C(118)	C(119)	C(120)	3(1)	C(118)	C(119)	C(120)	C(115)	-2(1)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table S4.
[Cu(μBr)dppb]₂ (2)

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	C ₆₀ H ₄₈ Br ₂ Cu ₂ P ₄
Formula Weight	1179.83
Crystal Color, Habit	yellow, block
Crystal Dimensions	0.20 X 0.20 X 0.10 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 30.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 11.20(1) Å b = 18.73(2) Å c = 12.12(1) Å β = 97.59(4) ° V = 2520(4) Å ³
Space Group	P2 ₁ (#4)
Z value	2
D _{calc}	1.554 g/cm ³
F ₀₀₀	1192.00
μ(MoKα)	26.01 cm ⁻¹

B. Intensity Measurements

Diffraction	Rigaku RAXIS-RAPID
Radiation	MoKα ($\lambda = 0.71075 \text{ \AA}$) graphite monochromated
Detector Aperture	280 mm x 256 mm
Data Images	44 exposures
ω oscillation Range ($\chi=45.0, \phi=30.0$)	130.0 - 190.0°
Exposure Rate	10.2 sec./°
ω oscillation Range ($\chi=45.0, \phi=180.0$)	0.0 - 160.0°
Exposure Rate	10.2 sec./°
Detector Position	127.40 mm
Pixel Size	0.100 mm
2θ _{max}	54.9°

No. of Reflections Measured	Total: 24210 Unique: 24182 ($R_{\text{int}} = 0.082$)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.5955 - 1.0000)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\sum w (F_o^2 - F_c^2)^2$
Least Squares Weights	$1/[0.0003F_o^2 + 0.2000\sigma(F_o^2)]/(4F_o^2)$
20 _{max} cutoff	54.9°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	24182
No. Variables	661
Reflection/Parameter Ratio	36.58
Residuals: R (All reflections)	0.069
Residuals: R1 ($>2.00\sigma(I)$)	0.045
Residuals: wR2 (All reflections)	0.109
Goodness of Fit Indicator	1.396
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	3.08 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-2.46 e ⁻ /Å ³

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Br(1)	Cu(1)	2.4536(6)	Br(1)	Cu(2)	2.4948(6)
Br(2)	Cu(1)	2.5328(6)	Br(2)	Cu(2)	2.4290(7)
Cu(1)	P(1)	2.262(1)	Cu(1)	P(2)	2.257(1)
Cu(2)	P(3)	2.259(1)	Cu(2)	P(4)	2.259(1)
P(1)	C(1)	1.839(4)	P(1)	C(7)	1.825(4)
P(1)	C(13)	1.824(4)	P(2)	C(6)	1.856(5)
P(2)	C(19)	1.828(4)	P(2)	C(25)	1.832(4)
P(3)	C(31)	1.849(4)	P(3)	C(37)	1.824(5)
P(3)	C(43)	1.830(4)	P(4)	C(36)	1.822(5)
P(4)	C(49)	1.821(4)	P(4)	C(55)	1.827(4)
C(1)	C(2)	1.401(6)	C(1)	C(6)	1.417(5)
C(2)	C(3)	1.384(6)	C(3)	C(2)	1.384(6)
C(3)	C(4)	1.388(6)	C(4)	C(3)	1.388(6)
C(4)	C(5)	1.378(6)	C(5)	C(6)	1.388(6)
C(7)	C(8)	1.408(5)	C(7)	C(12)	1.371(6)
C(8)	C(9)	1.386(5)	C(9)	C(10)	1.371(7)
C(10)	C(11)	1.395(6)	C(11)	C(12)	1.408(5)
C(13)	C(14)	1.402(6)	C(13)	C(18)	1.386(6)

C(14)	C(15)	1.379(6)	C(15)	C(16)	1.383(6)
C(16)	C(17)	1.385(7)	C(17)	C(18)	1.382(7)
C(19)	C(20)	1.370(7)	C(19)	C(24)	1.397(6)
C(20)	C(21)	1.391(6)	C(21)	C(22)	1.381(7)
C(22)	C(23)	1.362(8)	C(23)	C(24)	1.384(7)
C(25)	C(26)	1.386(6)	C(25)	C(30)	1.386(6)
C(26)	C(27)	1.398(6)	C(27)	C(28)	1.375(7)
C(28)	C(29)	1.384(7)	C(29)	C(30)	1.379(6)
C(31)	C(32)	1.383(6)	C(31)	C(36)	1.434(6)
C(32)	C(33)	1.386(7)	C(33)	C(34)	1.389(7)
C(34)	C(35)	1.390(7)	C(35)	C(36)	1.384(6)
C(37)	C(38)	1.392(6)	C(37)	C(42)	1.389(6)
C(38)	C(39)	1.400(7)	C(39)	C(40)	1.380(7)
C(40)	C(41)	1.372(7)	C(41)	C(42)	1.368(7)
C(43)	C(44)	1.377(7)	C(43)	C(48)	1.407(6)
C(44)	C(45)	1.393(6)	C(45)	C(46)	1.386(7)
C(46)	C(47)	1.372(8)	C(47)	C(48)	1.400(6)
C(49)	C(50)	1.387(6)	C(49)	C(54)	1.396(6)
C(50)	C(51)	1.379(6)	C(51)	C(52)	1.384(6)

Table 4. Bond lengths (\AA) -- continued

atom	atom	distance	atom	atom	distance
C(52)	C(53)	1.386(6)	C(53)	C(54)	1.387(6)
C(55)	C(56)	1.403(6)	C(55)	C(60)	1.386(7)
C(56)	C(57)	1.383(6)	C(57)	C(58)	1.377(8)
C(58)	C(59)	1.380(7)	C(59)	C(60)	1.378(6)

Table 6. Bond angles ($^{\circ}$)

atom	atom	atom	angle	atom	atom	atom	angle
Cu(2)	Br(1)	Cu(1)	69.96(2)	Br(1)	Cu(1)	Br(2)	106.61(2)
Br(1)	Cu(1)	P(1)	121.14(3)	Br(1)	Cu(1)	P(2)	120.62(4)
Br(1)	Cu(2)	Br(2)	108.59(2)	Br(1)	Cu(2)	P(3)	108.99(4)
Br(1)	Cu(2)	P(4)	110.41(4)	Cu(2)	Br(2)	Cu(1)	69.71(2)
Br(2)	Cu(1)	P(1)	109.79(3)	Br(2)	Cu(1)	P(2)	106.80(3)
Br(2)	Cu(2)	P(3)	121.35(4)	Br(2)	Cu(2)	P(4)	118.14(4)
P(2)	Cu(1)	P(1)	90.59(4)	Cu(1)	P(1)	C(1)	102.2(1)
Cu(1)	P(1)	C(7)	116.3(1)	Cu(1)	P(1)	C(13)	123.2(1)
Cu(1)	P(2)	C(6)	102.3(1)	Cu(1)	P(2)	C(19)	119.6(1)
Cu(1)	P(2)	C(25)	121.2(1)	P(4)	Cu(2)	P(3)	87.82(4)
Cu(2)	P(3)	C(31)	101.0(1)	Cu(2)	P(3)	C(43)	114.8(2)
Cu(2)	P(3)	C(37)	125.7(1)	Cu(2)	P(4)	C(36)	101.6(1)
Cu(2)	P(4)	C(55)	113.8(1)	Cu(2)	P(4)	C(49)	124.7(1)
P(1)	C(1)	C(6)	119.8(3)	C(7)	P(1)	C(1)	105.1(2)
P(1)	C(1)	C(2)	122.1(3)	C(13)	P(1)	C(1)	104.2(2)
P(1)	C(7)	C(8)	123.8(3)	P(1)	C(7)	C(12)	117.5(3)
C(13)	P(1)	C(7)	103.8(2)	P(1)	C(13)	C(14)	117.0(3)
P(1)	C(13)	C(18)	125.1(3)	P(2)	C(6)	C(1)	118.4(3)
C(19)	P(2)	C(6)	102.9(2)	C(25)	P(2)	C(6)	103.6(2)

P(2)	C(6)	C(5)	121.9(3)	C(25)	P(2)	C(19)	104.6(2)
P(2)	C(19)	C(20)	120.1(3)	P(2)	C(19)	C(24)	121.4(4)
P(2)	C(25)	C(26)	122.9(3)	P(2)	C(25)	C(30)	118.5(3)
P(3)	C(31)	C(36)	116.0(3)	C(43)	P(3)	C(31)	101.3(2)
P(3)	C(31)	C(32)	124.1(3)	C(37)	P(3)	C(31)	104.4(2)
C(43)	P(3)	C(37)	106.2(2)	P(3)	C(37)	C(38)	122.4(3)
P(3)	C(37)	C(42)	118.6(3)	P(3)	C(43)	C(44)	118.8(3)
P(3)	C(43)	C(48)	121.0(4)	P(4)	C(36)	C(31)	119.0(3)
C(55)	P(4)	C(36)	104.4(2)	P(4)	C(36)	C(35)	122.9(3)
C(49)	P(4)	C(36)	104.6(2)	C(55)	P(4)	C(49)	105.4(2)
P(4)	C(49)	C(50)	124.2(3)	P(4)	C(49)	C(54)	117.4(3)
P(4)	C(55)	C(56)	123.2(4)	P(4)	C(55)	C(60)	118.0(3)
C(6)	C(1)	C(2)	118.2(4)	C(1)	C(2)	C(3)	121.4(4)
C(1)	C(6)	C(5)	119.7(4)	C(2)	C(3)	C(4)	119.4(4)
C(3)	C(4)	C(5)	120.4(4)	C(4)	C(5)	C(6)	120.8(4)
C(12)	C(7)	C(8)	118.7(3)	C(7)	C(8)	C(9)	120.1(4)
C(7)	C(12)	C(11)	121.6(4)	C(8)	C(9)	C(10)	120.7(4)
C(9)	C(10)	C(11)	120.4(4)	C(10)	C(11)	C(12)	118.5(4)

Table 6. Bond angles ($^{\circ}$) -- continued

atom	atom	atom	angle	atom	atom	atom	angle
C(18)	C(13)	C(14)	117.9(4)	C(13)	C(14)	C(15)	120.8(4)
C(13)	C(18)	C(17)	120.9(4)	C(14)	C(15)	C(16)	120.9(4)
C(15)	C(16)	C(17)	118.5(4)	C(16)	C(17)	C(18)	120.9(4)
C(24)	C(19)	C(20)	118.4(4)	C(19)	C(20)	C(21)	121.7(4)
C(19)	C(24)	C(23)	119.6(5)	C(20)	C(21)	C(22)	119.2(5)
C(21)	C(22)	C(23)	119.7(4)	C(22)	C(23)	C(24)	121.4(4)
C(30)	C(25)	C(26)	118.4(4)	C(25)	C(26)	C(27)	120.4(4)
C(25)	C(30)	C(29)	121.4(4)	C(26)	C(27)	C(28)	120.1(4)
C(27)	C(28)	C(29)	119.8(4)	C(28)	C(29)	C(30)	119.8(5)
C(36)	C(31)	C(32)	119.9(4)	C(31)	C(32)	C(33)	120.4(4)
C(31)	C(36)	C(35)	118.1(4)	C(32)	C(33)	C(34)	120.4(4)
C(33)	C(34)	C(35)	119.5(4)	C(34)	C(35)	C(36)	121.6(4)
C(42)	C(37)	C(38)	118.6(4)	C(37)	C(38)	C(39)	119.9(4)
C(37)	C(42)	C(41)	120.7(4)	C(38)	C(39)	C(40)	120.3(4)
C(39)	C(40)	C(41)	119.1(4)	C(40)	C(41)	C(42)	121.4(5)
C(48)	C(43)	C(44)	119.7(4)	C(43)	C(44)	C(45)	120.8(4)
C(43)	C(48)	C(47)	118.7(5)	C(44)	C(45)	C(46)	119.7(5)
C(45)	C(46)	C(47)	119.9(4)	C(46)	C(47)	C(48)	121.2(4)
C(54)	C(49)	C(50)	118.2(4)	C(49)	C(50)	C(51)	121.3(4)
C(49)	C(54)	C(53)	120.5(4)	C(50)	C(51)	C(52)	120.3(4)
C(51)	C(52)	C(53)	119.2(4)	C(52)	C(53)	C(54)	120.4(4)
C(60)	C(55)	C(56)	118.6(4)	C(55)	C(56)	C(57)	119.7(5)
C(55)	C(60)	C(59)	120.8(4)	C(56)	C(57)	C(58)	121.0(4)
C(57)	C(58)	C(59)	119.3(4)	C(58)	C(59)	C(60)	120.5(5)

Table 8. Torsion Angles($^{\circ}$)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle

Cu(2)	Br(1)	Cu(1)	Br(2)	-17.02(3)	Cu(2)	Br(1)	Cu(1)	P(1)	-143.39(4)
Cu(2)	Br(1)	Cu(1)	P(2)	104.78(4)	Cu(1)	Br(1)	Cu(2)	Br(2)	17.97(3)
Cu(1)	Br(1)	Cu(2)	P(3)	152.09(4)	Cu(1)	Br(1)	Cu(2)	P(4)	-113.03(4)
Cu(2)	Br(2)	Cu(1)	Br(1)	17.52(3)	Cu(2)	Br(2)	Cu(1)	P(1)	150.44(4)
Cu(2)	Br(2)	Cu(1)	P(2)	-112.66(4)	Cu(1)	Br(2)	Cu(2)	Br(1)	-17.42(3)
Cu(1)	Br(2)	Cu(2)	P(3)	-144.78(4)	Cu(1)	Br(2)	Cu(2)	P(4)	109.25(4)
Br(1)	Cu(1)	P(1)	C(1)	-149.0(1)	Br(1)	Cu(1)	P(1)	C(7)	-35.2(2)
Br(1)	Cu(1)	P(1)	C(13)	94.8(2)	Br(2)	Cu(1)	P(1)	C(1)	86.0(1)
Br(2)	Cu(1)	P(1)	C(7)	-160.1(1)	Br(2)	Cu(1)	P(1)	C(13)	-30.1(2)
P(2)	Cu(1)	P(1)	C(1)	-22.1(1)	P(2)	Cu(1)	P(1)	C(7)	91.8(1)
P(2)	Cu(1)	P(1)	C(13)	-138.2(2)	Br(1)	Cu(1)	P(2)	C(6)	149.8(1)
Br(1)	Cu(1)	P(2)	C(19)	37.1(2)	Br(1)	Cu(1)	P(2)	C(25)	-95.9(2)
Br(2)	Cu(1)	P(2)	C(6)	-88.5(1)	Br(2)	Cu(1)	P(2)	C(19)	158.8(2)
Br(2)	Cu(1)	P(2)	C(25)	25.8(2)	P(1)	Cu(1)	P(2)	C(6)	22.4(1)
P(1)	Cu(1)	P(2)	C(19)	-90.3(2)	P(1)	Cu(1)	P(2)	C(25)	136.7(2)
Br(1)	Cu(2)	P(3)	C(31)	77.7(1)	Br(1)	Cu(2)	P(3)	C(37)	-39.1(2)
Br(1)	Cu(2)	P(3)	C(43)	-174.3(2)	Br(2)	Cu(2)	P(3)	C(31)	-155.1(1)
Br(2)	Cu(2)	P(3)	C(37)	88.1(2)	Br(2)	Cu(2)	P(3)	C(43)	-47.1(2)
P(4)	Cu(2)	P(3)	C(31)	-33.2(1)	P(4)	Cu(2)	P(3)	C(37)	-150.0(2)
P(4)	Cu(2)	P(3)	C(43)	74.9(2)	Br(1)	Cu(2)	P(4)	C(36)	-78.7(1)
Br(1)	Cu(2)	P(4)	C(49)	38.4(2)	Br(1)	Cu(2)	P(4)	C(55)	169.6(2)
Br(2)	Cu(2)	P(4)	C(36)	155.5(1)	Br(2)	Cu(2)	P(4)	C(49)	-87.4(2)
Br(2)	Cu(2)	P(4)	C(55)	43.8(2)	P(3)	Cu(2)	P(4)	C(36)	30.7(1)
P(3)	Cu(2)	P(4)	C(49)	147.8(2)	P(3)	Cu(2)	P(4)	C(55)	-80.9(2)
Cu(1)	P(1)	C(1)	C(2)	-162.7(3)	Cu(1)	P(1)	C(1)	C(6)	17.1(3)
C(7)	P(1)	C(1)	C(2)	75.4(3)	C(7)	P(1)	C(1)	C(6)	-104.8(3)
C(13)	P(1)	C(1)	C(2)	-33.5(3)	C(13)	P(1)	C(1)	C(6)	146.4(3)
Cu(1)	P(1)	C(7)	C(8)	-145.6(3)	Cu(1)	P(1)	C(7)	C(12)	34.6(4)
C(1)	P(1)	C(7)	C(8)	-33.4(4)	C(1)	P(1)	C(7)	C(12)	146.7(3)
C(13)	P(1)	C(7)	C(8)	75.7(4)	C(13)	P(1)	C(7)	C(12)	-104.1(3)
Cu(1)	P(1)	C(13)	C(14)	16.0(4)	Cu(1)	P(1)	C(13)	C(18)	-161.9(4)
C(1)	P(1)	C(13)	C(14)	-99.2(3)	C(1)	P(1)	C(13)	C(18)	82.9(4)
C(7)	P(1)	C(13)	C(14)	151.0(3)	C(7)	P(1)	C(13)	C(18)	-26.9(4)
Cu(1)	P(2)	C(6)	C(1)	-18.3(3)	Cu(1)	P(2)	C(6)	C(5)	162.7(3)
C(19)	P(2)	C(6)	C(1)	106.3(3)	C(19)	P(2)	C(6)	C(5)	-72.7(3)
C(25)	P(2)	C(6)	C(1)	-145.0(3)	C(25)	P(2)	C(6)	C(5)	36.0(3)
Cu(1)	P(2)	C(19)	C(20)	-14.2(4)	Cu(1)	P(2)	C(19)	C(24)	168.6(3)

Table 8. Torsion angles ($^{\circ}$) -- continued

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(6)	P(2)	C(19)	C(20)	-126.5(3)	C(6)	P(2)	C(19)	C(24)	56.2(4)
C(25)	P(2)	C(19)	C(20)	125.5(3)	C(25)	P(2)	C(19)	C(24)	-51.7(4)
Cu(1)	P(2)	C(25)	C(26)	121.8(3)	Cu(1)	P(2)	C(25)	C(30)	-52.9(4)
C(6)	P(2)	C(25)	C(26)	-124.5(4)	C(6)	P(2)	C(25)	C(30)	60.8(4)
C(19)	P(2)	C(25)	C(26)	-17.1(4)	C(19)	P(2)	C(25)	C(30)	168.2(3)
Cu(2)	P(3)	C(31)	C(32)	-152.8(3)	Cu(2)	P(3)	C(31)	C(36)	29.7(3)
C(37)	P(3)	C(31)	C(32)	-21.3(3)	C(37)	P(3)	C(31)	C(36)	161.3(3)
C(43)	P(3)	C(31)	C(32)	88.8(3)	C(43)	P(3)	C(31)	C(36)	-88.6(3)
Cu(2)	P(3)	C(37)	C(38)	-121.2(4)	Cu(2)	P(3)	C(37)	C(42)	50.6(5)
C(31)	P(3)	C(37)	C(38)	123.6(4)	C(31)	P(3)	C(37)	C(42)	-64.7(4)

C(43)	P(3)	C(37)	C(38)	17.0(4)	C(43)	P(3)	C(37)	C(42)	-171.2(4)
Cu(2)	P(3)	C(43)	C(44)	18.7(4)	Cu(2)	P(3)	C(43)	C(48)	-153.7(3)
C(31)	P(3)	C(43)	C(44)	126.5(3)	C(31)	P(3)	C(43)	C(48)	-45.9(3)
C(37)	P(3)	C(43)	C(44)	-124.7(3)	C(37)	P(3)	C(43)	C(48)	62.9(4)
Cu(2)	P(4)	C(36)	C(31)	-21.1(3)	Cu(2)	P(4)	C(36)	C(35)	157.8(3)
C(49)	P(4)	C(36)	C(31)	-151.9(3)	C(49)	P(4)	C(36)	C(35)	27.0(3)
C(55)	P(4)	C(36)	C(31)	97.5(3)	C(55)	P(4)	C(36)	C(35)	-83.6(3)
Cu(2)	P(4)	C(49)	C(50)	148.7(4)	Cu(2)	P(4)	C(49)	C(54)	-27.5(5)
C(36)	P(4)	C(49)	C(50)	-95.6(4)	C(36)	P(4)	C(49)	C(54)	88.2(4)
C(55)	P(4)	C(49)	C(50)	14.2(5)	C(55)	P(4)	C(49)	C(54)	-162.0(3)
Cu(2)	P(4)	C(55)	C(56)	120.1(3)	Cu(2)	P(4)	C(55)	C(60)	-55.1(4)
C(36)	P(4)	C(55)	C(56)	10.2(4)	C(36)	P(4)	C(55)	C(60)	-165.0(3)
C(49)	P(4)	C(55)	C(56)	-99.8(3)	C(49)	P(4)	C(55)	C(60)	85.1(3)
P(1)	C(1)	C(2)	C(3)	-179.3(3)	C(6)	C(1)	C(2)	C(3)	0.8(6)
P(1)	C(1)	C(6)	P(2)	0.8(4)	P(1)	C(1)	C(6)	C(5)	179.8(3)
C(2)	C(1)	C(6)	P(2)	-179.4(3)	C(2)	C(1)	C(6)	C(5)	-0.3(5)
C(1)	C(2)	C(3)	C(4)	-0.6(6)	C(2)	C(3)	C(4)	C(5)	-0.1(5)
C(3)	C(4)	C(5)	C(6)	0.6(6)	C(4)	C(5)	C(6)	P(2)	178.6(3)
C(4)	C(5)	C(6)	C(1)	-0.4(6)	P(1)	C(7)	C(8)	C(9)	-178.6(3)
C(12)	C(7)	C(8)	C(9)	1.2(6)	P(1)	C(7)	C(12)	C(11)	179.4(4)
C(8)	C(7)	C(12)	C(11)	-0.5(6)	C(7)	C(8)	C(9)	C(10)	-1.3(6)
C(8)	C(9)	C(10)	C(11)	0.6(7)	C(9)	C(10)	C(11)	C(12)	0.1(5)
C(10)	C(11)	C(12)	C(7)	-0.2(5)	P(1)	C(13)	C(14)	C(15)	-179.1(4)
C(18)	C(13)	C(14)	C(15)	-1.1(7)	P(1)	C(13)	C(18)	C(17)	-179.8(4)
C(14)	C(13)	C(18)	C(17)	2.3(7)	C(13)	C(14)	C(15)	C(16)	-0.1(6)
C(14)	C(15)	C(16)	C(17)	0.1(6)	C(15)	C(16)	C(17)	C(18)	1.1(8)
C(16)	C(17)	C(18)	C(13)	-2.4(8)	P(2)	C(19)	C(20)	C(21)	-177.3(4)

Table 8. Torsion angles ($^{\circ}$) -- continued

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(24)	C(19)	C(20)	C(21)	-0.0(6)	P(2)	C(19)	C(24)	C(23)	177.3(4)
C(20)	C(19)	C(24)	C(23)	0.0(5)	C(19)	C(20)	C(21)	C(22)	0.6(7)
C(20)	C(21)	C(22)	C(23)	-1.3(7)	C(21)	C(22)	C(23)	C(24)	1.3(7)
C(22)	C(23)	C(24)	C(19)	-0.7(7)	P(2)	C(25)	C(26)	C(27)	-176.2(4)
C(30)	C(25)	C(26)	C(27)	-1.5(7)	P(2)	C(25)	C(30)	C(29)	176.5(4)
C(26)	C(25)	C(30)	C(29)	1.5(7)	C(25)	C(26)	C(27)	C(28)	-1.1(7)
C(26)	C(27)	C(28)	C(29)	3.7(8)	C(27)	C(28)	C(29)	C(30)	-3.8(8)
C(28)	C(29)	C(30)	C(25)	1.1(8)	P(3)	C(31)	C(32)	C(33)	-175.5(3)
C(36)	C(31)	C(32)	C(33)	1.8(5)	P(3)	C(31)	C(36)	P(4)	-5.9(4)
P(3)	C(31)	C(36)	C(35)	175.1(3)	C(32)	C(31)	C(36)	P(4)	176.5(3)
C(32)	C(31)	C(36)	C(35)	-2.4(5)	C(31)	C(32)	C(33)	C(34)	0.4(6)
C(32)	C(33)	C(34)	C(35)	-2.0(6)	C(33)	C(34)	C(35)	C(36)	1.3(6)
C(34)	C(35)	C(36)	P(4)	-178.1(3)	C(34)	C(35)	C(36)	C(31)	0.8(5)
P(3)	C(37)	C(38)	C(39)	170.7(4)	C(42)	C(37)	C(38)	C(39)	-1.1(7)
P(3)	C(37)	C(42)	C(41)	-171.8(4)	C(38)	C(37)	C(42)	C(41)	0.3(7)
C(37)	C(38)	C(39)	C(40)	1.5(8)	C(38)	C(39)	C(40)	C(41)	-1.1(9)
C(39)	C(40)	C(41)	C(42)	0.3(7)	C(40)	C(41)	C(42)	C(37)	0.1(7)
P(3)	C(43)	C(44)	C(45)	-172.4(3)	C(48)	C(43)	C(44)	C(45)	0.0(5)
P(3)	C(43)	C(48)	C(47)	172.9(3)	C(44)	C(43)	C(48)	C(47)	0.6(6)
C(43)	C(44)	C(45)	C(46)	-0.0(6)	C(44)	C(45)	C(46)	C(47)	-0.7(7)

C(45)	C(46)	C(47)	C(48)	1.4(7)	C(46)	C(47)	C(48)	C(43)	-1.3(6)
P(4)	C(49)	C(50)	C(51)	-174.5(4)	C(54)	C(49)	C(50)	C(51)	1.7(7)
P(4)	C(49)	C(54)	C(53)	176.4(4)	C(50)	C(49)	C(54)	C(53)	-0.1(6)
C(49)	C(50)	C(51)	C(52)	-2.0(8)	C(50)	C(51)	C(52)	C(53)	0.7(8)
C(51)	C(52)	C(53)	C(54)	0.8(8)	C(52)	C(53)	C(54)	C(49)	-1.2(8)
P(4)	C(55)	C(56)	C(57)	-175.2(4)	C(60)	C(55)	C(56)	C(57)	-0.1(5)
P(4)	C(55)	C(60)	C(59)	175.2(4)	C(56)	C(55)	C(60)	C(59)	-0.1(5)
C(55)	C(56)	C(57)	C(58)	0.9(7)	C(56)	C(57)	C(58)	C(59)	-1.5(7)
C(57)	C(58)	C(59)	C(60)	1.2(7)	C(58)	C(59)	C(60)	C(55)	-0.4(6)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table S5.
[Cu(μCl)dppb]₂ (3)

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	C ₆₀ H ₄₈ P ₄ Cu ₂ Cl ₂
Formula Weight	1090.93
Crystal Color, Habit	yellow, platelet
Crystal Dimensions	0.30 X 0.25 X 0.10 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 90.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm

Lattice Parameters	a = 11.137(8) Å b = 18.74(2) Å c = 12.303(8) Å β = 97.45(3) ° V = 2545(3) Å ³
--------------------	------------------------------------------------------------------------------------------------------

Space Group	P2 ₁ (#4)
Z value	2
D _{calc}	1.423 g/cm ³
F ₀₀₀	1120.00
μ(MoKα)	11.06 cm ⁻¹

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated

Detector Aperture	280 mm x 256 mm
Data Images	83 exposures
ω oscillation Range (χ =45.0, ϕ =30.0)	130.0 - 190.0°
Exposure Rate	30.0 sec./°
ω oscillation Range (χ =45.0, ϕ =180.0)	0.0 - 159.0°
Exposure Rate	30.0 sec./°
Detector Position	127.40 mm
Pixel Size	0.100 mm
2θ _{max}	54.9°

No. of Reflections Measured	Total: 23769
Corrections	Unique: 11026 ($R_{\text{int}} = 0.058$)
	Lorentz-polarization
	Absorption
	(trans. factors: 0.7248 - 1.0000)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF99 PATTY)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\sum w (F_o^2 - F_c^2)^2$
Least Squares Weights	$1/[0.7720\sigma(F_o^2)]/(4F_o^2)$
$2\theta_{\text{max}}$ cutoff	54.9°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	11026
No. Variables	661
Reflection/Parameter Ratio	16.68
Residuals: R (All reflections)	0.088
Residuals: R1 ($I > 2.00\sigma(I)$)	0.042
Residuals: wR2 (All reflections)	0.052
Goodness of Fit Indicator	0.960
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	$1.51 \text{ e}^-/\text{\AA}^3$
Minimum peak in Final Diff. Map	$-1.01 \text{ e}^-/\text{\AA}^3$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Cu(1)	Cl(1)	2.383(1)	Cu(1)	Cl(2)	2.316(1)
Cu(1)	P(1)	2.255(2)	Cu(1)	P(2)	2.260(2)
Cu(2)	Cl(1)	2.324(1)	Cu(2)	Cl(2)	2.414(1)
Cu(2)	P(3)	2.246(2)	Cu(2)	P(4)	2.255(1)
P(1)	C(1)	1.829(5)	P(1)	C(7)	1.814(5)
P(1)	C(25)	1.837(4)	P(2)	C(13)	1.817(5)
P(2)	C(19)	1.802(6)	P(2)	C(30)	1.831(5)
P(3)	C(31)	1.825(5)	P(3)	C(37)	1.804(5)
P(3)	C(60)	1.848(4)	P(4)	C(43)	1.824(4)
P(4)	C(49)	1.809(5)	P(4)	C(55)	1.845(5)
C(1)	C(2)	1.390(7)	C(1)	C(6)	1.369(6)
C(2)	C(3)	1.383(9)	C(3)	C(4)	1.381(8)
C(4)	C(5)	1.357(9)	C(5)	C(6)	1.383(8)
C(7)	C(8)	1.377(8)	C(7)	C(12)	1.362(8)
C(8)	C(9)	1.358(9)	C(9)	C(10)	1.376(9)
C(10)	C(9)	1.376(9)	C(10)	C(11)	1.36(1)
C(11)	C(10)	1.36(1)	C(11)	C(12)	1.374(9)
C(13)	C(14)	1.370(8)	C(13)	C(18)	1.385(7)
C(14)	C(15)	1.382(9)	C(15)	C(16)	1.363(9)

C(16)	C(17)	1.37(1)	C(17)	C(18)	1.384(8)
C(19)	C(20)	1.361(9)	C(19)	C(24)	1.383(9)
C(20)	C(21)	1.39(1)	C(21)	C(22)	1.34(1)
C(22)	C(23)	1.36(1)	C(23)	C(24)	1.362(9)
C(25)	C(26)	1.362(7)	C(25)	C(30)	1.396(7)
C(26)	C(27)	1.373(7)	C(27)	C(28)	1.36(1)
C(28)	C(29)	1.385(7)	C(29)	C(30)	1.401(7)
C(31)	C(32)	1.381(7)	C(31)	C(36)	1.382(8)
C(32)	C(33)	1.377(8)	C(33)	C(34)	1.38(1)
C(34)	C(35)	1.35(1)	C(35)	C(34)	1.35(1)
C(35)	C(36)	1.357(9)	C(36)	C(35)	1.357(9)
C(37)	C(38)	1.373(7)	C(37)	C(42)	1.383(7)
C(38)	C(39)	1.379(8)	C(39)	C(40)	1.352(9)
C(40)	C(41)	1.352(9)	C(41)	C(42)	1.399(9)
C(43)	C(44)	1.365(7)	C(43)	C(48)	1.374(6)
C(44)	C(45)	1.391(7)	C(45)	C(46)	1.340(7)
C(46)	C(47)	1.371(8)	C(47)	C(48)	1.382(7)
C(49)	C(50)	1.384(7)	C(49)	C(54)	1.383(7)

Table 4. Bond lengths (Å) -- continued

atom	atom	distance	atom	atom	distance
C(50)	C(51)	1.366(8)	C(51)	C(52)	1.358(8)
C(52)	C(53)	1.353(9)	C(53)	C(54)	1.399(9)
C(55)	C(56)	1.384(6)	C(55)	C(60)	1.403(6)
C(56)	C(57)	1.362(7)	C(57)	C(58)	1.387(8)
C(58)	C(59)	1.378(6)	C(59)	C(60)	1.396(7)

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cu(1)	Cl(1)	Cu(2)	74.99(4)	Cl(2)	Cu(1)	Cl(1)	102.87(4)
P(1)	Cu(1)	Cl(1)	112.02(6)	P(2)	Cu(1)	Cl(1)	112.21(5)
Cu(1)	Cl(2)	Cu(2)	74.54(4)	P(1)	Cu(1)	Cl(2)	118.75(6)
P(2)	Cu(1)	Cl(2)	123.49(6)	P(2)	Cu(1)	P(1)	87.50(5)
Cu(1)	P(1)	C(1)	114.4(2)	Cu(1)	P(1)	C(25)	101.8(2)
Cu(1)	P(1)	C(7)	124.8(2)	Cu(1)	P(2)	C(13)	114.0(2)
Cu(1)	P(2)	C(30)	100.6(2)	Cu(1)	P(2)	C(19)	126.1(2)
Cl(2)	Cu(2)	Cl(1)	101.67(4)	P(3)	Cu(2)	Cl(1)	122.47(6)
P(4)	Cu(2)	Cl(1)	121.40(5)	P(3)	Cu(2)	Cl(2)	109.31(5)
P(4)	Cu(2)	Cl(2)	111.36(5)	P(4)	Cu(2)	P(3)	90.56(5)
Cu(2)	P(3)	C(31)	121.3(2)	Cu(2)	P(3)	C(37)	119.6(2)
Cu(2)	P(3)	C(60)	102.3(2)	Cu(2)	P(4)	C(43)	115.8(1)
Cu(2)	P(4)	C(49)	122.5(2)	Cu(2)	P(4)	C(55)	102.9(1)
C(25)	P(1)	C(1)	103.8(2)	P(1)	C(1)	C(2)	116.1(4)
P(1)	C(1)	C(6)	124.7(4)	C(7)	P(1)	C(1)	105.1(2)
C(25)	P(1)	C(7)	104.5(2)	P(1)	C(7)	C(8)	117.9(4)
P(1)	C(7)	C(12)	124.2(4)	P(1)	C(25)	C(30)	117.7(3)
P(1)	C(25)	C(26)	123.1(4)	P(2)	C(13)	C(14)	118.6(4)
C(30)	P(2)	C(13)	100.7(2)	P(2)	C(13)	C(18)	122.8(4)

C(19)	P(2)	C(13)	106.5(2)	C(30)	P(2)	C(19)	105.3(2)
P(2)	C(19)	C(20)	125.7(5)	P(2)	C(19)	C(24)	118.0(4)
P(2)	C(30)	C(25)	118.2(3)	P(2)	C(30)	C(29)	123.0(4)
C(37)	P(3)	C(31)	104.9(2)	C(60)	P(3)	C(31)	103.3(2)
P(3)	C(31)	C(32)	117.9(4)	P(3)	C(31)	C(36)	124.2(4)
C(60)	P(3)	C(37)	102.5(2)	P(3)	C(37)	C(38)	123.4(4)
P(3)	C(37)	C(42)	119.9(4)	P(3)	C(60)	C(55)	119.8(3)
P(3)	C(60)	C(59)	122.0(3)	C(49)	P(4)	C(43)	104.1(2)
C(55)	P(4)	C(43)	105.0(2)	P(4)	C(43)	C(44)	117.6(3)
P(4)	C(43)	C(48)	125.0(4)	C(55)	P(4)	C(49)	104.8(2)
P(4)	C(49)	C(50)	117.3(3)	P(4)	C(49)	C(54)	125.8(4)
P(4)	C(55)	C(60)	118.4(3)	P(4)	C(55)	C(56)	121.7(4)
C(6)	C(1)	C(2)	119.1(5)	C(1)	C(2)	C(3)	119.9(5)
C(1)	C(6)	C(5)	120.4(5)	C(2)	C(3)	C(4)	120.2(6)
C(3)	C(4)	C(5)	119.5(6)	C(4)	C(5)	C(6)	120.8(5)
C(12)	C(7)	C(8)	117.9(5)	C(7)	C(8)	C(9)	121.3(5)
C(7)	C(12)	C(11)	121.3(5)	C(8)	C(9)	C(10)	120.3(6)
C(9)	C(10)	C(11)	118.9(6)	C(10)	C(11)	C(12)	120.2(6)

Table 6. Bond angles ($^{\circ}$) -- continued

atom	atom	atom	angle	atom	atom	atom	angle
C(18)	C(13)	C(14)	118.2(5)	C(13)	C(14)	C(15)	121.4(5)
C(13)	C(18)	C(17)	120.8(5)	C(14)	C(15)	C(16)	119.5(6)
C(15)	C(16)	C(17)	120.6(6)	C(16)	C(17)	C(18)	119.4(5)
C(24)	C(19)	C(20)	116.0(5)	C(19)	C(20)	C(21)	121.4(6)
C(19)	C(24)	C(23)	121.9(6)	C(20)	C(21)	C(22)	121.8(7)
C(21)	C(22)	C(23)	117.5(7)	C(22)	C(23)	C(24)	121.4(6)
C(30)	C(25)	C(26)	119.2(4)	C(25)	C(26)	C(27)	121.9(5)
C(25)	C(30)	C(29)	118.7(4)	C(26)	C(27)	C(28)	120.0(5)
C(27)	C(28)	C(29)	119.8(5)	C(28)	C(29)	C(30)	120.4(5)
C(36)	C(31)	C(32)	117.7(5)	C(31)	C(32)	C(33)	120.6(5)
C(31)	C(36)	C(35)	121.8(5)	C(32)	C(33)	C(34)	119.6(6)
C(33)	C(34)	C(35)	120.2(6)	C(34)	C(35)	C(36)	120.0(6)
C(42)	C(37)	C(38)	116.7(5)	C(37)	C(38)	C(39)	123.0(5)
C(37)	C(42)	C(41)	120.4(5)	C(38)	C(39)	C(40)	118.9(5)
C(39)	C(40)	C(41)	120.7(6)	C(40)	C(41)	C(42)	120.3(6)
C(48)	C(43)	C(44)	117.3(4)	C(43)	C(44)	C(45)	122.0(4)
C(43)	C(48)	C(47)	121.1(5)	C(44)	C(45)	C(46)	119.4(5)
C(45)	C(46)	C(47)	120.3(5)	C(46)	C(47)	C(48)	119.7(5)
C(54)	C(49)	C(50)	116.9(5)	C(49)	C(50)	C(51)	121.7(4)
C(49)	C(54)	C(53)	120.9(5)	C(50)	C(51)	C(52)	120.6(5)
C(51)	C(52)	C(53)	119.9(6)	C(52)	C(53)	C(54)	120.0(5)
C(60)	C(55)	C(56)	119.9(4)	C(55)	C(56)	C(57)	120.8(4)
C(55)	C(60)	C(59)	118.3(4)	C(56)	C(57)	C(58)	120.5(4)
C(57)	C(58)	C(59)	119.3(5)	C(58)	C(59)	C(60)	121.2(4)

Table 8. Torsion Angles($^{\circ}$)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl(2)	Cu(1)	Cl(1)	Cu(2)	19.00(5)	P(1)	Cu(1)	Cl(1)	Cu(2)	-109.65(5)

P(2)	Cu(1)	Cl(1)	Cu(2)	153.80(5)	Cl(1)	Cu(1)	Cl(2)	Cu(2)	-18.31(5)
P(1)	Cu(1)	Cl(2)	Cu(2)	106.02(5)	P(2)	Cu(1)	Cl(2)	Cu(2)	-146.33(5)
Cl(1)	Cu(1)	P(1)	C(1)	166.0(2)	Cl(1)	Cu(1)	P(1)	C(7)	34.4(2)
Cl(1)	Cu(1)	P(1)	C(25)	-82.7(1)	Cl(2)	Cu(1)	P(1)	C(1)	46.3(2)
Cl(2)	Cu(1)	P(1)	C(7)	-85.3(2)	Cl(2)	Cu(1)	P(1)	C(25)	157.5(1)
P(2)	Cu(1)	P(1)	C(1)	-81.0(2)	P(2)	Cu(1)	P(1)	C(7)	147.4(2)
P(2)	Cu(1)	P(1)	C(25)	30.2(1)	Cl(1)	Cu(1)	P(2)	C(13)	-172.8(2)
Cl(1)	Cu(1)	P(2)	C(19)	-37.6(2)	Cl(1)	Cu(1)	P(2)	C(30)	80.3(2)
Cl(2)	Cu(1)	P(2)	C(13)	-48.8(2)	Cl(2)	Cu(1)	P(2)	C(19)	86.3(2)
Cl(2)	Cu(1)	P(2)	C(30)	-155.7(2)	P(1)	Cu(1)	P(2)	C(13)	74.4(2)
P(1)	Cu(1)	P(2)	C(19)	-150.4(2)	P(1)	Cu(1)	P(2)	C(30)	-32.5(2)
Cl(2)	Cu(2)	Cl(1)	Cu(1)	-18.12(5)	P(3)	Cu(2)	Cl(1)	Cu(1)	103.99(5)
P(4)	Cu(2)	Cl(1)	Cu(1)	-142.30(5)	Cl(1)	Cu(2)	Cl(2)	Cu(1)	18.70(5)
P(3)	Cu(2)	Cl(2)	Cu(1)	-112.08(4)	P(4)	Cu(2)	Cl(2)	Cu(1)	149.39(4)
Cl(1)	Cu(2)	P(3)	C(31)	-96.3(2)	Cl(1)	Cu(2)	P(3)	C(37)	37.4(2)
Cl(1)	Cu(2)	P(3)	C(60)	149.6(1)	Cl(2)	Cu(2)	P(3)	C(31)	22.2(2)
Cl(2)	Cu(2)	P(3)	C(37)	155.9(2)	Cl(2)	Cu(2)	P(3)	C(60)	-91.9(2)
P(4)	Cu(2)	P(3)	C(31)	135.1(2)	P(4)	Cu(2)	P(3)	C(37)	-91.2(2)
P(4)	Cu(2)	P(3)	C(60)	21.1(2)	Cl(1)	Cu(2)	P(4)	C(43)	-36.3(2)
Cl(1)	Cu(2)	P(4)	C(49)	92.6(2)	Cl(1)	Cu(2)	P(4)	C(55)	-150.2(1)
Cl(2)	Cu(2)	P(4)	C(43)	-155.8(2)	Cl(2)	Cu(2)	P(4)	C(49)	-26.9(2)
Cl(2)	Cu(2)	P(4)	C(55)	90.3(2)	P(3)	Cu(2)	P(4)	C(43)	93.1(2)
P(3)	Cu(2)	P(4)	C(49)	-138.0(2)	P(3)	Cu(2)	P(4)	C(55)	-20.8(2)
Cu(1)	P(1)	C(1)	C(2)	-55.8(4)	Cu(1)	P(1)	C(1)	C(6)	119.4(4)
C(7)	P(1)	C(1)	C(2)	84.8(4)	C(7)	P(1)	C(1)	C(6)	-100.1(4)
C(25)	P(1)	C(1)	C(2)	-165.8(3)	C(25)	P(1)	C(1)	C(6)	9.4(5)
Cu(1)	P(1)	C(7)	C(8)	-28.8(5)	Cu(1)	P(1)	C(7)	C(12)	150.3(3)
C(1)	P(1)	C(7)	C(8)	-164.0(4)	C(1)	P(1)	C(7)	C(12)	15.2(5)
C(25)	P(1)	C(7)	C(8)	87.0(4)	C(25)	P(1)	C(7)	C(12)	-93.8(4)
Cu(1)	P(1)	C(25)	C(26)	157.6(3)	Cu(1)	P(1)	C(25)	C(30)	-20.7(4)
C(1)	P(1)	C(25)	C(26)	-83.3(4)	C(1)	P(1)	C(25)	C(30)	98.3(3)
C(7)	P(1)	C(25)	C(26)	26.6(4)	C(7)	P(1)	C(25)	C(30)	-151.8(3)
Cu(1)	P(2)	C(13)	C(14)	20.8(5)	Cu(1)	P(2)	C(13)	C(18)	-151.4(4)
C(19)	P(2)	C(13)	C(14)	-122.7(4)	C(19)	P(2)	C(13)	C(18)	65.0(5)
C(30)	P(2)	C(13)	C(14)	127.6(4)	C(30)	P(2)	C(13)	C(18)	-44.6(5)
Cu(1)	P(2)	C(19)	C(20)	-127.3(4)	Cu(1)	P(2)	C(19)	C(24)	47.3(5)

Table 8. Torsion angles ($^{\circ}$) -- continued

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(13)	P(2)	C(19)	C(20)	10.5(5)	C(13)	P(2)	C(19)	C(24)	-174.9(4)
C(30)	P(2)	C(19)	C(20)	116.9(4)	C(30)	P(2)	C(19)	C(24)	-68.5(4)
Cu(1)	P(2)	C(30)	C(25)	29.7(4)	Cu(1)	P(2)	C(30)	C(29)	-153.8(4)
C(13)	P(2)	C(30)	C(25)	-87.5(3)	C(13)	P(2)	C(30)	C(29)	89.0(4)
C(19)	P(2)	C(30)	C(25)	162.0(3)	C(19)	P(2)	C(30)	C(29)	-21.5(4)
Cu(2)	P(3)	C(31)	C(32)	-52.8(4)	Cu(2)	P(3)	C(31)	C(36)	121.6(4)
C(37)	P(3)	C(31)	C(32)	167.8(3)	C(37)	P(3)	C(31)	C(36)	-17.8(4)
C(60)	P(3)	C(31)	C(32)	60.8(4)	C(60)	P(3)	C(31)	C(36)	-124.8(4)
Cu(2)	P(3)	C(37)	C(38)	169.0(3)	Cu(2)	P(3)	C(37)	C(42)	-12.8(4)
C(31)	P(3)	C(37)	C(38)	-50.8(4)	C(31)	P(3)	C(37)	C(42)	127.5(4)
C(60)	P(3)	C(37)	C(38)	56.8(4)	C(60)	P(3)	C(37)	C(42)	-124.9(4)

Cu(2)	P(3)	C(60)	C(55)	-17.6(4)	Cu(2)	P(3)	C(60)	C(59)	162.6(4)
C(31)	P(3)	C(60)	C(55)	-144.3(3)	C(31)	P(3)	C(60)	C(59)	35.9(4)
C(37)	P(3)	C(60)	C(55)	106.8(4)	C(37)	P(3)	C(60)	C(59)	-72.9(4)
Cu(2)	P(4)	C(43)	C(44)	39.1(5)	Cu(2)	P(4)	C(43)	C(48)	-143.1(4)
C(49)	P(4)	C(43)	C(44)	-98.3(4)	C(49)	P(4)	C(43)	C(48)	79.5(5)
C(55)	P(4)	C(43)	C(44)	151.8(4)	C(55)	P(4)	C(43)	C(48)	-30.4(5)
Cu(2)	P(4)	C(49)	C(50)	17.7(5)	Cu(2)	P(4)	C(49)	C(54)	-162.2(4)
C(43)	P(4)	C(49)	C(50)	151.4(4)	C(43)	P(4)	C(49)	C(54)	-28.5(5)
C(55)	P(4)	C(49)	C(50)	-98.6(4)	C(55)	P(4)	C(49)	C(54)	81.5(5)
Cu(2)	P(4)	C(55)	C(56)	-163.0(3)	Cu(2)	P(4)	C(55)	C(60)	15.8(4)
C(43)	P(4)	C(55)	C(56)	75.5(4)	C(43)	P(4)	C(55)	C(60)	-105.8(3)
C(49)	P(4)	C(55)	C(56)	-33.9(4)	C(49)	P(4)	C(55)	C(60)	144.9(3)
P(1)	C(1)	C(2)	C(3)	175.3(5)	C(6)	C(1)	C(2)	C(3)	-0.1(6)
P(1)	C(1)	C(6)	C(5)	-174.1(5)	C(2)	C(1)	C(6)	C(5)	0.9(8)
C(1)	C(2)	C(3)	C(4)	-0.5(8)	C(2)	C(3)	C(4)	C(5)	0.3(7)
C(3)	C(4)	C(5)	C(6)	0.5(8)	C(4)	C(5)	C(6)	C(1)	-1.1(9)
P(1)	C(7)	C(8)	C(9)	178.2(5)	C(12)	C(7)	C(8)	C(9)	-1.0(8)
P(1)	C(7)	C(12)	C(11)	-177.5(4)	C(8)	C(7)	C(12)	C(11)	1.7(7)
C(7)	C(8)	C(9)	C(10)	-0.4(8)	C(8)	C(9)	C(10)	C(11)	1.1(9)
C(9)	C(10)	C(11)	C(12)	-0.4(8)	C(10)	C(11)	C(12)	C(7)	-1.0(8)
P(2)	C(13)	C(14)	C(15)	-172.3(4)	C(18)	C(13)	C(14)	C(15)	0.3(7)
P(2)	C(13)	C(18)	C(17)	173.3(5)	C(14)	C(13)	C(18)	C(17)	1.0(8)
C(13)	C(14)	C(15)	C(16)	0.2(6)	C(14)	C(15)	C(16)	C(17)	-2.0(9)
C(15)	C(16)	C(17)	C(18)	3.3(9)	C(16)	C(17)	C(18)	C(13)	-2.8(9)
P(2)	C(19)	C(20)	C(21)	172.9(5)	C(24)	C(19)	C(20)	C(21)	-1.7(8)
P(2)	C(19)	C(24)	C(23)	-174.2(5)	C(20)	C(19)	C(24)	C(23)	0.9(8)

Table 8. Torsion angles ($^{\circ}$) -- continued

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(19)	C(20)	C(21)	C(22)	1(1)	C(20)	C(21)	C(22)	C(23)	0(1)
C(21)	C(22)	C(23)	C(24)	-0.1(8)	C(22)	C(23)	C(24)	C(19)	0.0(8)
P(1)	C(25)	C(26)	C(27)	-178.6(4)	C(30)	C(25)	C(26)	C(27)	-0.3(5)
P(1)	C(25)	C(30)	P(2)	-6.2(5)	P(1)	C(25)	C(30)	C(29)	177.1(4)
C(26)	C(25)	C(30)	P(2)	175.4(3)	C(26)	C(25)	C(30)	C(29)	-1.3(6)
C(25)	C(26)	C(27)	C(28)	2.0(7)	C(26)	C(27)	C(28)	C(29)	-2.2(7)
C(27)	C(28)	C(29)	C(30)	0.6(7)	C(28)	C(29)	C(30)	P(2)	-175.4(3)
C(28)	C(29)	C(30)	C(25)	1.1(7)	P(3)	C(31)	C(32)	C(33)	177.9(4)
C(36)	C(31)	C(32)	C(33)	3.1(7)	P(3)	C(31)	C(36)	C(35)	-176.3(5)
C(32)	C(31)	C(36)	C(35)	-1.9(7)	C(31)	C(32)	C(33)	C(34)	-1.8(8)
C(32)	C(33)	C(34)	C(35)	0(1)	C(33)	C(34)	C(35)	C(36)	2(1)
C(34)	C(35)	C(36)	C(31)	-0.8(9)	P(3)	C(37)	C(38)	C(39)	179.1(4)
C(42)	C(37)	C(38)	C(39)	0.8(7)	P(3)	C(37)	C(42)	C(41)	-179.0(4)
C(38)	C(37)	C(42)	C(41)	-0.6(7)	C(37)	C(38)	C(39)	C(40)	-1.2(8)
C(38)	C(39)	C(40)	C(41)	1.3(8)	C(39)	C(40)	C(41)	C(42)	-1.1(9)
C(40)	C(41)	C(42)	C(37)	0.8(8)	P(4)	C(43)	C(44)	C(45)	179.3(5)
C(48)	C(43)	C(44)	C(45)	1.3(8)	P(4)	C(43)	C(48)	C(47)	-177.8(5)
C(44)	C(43)	C(48)	C(47)	-0.1(7)	C(43)	C(44)	C(45)	C(46)	0.5(9)
C(44)	C(45)	C(46)	C(47)	-3.6(9)	C(45)	C(46)	C(47)	C(48)	4.8(9)
C(46)	C(47)	C(48)	C(43)	-3.0(9)	P(4)	C(49)	C(50)	C(51)	-178.8(4)
C(54)	C(49)	C(50)	C(51)	1.1(7)	P(4)	C(49)	C(54)	C(53)	179.9(4)

C(50)	C(49)	C(54)	C(53)	-0.0(7)	C(49)	C(50)	C(51)	C(52)	-1.6(9)
C(50)	C(51)	C(52)	C(53)	1.0(9)	C(51)	C(52)	C(53)	C(54)	0(1)
C(52)	C(53)	C(54)	C(49)	-0.5(9)	P(4)	C(55)	C(56)	C(57)	-179.4(4)
C(60)	C(55)	C(56)	C(57)	1.9(7)	P(4)	C(55)	C(60)	P(3)	1.2(5)
P(4)	C(55)	C(60)	C(59)	-179.0(4)	C(56)	C(55)	C(60)	P(3)	-180.0(3)
C(56)	C(55)	C(60)	C(59)	-0.2(6)	C(55)	C(56)	C(57)	C(58)	-2.5(7)
C(56)	C(57)	C(58)	C(59)	1.5(8)	C(57)	C(58)	C(59)	C(60)	0.1(6)
C(58)	C(59)	C(60)	P(3)	179.0(4)	C(58)	C(59)	C(60)	C(55)	-0.7(7)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table S6.
CuI(dppb)PPh₃ (4)

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	C ₄₈ H ₄₀ CuP ₃ I
Formula Weight	900.22
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.20 X 0.20 X 0.20 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 60.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 15.11(1) Å b = 14.67(1) Å c = 18.33(2) Å β = 99.60(4) ° V = 4004(5) Å ³
Space Group	P2 ₁ (#4)
Z value	4
D _{calc}	1.493 g/cm ³
F ₀₀₀	1820.00
μ(MoKα)	14.70 cm ⁻¹

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Detector Aperture	280 mm x 256 mm
Data Images	55 exposures
ω oscillation Range (χ =45.0, ϕ =0.0)	130.0 - 190.0°
Exposure Rate	30.0 sec./°
ω oscillation Range (χ =45.0, ϕ =210.0)	0.0 - 160.0°
Exposure Rate	30.0 sec./°
Detector Position	127.40 mm
Pixel Size	0.100 mm
2θ _{max}	55.0
No. of Reflections Measured	Total: 35524 Unique: 35498 (R _{int} = 0.045)

Corrections

Lorentz-polarization
Absorption
(trans. factors: 0.4919 - 1.0000)

C. Structure Solution and Refinement

Structure Solution

Direct Methods (SIR92)

Refinement

Full-matrix least-squares on F^2

Function Minimized

$\Sigma w (Fo^2 - Fc^2)^2$

Least Squares Weights

$1/[0.0002Fo^2 + 0.5000\sigma(Fo^2)]/(4Fo^2)$

$2\theta_{\text{max}}$ cutoff

55.0°

Anomalous Dispersion

All non-hydrogen atoms

No. Observations (All reflections)

35498

No. Variables

1034

Reflection/Parameter Ratio

34.33

Residuals: R (All reflections)

0.044

Residuals: R1 ($I > 2.00\sigma(I)$)

0.037

Residuals: wR2 (All reflections)

0.082

Goodness of Fit Indicator

1.269

Flack Parameter

0.029(6)

Max Shift/Error in Final Cycle

0.000

Maximum peak in Final Diff. Map

5.36 e⁻/Å³

Minimum peak in Final Diff. Map

-3.69 e⁻/Å³

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
I(1)	Cu(1)	2.5975(4)	I(2)	Cu(2)	2.6409(4)
Cu(1)	P(1)	2.2609(9)	Cu(1)	P(2)	2.278(1)
Cu(1)	P(3)	2.271(1)	Cu(2)	P(4)	2.237(1)
Cu(2)	P(5)	2.2617(9)	Cu(2)	P(6)	2.2774(8)
P(1)	C(31)	1.825(3)	P(1)	C(37)	1.829(3)
P(1)	C(43)	1.826(3)	P(2)	C(1)	1.817(3)
P(2)	C(7)	1.839(3)	P(2)	C(13)	1.826(3)
P(3)	C(6)	1.840(3)	P(3)	C(19)	1.825(3)
P(3)	C(25)	1.840(3)	P(4)	C(79)	1.821(3)
P(4)	C(85)	1.821(3)	P(4)	C(91)	1.834(3)
P(5)	C(49)	1.828(3)	P(5)	C(55)	1.821(3)
P(5)	C(61)	1.821(3)	P(6)	C(54)	1.850(3)
P(6)	C(67)	1.826(3)	P(6)	C(73)	1.815(3)
C(1)	C(2)	1.396(5)	C(1)	C(6)	1.408(4)
C(2)	C(3)	1.384(5)	C(3)	C(4)	1.381(5)
C(4)	C(5)	1.377(5)	C(5)	C(6)	1.395(4)
C(7)	C(8)	1.389(5)	C(7)	C(12)	1.386(5)
C(8)	C(9)	1.414(4)	C(9)	C(10)	1.370(5)
C(10)	C(11)	1.382(5)	C(11)	C(12)	1.395(4)
C(13)	C(14)	1.389(4)	C(13)	C(18)	1.392(5)
C(14)	C(15)	1.380(5)	C(15)	C(16)	1.382(5)
C(16)	C(17)	1.377(5)	C(17)	C(18)	1.381(5)
C(19)	C(20)	1.384(5)	C(19)	C(24)	1.391(4)
C(20)	C(21)	1.398(5)	C(21)	C(22)	1.360(5)

C(22)	C(23)	1.372(5)	C(23)	C(24)	1.384(5)
C(25)	C(26)	1.363(5)	C(25)	C(30)	1.397(5)
C(26)	C(27)	1.406(5)	C(27)	C(28)	1.377(6)
C(28)	C(29)	1.372(6)	C(29)	C(30)	1.382(4)
C(31)	C(32)	1.365(5)	C(31)	C(36)	1.398(5)
C(32)	C(33)	1.392(5)	C(33)	C(32)	1.392(5)
C(33)	C(34)	1.343(6)	C(34)	C(33)	1.343(6)
C(34)	C(35)	1.364(6)	C(35)	C(36)	1.362(5)
C(37)	C(38)	1.380(5)	C(37)	C(42)	1.373(5)
C(38)	C(39)	1.381(6)	C(39)	C(40)	1.362(6)
C(40)	C(41)	1.351(5)	C(41)	C(42)	1.401(5)
C(43)	C(44)	1.391(5)	C(43)	C(48)	1.396(5)
C(44)	C(45)	1.378(5)	C(45)	C(46)	1.386(5)

Table 4. Bond lengths (Å) -- continued

atom	atom	distance	atom	atom	distance
C(46)	C(47)	1.373(5)	C(47)	C(48)	1.386(5)
C(49)	C(50)	1.383(5)	C(49)	C(54)	1.417(4)
C(50)	C(51)	1.405(5)	C(51)	C(52)	1.391(5)
C(52)	C(53)	1.371(5)	C(53)	C(54)	1.391(5)
C(55)	C(56)	1.378(4)	C(55)	C(60)	1.401(4)
C(56)	C(57)	1.385(4)	C(57)	C(58)	1.395(5)
C(58)	C(59)	1.372(5)	C(59)	C(60)	1.395(5)
C(61)	C(62)	1.399(5)	C(61)	C(66)	1.388(4)
C(62)	C(63)	1.371(5)	C(63)	C(64)	1.389(5)
C(64)	C(65)	1.367(5)	C(65)	C(66)	1.395(5)
C(67)	C(68)	1.391(5)	C(67)	C(72)	1.399(5)
C(68)	C(69)	1.384(5)	C(69)	C(70)	1.369(5)
C(70)	C(71)	1.382(5)	C(71)	C(72)	1.381(5)
C(73)	C(74)	1.397(5)	C(73)	C(78)	1.386(5)
C(74)	C(75)	1.389(5)	C(75)	C(76)	1.382(5)
C(76)	C(77)	1.363(5)	C(77)	C(78)	1.382(5)
C(79)	C(80)	1.389(4)	C(79)	C(84)	1.392(5)
C(80)	C(81)	1.386(5)	C(81)	C(82)	1.369(5)
C(82)	C(83)	1.391(5)	C(83)	C(84)	1.387(5)
C(85)	C(86)	1.380(5)	C(85)	C(90)	1.398(5)
C(86)	C(87)	1.382(5)	C(87)	C(88)	1.380(5)
C(88)	C(89)	1.362(6)	C(89)	C(90)	1.398(5)
C(91)	C(92)	1.384(5)	C(91)	C(96)	1.392(4)
C(92)	C(93)	1.376(5)	C(93)	C(94)	1.373(5)
C(94)	C(95)	1.378(6)	C(95)	C(96)	1.397(5)

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
I(1)	Cu(1)	P(1)	101.59(3)	I(1)	Cu(1)	P(2)	116.34(2)
I(1)	Cu(1)	P(3)	111.60(3)	I(2)	Cu(2)	P(4)	111.79(2)
I(2)	Cu(2)	P(5)	98.76(3)	I(2)	Cu(2)	P(6)	100.23(3)
P(2)	Cu(1)	P(1)	115.91(3)	P(3)	Cu(1)	P(1)	123.67(3)

Cu(1)	P(1)	C(31)	108.2(1)	Cu(1)	P(1)	C(37)	116.2(1)
Cu(1)	P(1)	C(43)	120.1(1)	P(3)	Cu(1)	P(2)	88.58(3)
Cu(1)	P(2)	C(1)	103.8(1)	Cu(1)	P(2)	C(7)	121.5(1)
Cu(1)	P(2)	C(13)	117.9(1)	Cu(1)	P(3)	C(6)	103.8(1)
Cu(1)	P(3)	C(25)	109.5(1)	Cu(1)	P(3)	C(19)	129.3(1)
P(5)	Cu(2)	P(4)	127.49(4)	P(6)	Cu(2)	P(4)	124.88(4)
Cu(2)	P(4)	C(79)	109.5(1)	Cu(2)	P(4)	C(85)	115.5(1)
Cu(2)	P(4)	C(91)	119.8(1)	P(6)	Cu(2)	P(5)	87.75(3)
Cu(2)	P(5)	C(49)	102.0(1)	Cu(2)	P(5)	C(61)	113.3(1)
Cu(2)	P(5)	C(55)	127.2(1)	Cu(2)	P(6)	C(54)	101.7(1)
Cu(2)	P(6)	C(67)	119.8(1)	Cu(2)	P(6)	C(73)	120.4(1)
C(37)	P(1)	C(31)	104.8(1)	C(43)	P(1)	C(31)	103.0(1)
P(1)	C(31)	C(32)	124.1(3)	P(1)	C(31)	C(36)	118.3(3)
C(43)	P(1)	C(37)	102.8(1)	P(1)	C(37)	C(38)	122.5(3)
P(1)	C(37)	C(42)	119.8(2)	P(1)	C(43)	C(44)	118.6(2)
P(1)	C(43)	C(48)	123.0(3)	P(2)	C(1)	C(6)	118.6(2)
C(7)	P(2)	C(1)	105.0(1)	C(13)	P(2)	C(1)	102.2(1)
P(2)	C(1)	C(2)	121.8(2)	C(13)	P(2)	C(7)	104.1(1)
P(2)	C(7)	C(8)	124.7(2)	P(2)	C(7)	C(12)	116.5(2)
P(2)	C(13)	C(14)	123.1(2)	P(2)	C(13)	C(18)	118.6(2)
P(3)	C(6)	C(1)	119.0(2)	C(25)	P(3)	C(6)	107.9(2)
P(3)	C(6)	C(5)	122.3(2)	C(19)	P(3)	C(6)	102.0(1)
C(25)	P(3)	C(19)	102.9(1)	P(3)	C(19)	C(20)	117.7(2)
P(3)	C(19)	C(24)	123.0(2)	P(3)	C(25)	C(26)	124.6(3)
P(3)	C(25)	C(30)	115.6(3)	P(4)	C(79)	C(84)	116.8(2)
C(85)	P(4)	C(79)	104.6(1)	C(91)	P(4)	C(79)	104.4(1)
P(4)	C(79)	C(80)	124.7(2)	P(4)	C(85)	C(90)	118.0(3)
C(91)	P(4)	C(85)	101.6(2)	P(4)	C(85)	C(86)	123.0(2)
P(4)	C(91)	C(92)	122.8(2)	P(4)	C(91)	C(96)	119.0(2)
P(5)	C(49)	C(54)	117.7(2)	C(61)	P(5)	C(49)	102.2(1)
P(5)	C(49)	C(50)	123.0(2)	C(55)	P(5)	C(49)	105.9(2)
C(61)	P(5)	C(55)	103.5(1)	P(5)	C(55)	C(56)	119.1(2)
P(5)	C(55)	C(60)	122.2(2)	P(5)	C(61)	C(62)	117.2(2)

Table 6. Bond angles ($^{\circ}$) -- continued

atom	atom	atom	angle	atom	atom	atom	angle
P(5)	C(61)	C(66)	124.1(3)	P(6)	C(54)	C(49)	118.3(2)
C(67)	P(6)	C(54)	105.2(1)	C(73)	P(6)	C(54)	104.2(1)
P(6)	C(54)	C(53)	122.9(2)	C(73)	P(6)	C(67)	103.5(1)
P(6)	C(67)	C(68)	121.2(2)	P(6)	C(67)	C(72)	120.3(2)
P(6)	C(73)	C(74)	117.7(2)	P(6)	C(73)	C(78)	124.2(3)
C(6)	C(1)	C(2)	119.5(3)	C(1)	C(2)	C(3)	120.9(3)
C(1)	C(6)	C(5)	118.5(3)	C(2)	C(3)	C(4)	119.4(3)
C(3)	C(4)	C(5)	120.6(3)	C(4)	C(5)	C(6)	121.1(3)
C(12)	C(7)	C(8)	118.7(3)	C(7)	C(8)	C(9)	119.9(3)
C(7)	C(12)	C(11)	121.2(3)	C(8)	C(9)	C(10)	120.3(3)
C(9)	C(10)	C(11)	120.2(3)	C(10)	C(11)	C(12)	119.6(3)
C(18)	C(13)	C(14)	118.2(3)	C(13)	C(14)	C(15)	120.8(3)
C(13)	C(18)	C(17)	120.9(3)	C(14)	C(15)	C(16)	120.1(3)
C(15)	C(16)	C(17)	119.8(3)	C(16)	C(17)	C(18)	120.1(3)

C(24)	C(19)	C(20)	119.2(3)	C(19)	C(20)	C(21)	119.5(3)
C(19)	C(24)	C(23)	120.1(3)	C(20)	C(21)	C(22)	120.9(4)
C(21)	C(22)	C(23)	119.8(3)	C(22)	C(23)	C(24)	120.5(3)
C(30)	C(25)	C(26)	119.4(3)	C(25)	C(26)	C(27)	119.2(3)
C(25)	C(30)	C(29)	120.9(3)	C(26)	C(27)	C(28)	121.3(3)
C(27)	C(28)	C(29)	119.2(3)	C(28)	C(29)	C(30)	120.1(3)
C(36)	C(31)	C(32)	117.6(3)	C(31)	C(32)	C(33)	120.2(3)
C(31)	C(36)	C(35)	121.8(4)	C(32)	C(33)	C(34)	120.5(4)
C(33)	C(34)	C(35)	120.8(4)	C(34)	C(35)	C(36)	119.1(4)
C(42)	C(37)	C(38)	117.6(3)	C(37)	C(38)	C(39)	120.6(4)
C(37)	C(42)	C(41)	121.3(3)	C(38)	C(39)	C(40)	121.3(4)
C(39)	C(40)	C(41)	119.3(4)	C(40)	C(41)	C(42)	120.0(4)
C(48)	C(43)	C(44)	118.4(3)	C(43)	C(44)	C(45)	121.2(3)
C(43)	C(48)	C(47)	120.2(3)	C(44)	C(45)	C(46)	119.8(3)
C(45)	C(46)	C(47)	119.9(3)	C(46)	C(47)	C(48)	120.6(3)
C(54)	C(49)	C(50)	119.3(3)	C(49)	C(50)	C(51)	121.0(3)
C(49)	C(54)	C(53)	118.9(3)	C(50)	C(51)	C(52)	118.9(3)
C(51)	C(52)	C(53)	120.6(3)	C(52)	C(53)	C(54)	121.3(3)
C(60)	C(55)	C(56)	118.6(3)	C(55)	C(56)	C(57)	121.7(3)
C(55)	C(60)	C(59)	120.1(3)	C(56)	C(57)	C(58)	119.1(3)
C(57)	C(58)	C(59)	120.3(3)	C(58)	C(59)	C(60)	120.2(3)
C(66)	C(61)	C(62)	118.3(3)	C(61)	C(62)	C(63)	121.3(3)
C(61)	C(66)	C(65)	120.4(3)	C(62)	C(63)	C(64)	119.4(3)

Table 6. Bond angles ($^{\circ}$) -- continued

atom	atom	atom	angle	atom	atom	atom	angle
C(63)	C(64)	C(65)	120.6(3)	C(64)	C(65)	C(66)	119.9(3)
C(72)	C(67)	C(68)	118.0(3)	C(67)	C(68)	C(69)	120.6(3)
C(67)	C(72)	C(71)	120.6(3)	C(68)	C(69)	C(70)	120.8(3)
C(69)	C(70)	C(71)	119.5(3)	C(70)	C(71)	C(72)	120.4(3)
C(78)	C(73)	C(74)	118.0(3)	C(73)	C(74)	C(75)	120.6(3)
C(73)	C(78)	C(77)	120.9(3)	C(74)	C(75)	C(76)	119.9(3)
C(75)	C(76)	C(77)	119.8(3)	C(76)	C(77)	C(78)	120.7(3)
C(84)	C(79)	C(80)	118.3(3)	C(79)	C(80)	C(81)	120.7(3)
C(79)	C(84)	C(83)	121.0(3)	C(80)	C(81)	C(82)	120.5(3)
C(81)	C(82)	C(83)	119.9(3)	C(82)	C(83)	C(84)	119.5(3)
C(90)	C(85)	C(86)	118.9(3)	C(85)	C(86)	C(87)	120.8(3)
C(85)	C(90)	C(89)	120.0(3)	C(86)	C(87)	C(88)	119.8(4)
C(87)	C(88)	C(89)	120.7(3)	C(88)	C(89)	C(90)	119.8(3)
C(96)	C(91)	C(92)	118.2(3)	C(91)	C(92)	C(93)	121.4(3)
C(91)	C(96)	C(95)	120.0(3)	C(92)	C(93)	C(94)	120.5(4)
C(93)	C(94)	C(95)	119.3(4)	C(94)	C(95)	C(96)	120.6(3)

Table 8. Torsion Angles($^{\circ}$)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
I(1)	Cu(1)	P(1)	C(31)	-43.0(1)	I(1)	Cu(1)	P(1)	C(37)	74.5(1)
I(1)	Cu(1)	P(1)	C(43)	-160.7(1)	P(2)	Cu(1)	P(1)	C(31)	84.1(1)
P(2)	Cu(1)	P(1)	C(37)	-158.4(1)	P(2)	Cu(1)	P(1)	C(43)	-33.6(1)

P(3)	Cu(1)	P(1)	C(31)	-169.1(1)	P(3)	Cu(1)	P(1)	C(37)	-51.6(1)
P(3)	Cu(1)	P(1)	C(43)	73.2(1)	I(1)	Cu(1)	P(2)	C(1)	-91.6(1)
I(1)	Cu(1)	P(2)	C(7)	26.0(1)	I(1)	Cu(1)	P(2)	C(13)	156.3(1)
P(1)	Cu(1)	P(2)	C(1)	149.10(9)	P(1)	Cu(1)	P(2)	C(7)	-93.4(1)
P(1)	Cu(1)	P(2)	C(13)	37.0(1)	P(3)	Cu(1)	P(2)	C(1)	21.92(9)
P(3)	Cu(1)	P(2)	C(7)	139.5(1)	P(3)	Cu(1)	P(2)	C(13)	-90.2(1)
I(1)	Cu(1)	P(3)	C(6)	98.6(1)	I(1)	Cu(1)	P(3)	C(19)	-19.9(1)
I(1)	Cu(1)	P(3)	C(25)	-146.4(1)	P(1)	Cu(1)	P(3)	C(6)	-139.8(1)
P(1)	Cu(1)	P(3)	C(19)	101.7(1)	P(1)	Cu(1)	P(3)	C(25)	-24.8(1)
P(2)	Cu(1)	P(3)	C(6)	-19.3(1)	P(2)	Cu(1)	P(3)	C(19)	-137.8(1)
P(2)	Cu(1)	P(3)	C(25)	95.7(1)	I(2)	Cu(2)	P(4)	C(79)	-30.6(1)
I(2)	Cu(2)	P(4)	C(85)	87.1(1)	I(2)	Cu(2)	P(4)	C(91)	-151.0(1)
P(5)	Cu(2)	P(4)	C(79)	90.3(1)	P(5)	Cu(2)	P(4)	C(85)	-152.0(1)
P(5)	Cu(2)	P(4)	C(91)	-30.1(1)	P(6)	Cu(2)	P(4)	C(79)	-151.4(1)
P(6)	Cu(2)	P(4)	C(85)	-33.7(1)	P(6)	Cu(2)	P(4)	C(91)	88.2(1)
I(2)	Cu(2)	P(5)	C(49)	-68.9(1)	I(2)	Cu(2)	P(5)	C(55)	51.9(1)
I(2)	Cu(2)	P(5)	C(61)	-177.9(1)	P(4)	Cu(2)	P(5)	C(49)	164.81(9)
P(4)	Cu(2)	P(5)	C(55)	-74.4(1)	P(4)	Cu(2)	P(5)	C(61)	55.8(1)
P(6)	Cu(2)	P(5)	C(49)	31.1(1)	P(6)	Cu(2)	P(5)	C(55)	151.9(1)
P(6)	Cu(2)	P(5)	C(61)	-77.9(1)	I(2)	Cu(2)	P(6)	C(54)	70.1(1)
I(2)	Cu(2)	P(6)	C(67)	-45.2(1)	I(2)	Cu(2)	P(6)	C(73)	-175.6(1)
P(4)	Cu(2)	P(6)	C(54)	-164.06(9)	P(4)	Cu(2)	P(6)	C(67)	80.7(1)
P(4)	Cu(2)	P(6)	C(73)	-49.8(1)	P(5)	Cu(2)	P(6)	C(54)	-28.4(1)
P(5)	Cu(2)	P(6)	C(67)	-143.7(1)	P(5)	Cu(2)	P(6)	C(73)	85.9(1)
Cu(1)	P(1)	C(31)	C(32)	122.8(3)	Cu(1)	P(1)	C(31)	C(36)	-55.1(3)
C(37)	P(1)	C(31)	C(32)	-1.8(3)	C(37)	P(1)	C(31)	C(36)	-179.7(2)
C(43)	P(1)	C(31)	C(32)	-109.0(3)	C(43)	P(1)	C(31)	C(36)	73.1(3)
Cu(1)	P(1)	C(37)	C(38)	147.7(3)	Cu(1)	P(1)	C(37)	C(42)	-29.2(3)
C(31)	P(1)	C(37)	C(38)	-93.0(3)	C(31)	P(1)	C(37)	C(42)	90.1(3)
C(43)	P(1)	C(37)	C(38)	14.4(3)	C(43)	P(1)	C(37)	C(42)	-162.5(3)
Cu(1)	P(1)	C(43)	C(44)	-49.0(3)	Cu(1)	P(1)	C(43)	C(48)	133.1(3)
C(31)	P(1)	C(43)	C(44)	-169.3(2)	C(31)	P(1)	C(43)	C(48)	12.7(3)
C(37)	P(1)	C(43)	C(44)	82.0(3)	C(37)	P(1)	C(43)	C(48)	-95.9(3)
Cu(1)	P(2)	C(1)	C(2)	161.7(2)	Cu(1)	P(2)	C(1)	C(6)	-21.3(2)

Table 8. Torsion angles ($^{\circ}$) -- continued

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(7)	P(2)	C(1)	C(2)	33.1(3)	C(7)	P(2)	C(1)	C(6)	-149.8(2)
C(13)	P(2)	C(1)	C(2)	-75.2(2)	C(13)	P(2)	C(1)	C(6)	101.8(2)
Cu(1)	P(2)	C(7)	C(8)	150.2(2)	Cu(1)	P(2)	C(7)	C(12)	-27.5(3)
C(1)	P(2)	C(7)	C(8)	-92.9(3)	C(1)	P(2)	C(7)	C(12)	89.5(3)
C(13)	P(2)	C(7)	C(8)	14.2(3)	C(13)	P(2)	C(7)	C(12)	-163.5(2)
Cu(1)	P(2)	C(13)	C(14)	105.4(3)	Cu(1)	P(2)	C(13)	C(18)	-72.3(3)
C(1)	P(2)	C(13)	C(14)	-7.6(3)	C(1)	P(2)	C(13)	C(18)	174.8(2)
C(7)	P(2)	C(13)	C(14)	-116.6(3)	C(7)	P(2)	C(13)	C(18)	65.7(3)
Cu(1)	P(3)	C(6)	C(1)	12.1(2)	Cu(1)	P(3)	C(6)	C(5)	-162.3(2)
C(19)	P(3)	C(6)	C(1)	148.1(2)	C(19)	P(3)	C(6)	C(5)	-26.3(3)
C(25)	P(3)	C(6)	C(1)	-104.0(2)	C(25)	P(3)	C(6)	C(5)	81.6(3)
Cu(1)	P(3)	C(19)	C(20)	36.9(3)	Cu(1)	P(3)	C(19)	C(24)	-147.5(3)
C(6)	P(3)	C(19)	C(20)	-82.3(3)	C(6)	P(3)	C(19)	C(24)	93.2(3)

C(25)	P(3)	C(19)	C(20)	165.9(3)	C(25)	P(3)	C(19)	C(24)	-18.5(3)
Cu(1)	P(3)	C(25)	C(26)	-103.9(3)	Cu(1)	P(3)	C(25)	C(30)	68.5(2)
C(6)	P(3)	C(25)	C(26)	8.5(3)	C(6)	P(3)	C(25)	C(30)	-179.2(2)
C(19)	P(3)	C(25)	C(26)	115.8(3)	C(19)	P(3)	C(25)	C(30)	-71.9(2)
Cu(2)	P(4)	C(79)	C(80)	130.4(3)	Cu(2)	P(4)	C(79)	C(84)	-45.0(3)
C(85)	P(4)	C(79)	C(80)	6.0(3)	C(85)	P(4)	C(79)	C(84)	-169.3(2)
C(91)	P(4)	C(79)	C(80)	-100.3(3)	C(91)	P(4)	C(79)	C(84)	84.4(3)
Cu(2)	P(4)	C(85)	C(86)	166.9(2)	Cu(2)	P(4)	C(85)	C(90)	-17.0(3)
C(79)	P(4)	C(85)	C(86)	-72.7(3)	C(79)	P(4)	C(85)	C(90)	103.4(2)
C(91)	P(4)	C(85)	C(86)	35.7(3)	C(91)	P(4)	C(85)	C(90)	-148.2(2)
Cu(2)	P(4)	C(91)	C(92)	101.6(3)	Cu(2)	P(4)	C(91)	C(96)	-75.9(3)
C(79)	P(4)	C(91)	C(92)	-21.3(3)	C(79)	P(4)	C(91)	C(96)	161.2(3)
C(85)	P(4)	C(91)	C(92)	-129.9(3)	C(85)	P(4)	C(91)	C(96)	52.6(3)
Cu(2)	P(5)	C(49)	C(50)	153.0(2)	Cu(2)	P(5)	C(49)	C(54)	-28.4(2)
C(55)	P(5)	C(49)	C(50)	18.4(3)	C(55)	P(5)	C(49)	C(54)	-163.1(2)
C(61)	P(5)	C(49)	C(50)	-89.6(2)	C(61)	P(5)	C(49)	C(54)	88.9(2)
Cu(2)	P(5)	C(55)	C(56)	-16.5(3)	Cu(2)	P(5)	C(55)	C(60)	160.6(2)
C(49)	P(5)	C(55)	C(56)	102.6(3)	C(49)	P(5)	C(55)	C(60)	-80.3(3)
C(61)	P(5)	C(55)	C(56)	-150.3(3)	C(61)	P(5)	C(55)	C(60)	26.7(3)
Cu(2)	P(5)	C(61)	C(62)	-57.0(3)	Cu(2)	P(5)	C(61)	C(66)	116.0(3)
C(49)	P(5)	C(61)	C(62)	-165.9(2)	C(49)	P(5)	C(61)	C(66)	7.1(3)
C(55)	P(5)	C(61)	C(62)	84.3(2)	C(55)	P(5)	C(61)	C(66)	-102.7(3)
Cu(2)	P(6)	C(54)	C(49)	19.4(2)	Cu(2)	P(6)	C(54)	C(53)	-160.2(2)
C(67)	P(6)	C(54)	C(49)	145.0(2)	C(67)	P(6)	C(54)	C(53)	-34.6(3)

Table 8. Torsion angles ($^{\circ}$) -- continued

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(73)	P(6)	C(54)	C(49)	-106.4(2)	C(73)	P(6)	C(54)	C(53)	74.0(3)
Cu(2)	P(6)	C(67)	C(68)	-98.9(3)	Cu(2)	P(6)	C(67)	C(72)	72.5(3)
C(54)	P(6)	C(67)	C(68)	147.7(2)	C(54)	P(6)	C(67)	C(72)	-40.8(3)
C(73)	P(6)	C(67)	C(68)	38.6(3)	C(73)	P(6)	C(67)	C(72)	-149.9(2)
Cu(2)	P(6)	C(73)	C(74)	-6.3(3)	Cu(2)	P(6)	C(73)	C(78)	174.3(3)
C(54)	P(6)	C(73)	C(74)	106.6(3)	C(54)	P(6)	C(73)	C(78)	-72.8(3)
C(67)	P(6)	C(73)	C(74)	-143.5(3)	C(67)	P(6)	C(73)	C(78)	37.1(3)
P(2)	C(1)	C(2)	C(3)	177.8(3)	C(6)	C(1)	C(2)	C(3)	0.8(4)
P(2)	C(1)	C(6)	P(3)	6.3(3)	P(2)	C(1)	C(6)	C(5)	-179.1(3)
C(2)	C(1)	C(6)	P(3)	-176.6(2)	C(2)	C(1)	C(6)	C(5)	-2.0(4)
C(1)	C(2)	C(3)	C(4)	0.2(4)	C(2)	C(3)	C(4)	C(5)	-0.0(5)
C(3)	C(4)	C(5)	C(6)	-1.3(5)	C(4)	C(5)	C(6)	P(3)	176.7(2)
C(4)	C(5)	C(6)	C(1)	2.3(5)	P(2)	C(7)	C(8)	C(9)	-176.2(3)
C(12)	C(7)	C(8)	C(9)	1.5(5)	P(2)	C(7)	C(12)	C(11)	177.0(3)
C(8)	C(7)	C(12)	C(11)	-0.8(5)	C(7)	C(8)	C(9)	C(10)	-0.4(5)
C(8)	C(9)	C(10)	C(11)	-1.4(5)	C(9)	C(10)	C(11)	C(12)	2.0(5)
C(10)	C(11)	C(12)	C(7)	-0.9(5)	P(2)	C(13)	C(14)	C(15)	-176.8(3)
C(18)	C(13)	C(14)	C(15)	0.9(5)	P(2)	C(13)	C(18)	C(17)	178.4(3)
C(14)	C(13)	C(18)	C(17)	0.6(5)	C(13)	C(14)	C(15)	C(16)	-2.2(5)
C(14)	C(15)	C(16)	C(17)	1.8(5)	C(15)	C(16)	C(17)	C(18)	-0.3(5)
C(16)	C(17)	C(18)	C(13)	-0.9(5)	P(3)	C(19)	C(20)	C(21)	177.5(3)
C(24)	C(19)	C(20)	C(21)	1.8(6)	P(3)	C(19)	C(24)	C(23)	-178.3(3)
C(20)	C(19)	C(24)	C(23)	-2.8(5)	C(19)	C(20)	C(21)	C(22)	-0.2(5)

C(20)	C(21)	C(22)	C(23)	-0.5(6)	C(21)	C(22)	C(23)	C(24)	-0.5(6)
C(22)	C(23)	C(24)	C(19)	2.1(6)	P(3)	C(25)	C(26)	C(27)	172.2(3)
C(30)	C(25)	C(26)	C(27)	0.2(4)	P(3)	C(25)	C(30)	C(29)	-173.8(3)
C(26)	C(25)	C(30)	C(29)	-1.0(5)	C(25)	C(26)	C(27)	C(28)	0.4(5)
C(26)	C(27)	C(28)	C(29)	-0.1(4)	C(27)	C(28)	C(29)	C(30)	-0.7(5)
C(28)	C(29)	C(30)	C(25)	1.3(5)	P(1)	C(31)	C(32)	C(33)	179.4(3)
C(36)	C(31)	C(32)	C(33)	-2.8(5)	P(1)	C(31)	C(36)	C(35)	-177.7(3)
C(32)	C(31)	C(36)	C(35)	4.3(5)	C(31)	C(32)	C(33)	C(34)	-0.1(4)
C(32)	C(33)	C(34)	C(35)	1.7(6)	C(33)	C(34)	C(35)	C(36)	-0.3(6)
C(34)	C(35)	C(36)	C(31)	-2.8(6)	P(1)	C(37)	C(38)	C(39)	-176.5(3)
C(42)	C(37)	C(38)	C(39)	0.5(6)	P(1)	C(37)	C(42)	C(41)	177.9(3)
C(38)	C(37)	C(42)	C(41)	0.8(5)	C(37)	C(38)	C(39)	C(40)	-0.8(7)
C(38)	C(39)	C(40)	C(41)	-0.2(5)	C(39)	C(40)	C(41)	C(42)	1.5(6)
C(40)	C(41)	C(42)	C(37)	-1.8(6)	P(1)	C(43)	C(44)	C(45)	-177.1(3)

Table 8. Torsion angles ($^{\circ}$) -- continued

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(48)	C(43)	C(44)	C(45)	1.0(5)	P(1)	C(43)	C(48)	C(47)	177.9(3)
C(44)	C(43)	C(48)	C(47)	0.0(5)	C(43)	C(44)	C(45)	C(46)	-1.2(5)
C(44)	C(45)	C(46)	C(47)	0.5(6)	C(45)	C(46)	C(47)	C(48)	0.5(6)
C(46)	C(47)	C(48)	C(43)	-0.7(5)	P(5)	C(49)	C(50)	C(51)	176.0(2)
C(54)	C(49)	C(50)	C(51)	-2.5(4)	P(5)	C(49)	C(54)	P(6)	6.0(3)
P(5)	C(49)	C(54)	C(53)	-174.4(2)	C(50)	C(49)	C(54)	P(6)	-175.4(2)
C(50)	C(49)	C(54)	C(53)	4.2(4)	C(49)	C(50)	C(51)	C(52)	-1.0(4)
C(50)	C(51)	C(52)	C(53)	3.0(5)	C(51)	C(52)	C(53)	C(54)	-1.3(5)
C(52)	C(53)	C(54)	P(6)	177.2(2)	C(52)	C(53)	C(54)	C(49)	-2.3(4)
P(5)	C(55)	C(56)	C(57)	178.2(3)	C(60)	C(55)	C(56)	C(57)	1.0(5)
P(5)	C(55)	C(60)	C(59)	-179.0(3)	C(56)	C(55)	C(60)	C(59)	-2.0(5)
C(55)	C(56)	C(57)	C(58)	-0.1(4)	C(56)	C(57)	C(58)	C(59)	0.1(4)
C(57)	C(58)	C(59)	C(60)	-1.0(6)	C(58)	C(59)	C(60)	C(55)	2.0(6)
P(5)	C(61)	C(62)	C(63)	173.2(3)	C(66)	C(61)	C(62)	C(63)	-0.2(5)
P(5)	C(61)	C(66)	C(65)	-172.3(3)	C(62)	C(61)	C(66)	C(65)	0.7(5)
C(61)	C(62)	C(63)	C(64)	-1.2(5)	C(62)	C(63)	C(64)	C(65)	2.1(5)
C(63)	C(64)	C(65)	C(66)	-1.7(5)	C(64)	C(65)	C(66)	C(61)	0.3(5)
P(6)	C(67)	C(68)	C(69)	174.0(3)	C(72)	C(67)	C(68)	C(69)	2.4(5)
P(6)	C(67)	C(72)	C(71)	-175.5(3)	C(68)	C(67)	C(72)	C(71)	-3.8(5)
C(67)	C(68)	C(69)	C(70)	-0.0(5)	C(68)	C(69)	C(70)	C(71)	-1.0(5)
C(69)	C(70)	C(71)	C(72)	-0.4(5)	C(70)	C(71)	C(72)	C(67)	2.9(5)
P(6)	C(73)	C(74)	C(75)	-177.6(3)	C(78)	C(73)	C(74)	C(75)	1.8(5)
P(6)	C(73)	C(78)	C(77)	178.0(3)	C(74)	C(73)	C(78)	C(77)	-1.4(5)
C(73)	C(74)	C(75)	C(76)	-1.4(5)	C(74)	C(75)	C(76)	C(77)	0.5(6)
C(75)	C(76)	C(77)	C(78)	0.0(6)	C(76)	C(77)	C(78)	C(73)	0.5(6)
P(4)	C(79)	C(80)	C(81)	-175.7(3)	C(84)	C(79)	C(80)	C(81)	-0.5(5)
P(4)	C(79)	C(84)	C(83)	176.6(3)	C(80)	C(79)	C(84)	C(83)	1.0(5)
C(79)	C(80)	C(81)	C(82)	-0.0(5)	C(80)	C(81)	C(82)	C(83)	0.0(5)
C(81)	C(82)	C(83)	C(84)	0.4(6)	C(82)	C(83)	C(84)	C(79)	-1.0(5)
P(4)	C(85)	C(86)	C(87)	177.6(3)	C(90)	C(85)	C(86)	C(87)	1.5(4)
P(4)	C(85)	C(90)	C(89)	-177.9(3)	C(86)	C(85)	C(90)	C(89)	-1.6(4)
C(85)	C(86)	C(87)	C(88)	-0.9(5)	C(86)	C(87)	C(88)	C(89)	0.3(5)
C(87)	C(88)	C(89)	C(90)	-0.5(5)	C(88)	C(89)	C(90)	C(85)	1.1(5)

P(4)	C(91)	C(92)	C(93)	-178.0(3)	C(96)	C(91)	C(92)	C(93)	-0.4(6)
P(4)	C(91)	C(96)	C(95)	177.4(3)	C(92)	C(91)	C(96)	C(95)	-0.2(5)
C(91)	C(92)	C(93)	C(94)	1.2(6)	C(92)	C(93)	C(94)	C(95)	-1.3(7)
C(93)	C(94)	C(95)	C(96)	0.7(6)	C(94)	C(95)	C(96)	C(91)	0.1(5)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.