A Highly Emissive Cu_2N_2 Diamond Core Complex Supported by a $[PNP]^-$ Ligand

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Supporting Information

Experimental Section

General. All manipulations were carried out using standard Schlenk or glove-box techniques under a dinitrogen atmosphere. Unless otherwise noted, solvents were deoxygenated and dried by thorough 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. Spectral grade THF was purchased from Aldrich and distilled from molten potassium prior to use. All reagents were purchased from commercial vendors and used without further purification unless otherwise stated. A volumetric solution of 0.1N NaOH was purchased from J.T. Baker and used as received. $[Cp_2Fe][B(C_6H_3(CF_3)_2)_4]$,[1] were prepared according to literature procedure. Elemental analyses was 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 Crystallographic Facility on a Brüker Smart 1000 CCD diffractometer and solved using SHELX v. 6.14.

Electrochemistry. Electrochemical measurements were carried out in a glove-box under a dinitrogen atmosphere in a one-compartment cell using a BAS model 100/W electrochemical analyzer. A glassy carbon electrode and platinum wire were used as the working and auxiliary electrodes, respectively. 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.

Spectroscopic measurements. High-resolution EI mass spectroscopy was carried out by the Caltech Chemistry Mass Spectral Facility using a JEOL JMS600. A Varian Mercury-300 or INOVA-500 NMR spectrometer was used to record ^1H, ^{13}C, ^{19}F, ^{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 NMR 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 spectro-fluorometer. 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 monochromator (Instruments SA DH-10) onto a photomultiplier tube (PMT) (Hamamatsu R928). The PMT current was amplified and recorded with a transient digitizer (Tektronix). UV-vis measurements were taken on a Cary 50 UV/Vis Spectrophotometer using a 1 cm quartz cell or 500 UV/Vis/NIR Spectrophotometer using either a 2 cm or 1 cm quartz cell sealed with a Teflon stopper.

Synthesis of Lithium Diisobutylphosphide. In a 500 mL Erlenmeyer flask diisobutylphosphine (25 g, 0.171 mol) was dissolved in 200 mL of petroleum ether and cooled to -80ºC, at which time at 1.6 M solution of ^{n}butyl lithium in hexane (107 mL, 0.171 mol) was added over 20 min. The reaction was then stirred at ambient temperature for 24 h, concentrated in vacuo to ca. 50 mL, and the white solids were then collected on a sintered-glass frit. Washing of the solids with petroleum ether afforded a single phosphorous containing product (21.1 g, 81%) as by ^{31}P NMR upon drying. $^{31}P\{^1H\}$ NMR (121.5 MHz, THF): -91.2.

Synthesis of Bis(2-(diisobutylphosphino)phenyl)amine, 1. In a 250 mL sealable reaction bomb, a 1.6 M ^{n}butyl lithium solution (7.9 mL, 12.6 mmol) in hexanes was added dropwise to a solution of bis(2-fluorophenyl)amine (2.46 g, 12.0 mmol) in THF (20 mL). After stirring for 15 min, the solution was concentrated in vacuo to remove the majority of the reaction volatiles after which time a solution of lithium diisobutylphosphide (5.47 g, 36 mmol) in THF (40 mL) was added and the vessel was sealed with a Teflon plug. The reaction was heated at 45ºC for 4 days and was monitored by ^{19}F NMR for the complete disappearance of the aryl fluoride resonance. The reaction was then quenched with methanol (5 mL) and the solution became yellow in color. Petroleum ether (50 mL) was added and the mixture was filtered twice through Celite to remove solids. Removal of the solvent in vacuo afforded an orange oil which was diluted in petroleum ether (30 mL) and flashed through two plugs of silica gel in a 60 mL sintered-glass frit. Evaporation of the solvent under reduced pressure afforded a spectroscopically pure, pale green oil (4.10 g, 75 %).

^1H NMR(300.1 MHz, $CDCl_3$): δ 8.03 (t, 1H), 7.52 (m, 2H), 7.33 (m, 2H), 7.26 (t, 2H), 7.00 (t, 2H), 1.73 (m, 12H), 1.08(d, 12), 1.03 (d, 12H). $^{13}C\{^1H\}$ NMR(75.5 MHz, $CDCl_3$): δ 147.8, 131.8, 129.4, 128.0, 121.0, 119.3, 116.7, 39.4, 26.6, 24.7, 24.3. $^{31}P\{^1H\}$ NMR (121.5 MHz, $CDCl_3$): δ -54.5. UV-vis (benzene, nm($M^{-1}cm^{-1}$)):

[1] Chávez, I.; et. al. *J. Organomet. Chem.* **2000**, *601*, 126.

302(18,700), sh 334(5900). FAB+ MS: calcd for $C_{28}H_{45}NP_2$: 457.3027. Found: 458.3122 [M+H], 400.2226 [M-^{i}Bu], 312.1904 [M-(^{i}Bu$_2$P)].

Synthesis of [Li][PNP], [1]Li. At ambient temperature a 1.6 M ^{n}butyl lithium solution (4.0 mL, 6.4 mmol) in hexanes was added dropwise to a solution of **1** (2.63 g, 5.76 mmol) in petroleum ether (50 mL) over 15 min. The reaction was stirred for 30 min, at which time a solid began to precipitate. The solution was concentrated to ca. 30 mL and cooled to -30 °C for 12 hrs. The resultant solids were collected on a sintered-glass frit as fine pale yellow powder, dried thoroughly (2.24 g, 84 %).

^{1}H NMR(499.9 MHz, C_6D_6): δ 7.21 (m, 2 H), 7.06 (m, 4 H), 6.71 (m, 2 H), 1.8-0.6 (br m, 36 H). ^{13}C{^{1}H} NMR(125.7 MHz, C_6D_6): δ 170.6, 132.4, 131.2, 128.7, 128.1, 118.6, 42.3, 36.2, 26.3, 25.3. ^{31}P{^{1}H} NMR (121.5MHz, C_6D_6): δ -49.4 (q, 61 Hz). UV-vis (cyclohexane, nm($M^{-1}cm^{-1}$)): 301(18,700), 357(31,400), sh 395(10,200). Anal. calcd. for $C_{56}H_{88}Li_2N_2P_4$: C, 72.55; H, 9.57; N, 3.02. Found: C, 73.21; H, 9.43; N, 3.14.

Synthesis of {(PNP)Cu}$_2$, 2: A solution of **[1]Li** (1.0 g, 2.16 mmol) in diethyl ether (20 mL) was added to a slurry of CuBr·S(CH$_3$)$_2$ (0.466 g, 2.27 mmol) in ether (30 mL) and stirred for 12 h. The solvent was removed in vacuo and the resultant yellow solids were dissolved in petroleum ether (50 ml) and filtered to remove insoluble materials. Removal of petroleum ether and drying the yellow solids in vacuo afforded analytically pure material (1.04 g, 92%). Crystals suitable for X-ray diffraction were obtained both by slow-evaporation of a petroleum ether solution of **2**.

^{1}H NMR(499.9 MHz, CD_2Cl_2): δ 7.20 (m, 4H), 6.93 (m, 4H), 6.71 (br d, 4H), 6.61 (t, 4H), 1.806 (m, 4H), 1.58 (m, 8H), 1.39 (m, 8H) , 1.29 (m, 4H) 0.99 (d, 12H), 0.73 (d, 12H), 0.70 (d, 12H), 0.60 (d, 12H). ^{13}C{^{1}H} NMR(125.7 MHz, CD_2Cl_2): δ 169.4, 131.8, 130.5, 128.7, 125.2, 117.8, 40.2, 36.4, 26.3, 26.2, 26.0, 25.7, 25.4, 25.1. ^{31}P{^{1}H} NMR (121.5MHz, C_6D_6): δ -33.9. UV-vis (cyclohexane, nm($M^{-1}cm^{-1}$)): 298(19,300), 314(19,900), 352(41,000), sh 387(14,300), 425(5100), sh 454(3400). Anal. calcd. for $C_{56}H_{88}Cu_2N_2P_4$: C, 64.65; H, 8.53; N, 2.69. Found: C, 64.54; H, 8.25; N, 2.62.

Quantum yield experiments

A volumetric solution of **2** (10 μM) in either cyclohexane (n = 1.426)[2] or tetrahydrofuran (n = 1.407)[2] was prepared in a nitrogen-filled glovebox. Three cuvettes (1 cm path) were charged with this solution, sparged briefly with argon, and sealed with a greased ground-glass stopper. The absorption spectra were acquired both before and after fluorescence measurements to ensure the sample was not degrading. A solution of fluorescein in an aqueous 0.1 N NaOH solution was prepared and sparged with argon, the concentration was adjusted such that the optical density (OD) at 440 nm was the same as that of the individual solutions of **2**. Fluorescent measurements were performed with λ_{ex} = 440 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[3] using eqn. 1.

$$\text{(eqn. 1)} \quad Q = (Q_R)(I / I_R)(OD_R / OD)(n^2 / n_R^2)$$

Q:	quantum yield of the sample.
Q_R:	quantum yield of fluorescein in aqueous 0.1 N NaOH solution (Q_R =0.9).
I:	integrated intensity of **2**.
I_R:	integrated intensity of fluorescein sample.
OD_R:	optical density of the fluorescein sample in absorption units.
OD:	optical density of **2** in absorption units.
n:	index of refraction of the solvent in which **2** was dissolved.
n_R:	index of refraction of 0.1N NaOH solution (n_R = 1.3351), measured on a Bausch & Lomb refractometer.

[2] Lide, D. R., Ed. *CRC Handbook of Chemistry and Physics, 77th Edition*; CRC Press: New York, NY, 1996.
[3] Demas, J. N.; Crosby, G. A. *J. Phys. Chem.* **1971**, *75*, 991

Table 1: Data for Quantum Yield Measurements.

Solution	OD (measured)	I (measured)	Q (calculated)
Fluorescein in 0.1N NaOH	0.0398	2.4725E+09	
10 μM **2** in cyclohexane	0.0352	1.5000E+09	0.70
10 μM **2** in cyclohexane	0.0369	1.5067E+09	0.67
10 μM **2** in cyclohexane	0.0408	1.6423E+09	0.67
		Average	**0.68**
		std. deviation	**0.02**
Solution	**OD (measured)**	**I (measured)**	**Q (calculated)**
Fluorescein in 0.1N NaOH	0.0119	6.5402E+08	
10 μM **2** in tetrahydrofuran	0.0174	6.6049E+08	0.69
10 μM **2** in tetrahydrofuran	0.0193	6.6209E+08	0.62
10 μM **2** in tetrahydrofuran	0.0137	5.3344E+08	0.71
		Average	**0.67**
		std. deviation	**0.04**

Lifetime measurements.

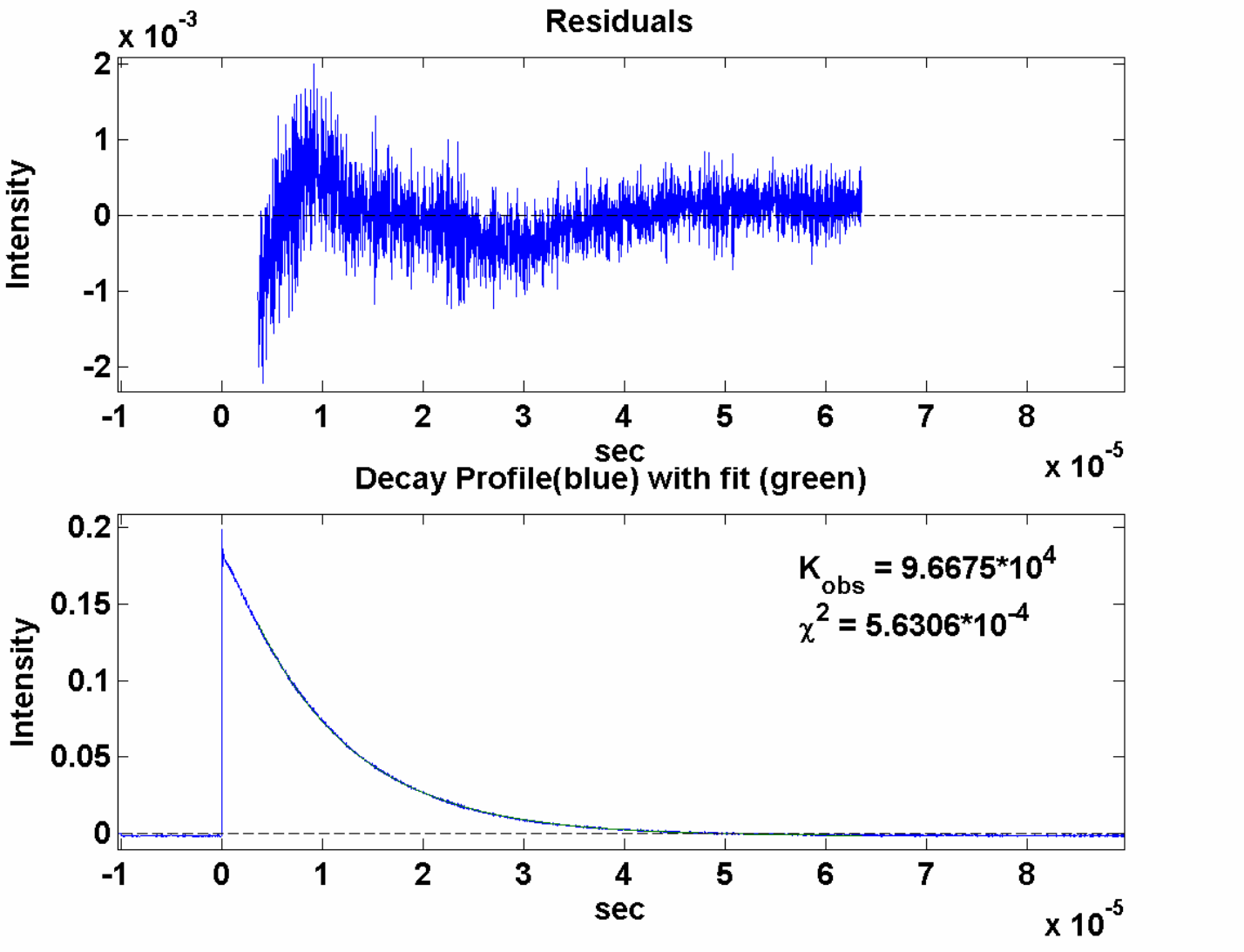
A solution of **2** (10 μM) in either cyclohexane or tetrahydrofuran was prepared in a nitrogen filled glovebox. The cuvettes (1 cm path) were charged with this solution, sparged briefly with argon, and sealed with a greased ground-glass stopper. The absorption spectra were acquired both before and after the fluorescence measurements to ensure the sample was not degrading. Fluorescent measurements were performed with λ_{ex} =460, λ_{em}= 510 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 (see Table 2).

Table 2: Data for Excited State Lifetime Measurements.

Entry	Solution	k_{obs} (s^{-1})	Lifetime (1/ k_{obs}) (μs)
1	10 μM **2** in tetrahydrofuran	8.9683E+04	11.15
2	10 μM **2** in tetrahydrofuran	8.9656E+04	11.15
3	10 μM **2** in tetrahydrofuran	9.4984E+04	10.53
		average	**10.94**
		std. deviation	**0.4**
	$t_{radiative}$[a](average)	6.22E+04	
	$t_{non\text{-}radiative}$[b] (average)	2.93E+04	
	Solution	k_{obs} (s^{-1})	Lifetime (1/ k_{obs}) (μs)
4	10 μM **2** in cyclohexane[c]	9.6675E+04	10.34
5	10 μM **2** in cyclohexane	9.9590E+04	10.04
		average	**10.19**
		std. deviation	**0.2**
	$k_{radiative}$[a] (average)	6.58E+04	
	$k_{non\text{-}radiative}$[b] (average)	3.24E+04	

(a) $k_{radiative}$ = (Quantum Yield)/(Lifetime); (b) $k_{non\text{-}radiative} = k_{obs} - k_{radiative}$ (c) indicates the representative fit shown below

Graph 1: Fit of the excited-state decay with residuals for Entry 4, Table 2.



Time-resolved luminescent quenching experiments.
A solution of **2** (20 μM) in tetrahydrofuran was prepared in a nitrogen-filled glovebox. Two cuvettes (1 cm path) were charged with 2 mL of this solution, sparged briefly with argon, and sealed with a rubber stopper. The initial emission decay of **2** in each cuvette was measured with λ_{ex} = 440 nm and λ_{em}= 500 nm prior to the introduction of the quencher. A solution of 2,6-dichloroquinone (DCQ) (10 mM) was then sequentially added to the cuvettes via syringe in volumes listed in Table 3, and the emission decay was measured. The combined data from the two runs is plotted in Graph 1, and a first order rate constant of $1.2 \cdot 10^{10}$ $M^{-1}s^{-1}$ was determined for the emission quenching.

Table 3: Time-resolved Emission Quenching Measurements.

Run 1		
μL of DCQ solution (total)	**μM of DCQ in sample**	**k_{obs} (s^{-1})**
0	0	2.1E+05
4	20	4.2E+05
20	99	1.3E+06
40	200	2.4E+06
80	380	4.7E+06
Run 2		
μL of DCQ solution (total)	**μM of DCQ in sample**	**k_{obs} (s^{-1})**
0	0	1.1E+05
10	50	9.7E+05
30	150	2.0E+06
50	240	3.2E+06
70	340	4.4E+06

Graph 2: Time-Resolved Emission Quenching with DCQ in THF.

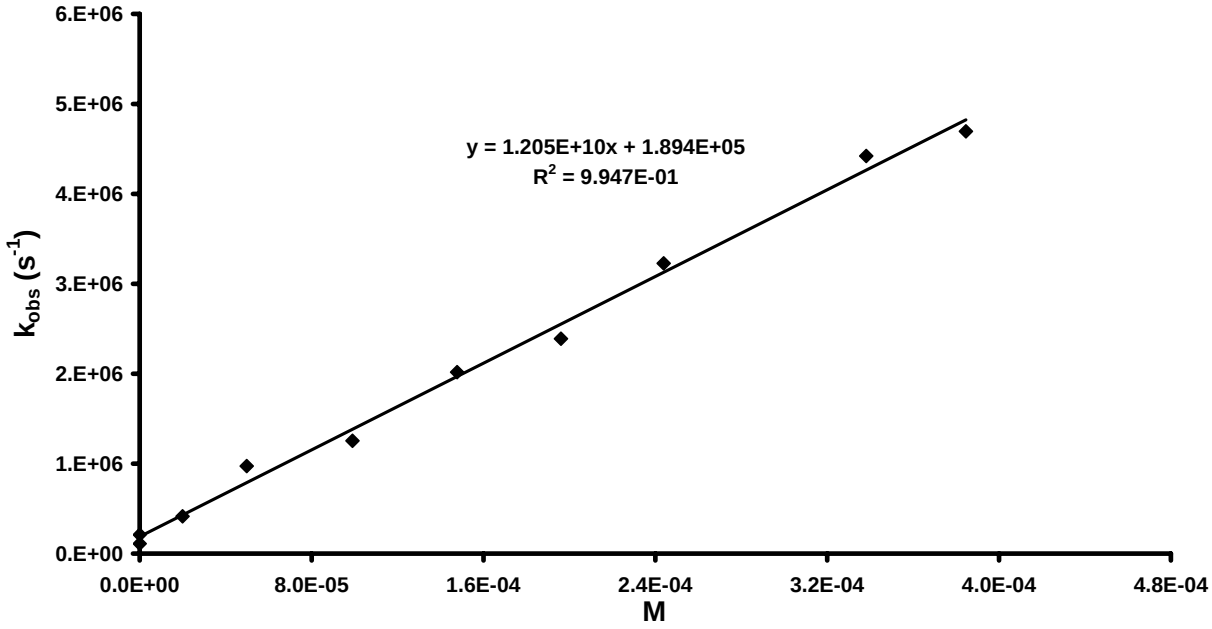


Figure 1: Cyclic voltammogram of **2** in CH_2Cl_2 (0.30 M [$^nBu_4N$][PF_6], 50 mV/s) referenced vs. Fc^+/Fc.

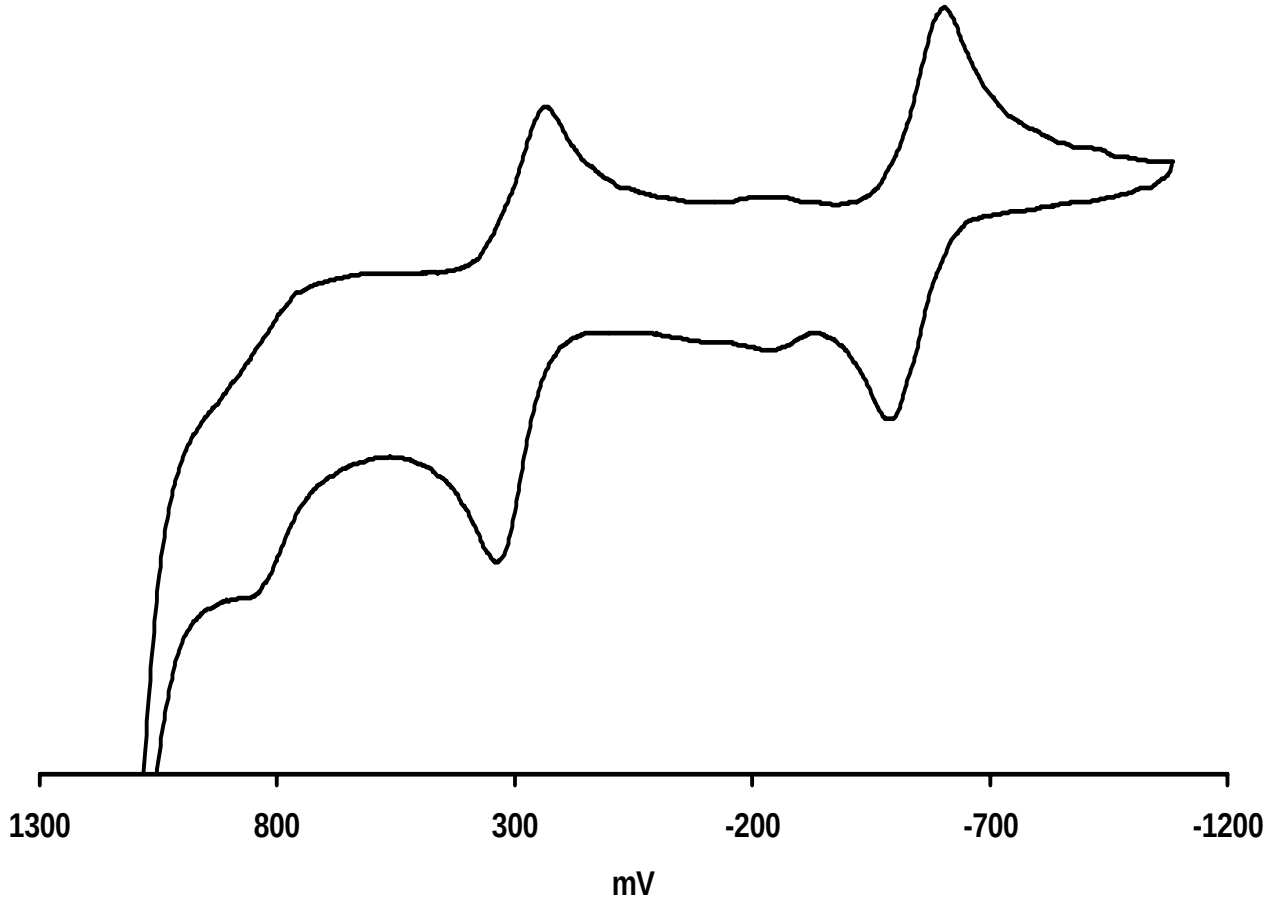


Figure 2: Solid State Molecular Structure of **2.** Hydrogen atoms have been omitted for clarity.

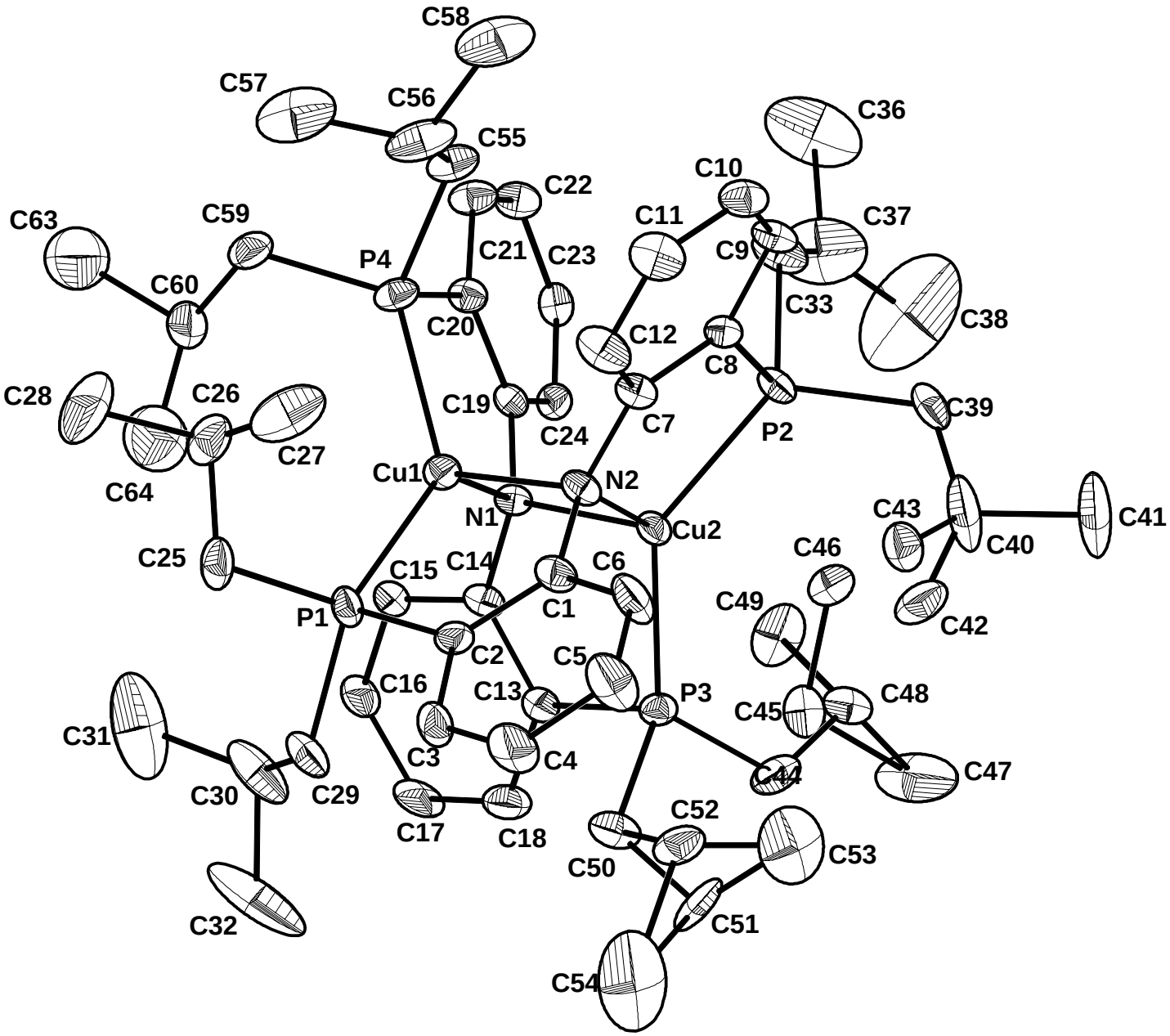


Table 4. Crystal data and structure refinement for **2**.

Name	$\{(PNP)Cu\}_2$	
Empirical formula	$C_{56}H_{88}Cu_2N_2P_4$	
Formula weight	1040.24	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca(#61)	
Unit cell dimensions	a = 21.5707(15) Å	α= 90°
	b = 21.4607(15) Å	β= 90°
	c = 23.8297(17) Å	γ = 90°
Volume	11031.3(13) $Å^3$	
Z	8	
Density (calculated)	1.253 Mg/m^3	
Absorption coefficient	0.924 mm^{-1}	
F(000)	4448	
Crystal size	0.36 x 0.21 x 0.18 mm^3	
Theta range for data collection	1.59 to 28.56°	
Index ranges	-28<=h<=27, -28<=k<=28, -31<=l<=31	
Reflections collected	158849	
Independent reflections	13443 [R_{int} = 0.0931]	
Completeness to theta = 28.56°	95.7 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13443 / 0 / 629	
Goodness-of-fit on F^2	1.129	
Final R indices [I>2sigma(I)]	R1 = 0.0789, wR2 = 0.1617	
R indices (all data)	R1 = 0.1118, wR2 = 0.1737	
Largest diff. peak and hole	1.635 and -0.691 e·$Å^{-3}$	

Special Refinement Details

Refinement of F^2 against all reflections. The weighted R-factor wR 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 > 2sigma(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. Several carbon atoms of the isobutyl groups were satisfactorily modeled by assuming a partial population over two sites.

Table 5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	974(1)	7198(1)	5954(1)	18(1)
Cu(2)	93(1)	7730(1)	6543(1)	17(1)
N(2)	1001(2)	7392(2)	6856(2)	18(1)
N(1)	81(2)	7466(2)	5661(2)	15(1)
P(1)	1801(1)	7798(1)	5842(1)	19(1)
P(2)	-366(1)	7084(1)	7143(1)	18(1)
P(3)	0(1)	8718(1)	6275(1)	18(1)
P(4)	760(1)	6218(1)	5705(1)	20(1)
C(1)	1494(2)	7805(2)	6981(2)	22(1)
C(2)	1900(2)	8043(2)	6572(2)	20(1)
C(3)	2366(2)	8464(2)	6716(2)	27(1)
C(4)	2459(3)	8646(3)	7265(2)	39(2)
C(5)	2074(3)	8395(3)	7677(3)	45(2)
C(6)	1609(3)	7992(3)	7539(2)	35(1)
C(7)	916(2)	6918(2)	7260(2)	18(1)
C(8)	327(2)	6705(2)	7422(2)	17(1)
C(9)	274(2)	6233(2)	7827(2)	22(1)
C(10)	783(2)	5970(2)	8083(2)	25(1)
C(11)	1365(3)	6176(3)	7923(2)	30(1)
C(12)	1432(2)	6633(3)	7517(2)	30(1)
C(13)	-2(2)	8602(2)	5517(2)	19(1)
C(14)	31(2)	7991(2)	5308(2)	18(1)
C(15)	32(2)	7910(2)	4715(2)	20(1)
C(16)	-13(2)	8415(2)	4357(2)	25(1)
C(17)	-59(3)	9015(2)	4571(2)	30(1)
C(18)	-49(3)	9103(2)	5143(2)	28(1)
C(19)	-275(2)	6951(2)	5482(2)	15(1)
C(20)	-49(2)	6333(2)	5514(2)	18(1)
C(21)	-431(2)	5837(2)	5362(2)	23(1)
C(22)	-1028(2)	5927(2)	5165(2)	23(1)
C(23)	-1243(2)	6534(2)	5114(2)	20(1)
C(24)	-882(2)	7031(2)	5273(2)	19(1)
C(25)	2537(2)	7413(3)	5647(2)	28(1)
C(26)	2601(3)	6731(3)	5802(3)	34(1)
C(27)	2704(4)	6643(3)	6422(3)	57(2)
C(28)	3114(4)	6428(4)	5458(4)	77(3)
C(29)	1890(2)	8559(3)	5475(2)	29(1)
C(30)	1601(3)	8633(3)	4900(3)	46(2)
C(31)	1921(4)	8271(5)	4449(3)	80(3)
C(32)	1597(4)	9322(4)	4732(4)	90(4)
C(33)	-838(2)	6397(3)	6947(3)	32(1)
C(36)	-1749(4)	5838(4)	6578(4)	75(3)
C(37)	-1470(3)	6470(4)	6712(4)	69(3)
C(38)	-1903(4)	6899(6)	6857(6)	129(6)
C(39)	-768(2)	7344(2)	7788(2)	25(1)
C(40)	-533(3)	7934(4)	8059(3)	52(2)
C(41)	-912(3)	8071(4)	8594(3)	62(2)
C(42)	-266(9)	8364(9)	7886(9)	37(6)
C(44)	-692(2)	9211(2)	6394(2)	30(1)
C(47)	-1828(2)	9414(2)	6386(2)	88(4)

C(43)	134(4)	8023(4)	8159(3)	28(2)
C(45)	-1331(4)	8935(5)	6142(7)	25(3)
C(46)	-1493(7)	8285(5)	6341(7)	45(3)
C(48)	-1285(6)	8934(5)	6467(7)	23(3)
C(49)	-1444(6)	8509(8)	5979(8)	45(6)
C(50)	631(3)	9294(2)	6353(2)	28(1)
C(51)	628(4)	9762(5)	6795(4)	35(3)
C(52)	896(7)	9408(7)	6962(7)	30(5)
C(53)	535(4)	9520(4)	7392(3)	61(2)
C(54)	1287(5)	10078(6)	6806(5)	125(5)
C(55)	721(2)	5557(2)	6198(2)	26(1)
C(56)	1323(3)	5367(3)	6505(3)	39(2)
C(57)	1820(3)	5098(3)	6132(3)	54(2)
C(58)	1152(4)	4902(3)	6967(3)	53(2)
C(59)	1060(2)	5845(2)	5060(2)	27(1)
C(60)	977(4)	6204(3)	4492(3)	51(2)
C(63)	1137(4)	5748(4)	3993(3)	61(2)
C(64)	1342(4)	6767(4)	4444(3)	60(2)

Table 6. Bond lengths [Å] and angles [°] for **2**.

Cu(1)-N(1)	2.127(4)	C(18)-H(18)	0.9500
Cu(1)-N(2)	2.191(4)	C(19)-C(20)	1.413(6)
Cu(1)-P(1)	2.2173(13)	C(19)-C(24)	1.413(6)
Cu(1)-P(4)	2.2339(13)	C(20)-C(21)	1.395(6)
Cu(1)-Cu(2)	2.6245(8)	C(21)-C(22)	1.384(7)
Cu(2)-N(1)	2.179(4)	C(21)-H(21)	0.9500
Cu(2)-N(2)	2.219(4)	C(22)-C(23)	1.388(7)
Cu(2)-P(3)	2.2235(13)	C(22)-H(22)	0.9500
Cu(2)-P(2)	2.2241(13)	C(23)-C(24)	1.375(7)
N(2)-C(7)	1.412(6)	C(23)-H(23)	0.9500
N(2)-C(1)	1.416(6)	C(24)-H(24)	0.9500
N(1)-C(14)	1.410(6)	C(25)-C(26)	1.515(8)
N(1)-C(19)	1.412(6)	C(25)-H(25A)	0.9900
P(1)-C(2)	1.829(5)	C(25)-H(25B)	0.9900
P(1)-C(25)	1.849(5)	C(26)-C(27)	1.507(10)
P(1)-C(29)	1.863(5)	C(26)-C(28)	1.523(8)
P(2)-C(8)	1.828(5)	C(26)-H(26)	0.98(6)
P(2)-C(39)	1.850(5)	C(27)-H(27A)	0.9800
P(2)-C(33)	1.851(5)	C(27)-H(27B)	0.9800
P(3)-C(13)	1.823(5)	C(27)-H(27C)	0.9800
P(3)-C(50)	1.848(5)	C(28)-H(28A)	0.9800
P(3)-C(44)	1.851(4)	C(28)-H(28B)	0.9800
P(4)-C(20)	1.820(5)	C(28)-H(28C)	0.9800
P(4)-C(55)	1.845(5)	C(29)-C(30)	1.514(8)
P(4)-C(59)	1.849(5)	C(29)-H(29A)	0.9900
C(1)-C(2)	1.406(7)	C(29)-H(29B)	0.9900
C(1)-C(6)	1.412(7)	C(30)-C(31)	1.496(11)
C(2)-C(3)	1.394(6)	C(30)-C(32)	1.531(11)
C(3)-C(4)	1.379(8)	C(30)-H(30)	0.9987
C(3)-H(3)	0.9500	C(31)-H(31A)	0.9800
C(4)-C(5)	1.396(8)	C(31)-H(31B)	0.9800
C(4)-H(4)	0.9500	C(31)-H(31C)	0.9800
C(5)-C(6)	1.364(7)	C(32)-H(32A)	0.9800
C(5)-H(5)	0.9500	C(32)-H(32B)	0.9800
C(6)-H(6)	0.9500	C(32)-H(32C)	0.9800
C(7)-C(8)	1.404(6)	C(33)-C(37)	1.482(8)
C(7)-C(12)	1.409(7)	C(33)-H(33A)	0.9900
C(8)-C(9)	1.403(6)	C(33)-H(33B)	0.9900
C(9)-C(10)	1.377(7)	C(36)-C(37)	1.519(10)
C(9)-H(9)	0.9500	C(36)-H(36A)	0.9800
C(10)-C(11)	1.385(8)	C(36)-H(36B)	0.9800
C(10)-H(10)	0.9500	C(36)-H(36C)	0.9800
C(11)-C(12)	1.385(7)	C(37)-C(38)	1.356(12)
C(11)-H(11)	0.9500	C(37)-H(37)	1.0002
C(12)-H(12)	0.9500	C(38)-H(38A)	0.9800
C(13)-C(18)	1.401(7)	C(38)-H(38B)	0.9800
C(13)-C(14)	1.404(6)	C(38)-H(38C)	0.9800
C(14)-C(15)	1.423(6)	C(39)-C(40)	1.509(9)
C(15)-C(16)	1.382(7)	C(39)-H(39A)	0.9900
C(15)-H(15)	0.9500	C(39)-H(39B)	0.9900
C(16)-C(17)	1.390(7)	C(40)-C(42)	1.16(2)
C(16)-H(16)	0.9500	C(40)-C(43)	1.470(10)
C(17)-C(18)	1.375(7)	C(40)-C(41)	1.542(8)
C(17)-H(17)	0.9500	C(40)-H(40A)	1.0149

C(40)-H(40B)	1.0016	C(52)-H(52)	0.9833
C(41)-H(41A)	0.9800	C(52)-H(50A)	1.5733
C(41)-H(41B)	0.9800	C(53)-H(53A)	0.9934
C(41)-H(41C)	0.9800	C(53)-H(53B)	0.9856
C(42)-H(40A)	0.8505	C(53)-H(53C)	1.0072
C(42)-H(42A)	0.9733	C(54)-H(54A)	0.9803
C(42)-H(42B)	0.9851	C(54)-H(54B)	0.9887
C(42)-H(42C)	1.0193	C(54)-H(54C)	0.9881
C(42)-H(43C)	1.3752	C(55)-C(56)	1.545(7)
C(42)-H(40B)	1.5856	C(55)-H(55A)	0.9900
C(44)-C(48)	1.421(12)	C(55)-H(55B)	0.9900
C(44)-C(45)	1.616(12)	C(56)-C(57)	1.510(10)
C(44)-H(44A)	1.0035	C(56)-C(58)	1.531(9)
C(44)-H(44B)	1.0139	C(56)-H(56)	0.94(7)
C(44)-H(44C)	1.0148	C(57)-H(57A)	0.9800
C(44)-H(44D)	1.0026	C(57)-H(57B)	0.9800
C(47)-C(48)	1.572(13)	C(57)-H(57C)	0.9800
C(47)-C(45)	1.595(11)	C(58)-H(58A)	0.9800
C(47)-H(47A)	1.0181	C(58)-H(58B)	0.9800
C(47)-H(47B)	0.9684	C(58)-H(58C)	0.9800
C(47)-H(47C)	0.9819	C(59)-C(60)	1.568(9)
C(43)-H(42A)	1.0105	C(59)-H(59A)	0.9900
C(43)-H(43A)	0.9867	C(59)-H(59B)	0.9900
C(43)-H(43B)	0.9913	C(60)-C(64)	1.448(10)
C(43)-H(43C)	0.9791	C(60)-C(63)	1.579(10)
C(43)-H(40B)	0.8825	C(60)-H(60B)	1.13(8)
C(45)-C(46)	1.513(18)	C(63)-H(63A)	0.9800
C(45)-H(45)	0.9664	C(63)-H(63B)	0.9800
C(45)-H(49A)	1.2741	C(63)-H(63C)	0.9800
C(46)-H(46A)	0.9800	C(64)-H(64A)	0.9800
C(46)-H(46B)	0.9800	C(64)-H(64B)	0.9800
C(46)-H(46C)	0.9800	C(64)-H(64C)	0.9800
C(46)-H(48)	1.5382		
C(46)-H(49B)	1.1980	N(1)-Cu(1)-N(2)	107.20(14)
C(46)-H(49C)	1.0629	N(1)-Cu(1)-P(1)	122.18(11)
C(48)-C(49)	1.52(2)	N(2)-Cu(1)-P(1)	89.20(10)
C(48)-H(48)	1.0018	N(1)-Cu(1)-P(4)	88.88(11)
C(49)-H(45)	1.1614	N(2)-Cu(1)-P(4)	116.39(11)
C(49)-H(46B)	1.4630	P(1)-Cu(1)-P(4)	132.93(5)
C(49)-H(46C)	1.2192	N(1)-Cu(1)-Cu(2)	53.34(10)
C(49)-H(49A)	0.9984	N(2)-Cu(1)-Cu(2)	53.98(10)
C(49)-H(49B)	0.9525	P(1)-Cu(1)-Cu(2)	113.25(4)
C(49)-H(49C)	0.9371	P(4)-Cu(1)-Cu(2)	113.73(4)
C(50)-C(51)	1.457(10)	N(1)-Cu(2)-N(2)	104.44(14)
C(50)-C(52)	1.579(16)	N(1)-Cu(2)-P(3)	88.23(10)
C(50)-H(50C)	1.0097	N(2)-Cu(2)-P(3)	119.26(10)
C(50)-H(50D)	0.9977	N(1)-Cu(2)-P(2)	116.91(11)
C(50)-H(50A)	0.9980	N(2)-Cu(2)-P(2)	88.45(10)
C(50)-H(50B)	1.0095	P(3)-Cu(2)-P(2)	137.69(5)
C(51)-C(53)	1.528(14)	N(1)-Cu(2)-Cu(1)	51.56(10)
C(51)-C(54)	1.574(13)	N(2)-Cu(2)-Cu(1)	52.99(10)
C(51)-H(50D)	1.4713	P(3)-Cu(2)-Cu(1)	109.03(4)
C(51)-H(51)	1.0253	P(2)-Cu(2)-Cu(1)	113.26(4)
C(51)-H(53A)	1.5320	C(7)-N(2)-C(1)	114.0(4)
C(52)-C(53)	1.311(17)	C(7)-N(2)-Cu(1)	122.0(3)
C(52)-C(54)	1.707(17)	C(1)-N(2)-Cu(1)	110.2(3)

C(7)-N(2)-Cu(2)	110.4(3)	C(7)-C(8)-P(2)	119.7(3)
C(1)-N(2)-Cu(2)	121.8(3)	C(10)-C(9)-C(8)	122.4(5)
Cu(1)-N(2)-Cu(2)	73.03(12)	C(10)-C(9)-H(9)	118.8
C(14)-N(1)-C(19)	113.9(4)	C(8)-C(9)-H(9)	118.8
C(14)-N(1)-Cu(1)	118.7(3)	C(9)-C(10)-C(11)	118.0(5)
C(19)-N(1)-Cu(1)	112.3(3)	C(9)-C(10)-H(10)	121.0
C(14)-N(1)-Cu(2)	111.6(3)	C(11)-C(10)-H(10)	121.0
C(19)-N(1)-Cu(2)	120.1(3)	C(10)-C(11)-C(12)	120.8(5)
Cu(1)-N(1)-Cu(2)	75.10(12)	C(10)-C(11)-H(11)	119.6
C(2)-P(1)-C(25)	105.5(2)	C(12)-C(11)-H(11)	119.6
C(2)-P(1)-C(29)	100.5(2)	C(11)-C(12)-C(7)	121.9(5)
C(25)-P(1)-C(29)	100.7(2)	C(11)-C(12)-H(12)	119.1
C(2)-P(1)-Cu(1)	98.39(15)	C(7)-C(12)-H(12)	119.1
C(25)-P(1)-Cu(1)	117.51(18)	C(18)-C(13)-C(14)	119.6(4)
C(29)-P(1)-Cu(1)	130.41(18)	C(18)-C(13)-P(3)	121.7(4)
C(8)-P(2)-C(39)	102.4(2)	C(14)-C(13)-P(3)	118.6(3)
C(8)-P(2)-C(33)	100.7(2)	C(13)-C(14)-N(1)	122.6(4)
C(39)-P(2)-C(33)	101.1(3)	C(13)-C(14)-C(15)	117.8(4)
C(8)-P(2)-Cu(2)	98.48(15)	N(1)-C(14)-C(15)	119.6(4)
C(39)-P(2)-Cu(2)	123.62(17)	C(16)-C(15)-C(14)	121.1(4)
C(33)-P(2)-Cu(2)	125.5(2)	C(16)-C(15)-H(15)	119.4
C(13)-P(3)-C(50)	101.1(2)	C(14)-C(15)-H(15)	119.4
C(13)-P(3)-C(44)	103.2(2)	C(15)-C(16)-C(17)	120.3(5)
C(50)-P(3)-C(44)	101.4(2)	C(15)-C(16)-H(16)	119.8
C(13)-P(3)-Cu(2)	98.92(15)	C(17)-C(16)-H(16)	119.8
C(50)-P(3)-Cu(2)	122.80(18)	C(18)-C(17)-C(16)	119.3(5)
C(44)-P(3)-Cu(2)	124.96(15)	C(18)-C(17)-H(17)	120.3
C(20)-P(4)-C(55)	102.7(2)	C(16)-C(17)-H(17)	120.3
C(20)-P(4)-C(59)	100.8(2)	C(17)-C(18)-C(13)	121.8(5)
C(55)-P(4)-C(59)	102.2(2)	C(17)-C(18)-H(18)	119.1
C(20)-P(4)-Cu(1)	97.81(15)	C(13)-C(18)-H(18)	119.1
C(55)-P(4)-Cu(1)	124.38(17)	N(1)-C(19)-C(20)	122.1(4)
C(59)-P(4)-Cu(1)	123.79(17)	N(1)-C(19)-C(24)	120.9(4)
C(2)-C(1)-C(6)	116.2(4)	C(20)-C(19)-C(24)	116.9(4)
C(2)-C(1)-N(2)	123.3(4)	C(21)-C(20)-C(19)	119.9(4)
C(6)-C(1)-N(2)	120.5(4)	C(21)-C(20)-P(4)	121.8(4)
C(3)-C(2)-C(1)	120.8(5)	C(19)-C(20)-P(4)	118.1(3)
C(3)-C(2)-P(1)	120.3(4)	C(22)-C(21)-C(20)	122.0(4)
C(1)-C(2)-P(1)	118.9(3)	C(22)-C(21)-H(21)	119.0
C(4)-C(3)-C(2)	121.6(5)	C(20)-C(21)-H(21)	119.0
C(4)-C(3)-H(3)	119.2	C(21)-C(22)-C(23)	118.2(4)
C(2)-C(3)-H(3)	119.2	C(21)-C(22)-H(22)	120.9
C(3)-C(4)-C(5)	118.0(5)	C(23)-C(22)-H(22)	120.9
C(3)-C(4)-H(4)	121.0	C(24)-C(23)-C(22)	121.0(4)
C(5)-C(4)-H(4)	121.0	C(24)-C(23)-H(23)	119.5
C(6)-C(5)-C(4)	120.9(5)	C(22)-C(23)-H(23)	119.5
C(6)-C(5)-H(5)	119.6	C(23)-C(24)-C(19)	121.8(4)
C(4)-C(5)-H(5)	119.6	C(23)-C(24)-H(24)	119.1
C(5)-C(6)-C(1)	122.4(5)	C(19)-C(24)-H(24)	119.1
C(5)-C(6)-H(6)	118.8	C(26)-C(25)-P(1)	116.7(4)
C(1)-C(6)-H(6)	118.8	C(26)-C(25)-H(25A)	108.1
C(8)-C(7)-C(12)	117.0(4)	P(1)-C(25)-H(25A)	108.1
C(8)-C(7)-N(2)	122.7(4)	C(26)-C(25)-H(25B)	108.1
C(12)-C(7)-N(2)	120.3(4)	P(1)-C(25)-H(25B)	108.1
C(9)-C(8)-C(7)	119.8(4)	H(25A)-C(25)-H(25B)	107.3
C(9)-C(8)-P(2)	120.4(4)	C(27)-C(26)-C(25)	111.9(5)

C(27)-C(26)-C(28)	111.5(6)	C(40)-C(39)-H(39B)	108.1
C(25)-C(26)-C(28)	110.3(6)	P(2)-C(39)-H(39B)	108.1
C(27)-C(26)-H(26)	107(4)	H(39A)-C(39)-H(39B)	107.3
C(25)-C(26)-H(26)	110(4)	C(42)-C(40)-C(43)	58.1(11)
C(28)-C(26)-H(26)	106(4)	C(42)-C(40)-C(39)	132.8(12)
C(26)-C(27)-H(27A)	109.5	C(43)-C(40)-C(39)	120.4(6)
C(26)-C(27)-H(27B)	109.5	C(42)-C(40)-C(41)	113.9(12)
H(27A)-C(27)-H(27B)	109.5	C(43)-C(40)-C(41)	111.1(6)
C(26)-C(27)-H(27C)	109.5	C(39)-C(40)-C(41)	109.6(5)
H(27A)-C(27)-H(27C)	109.5	C(42)-C(40)-H(40A)	45.3
H(27B)-C(27)-H(27C)	109.5	C(43)-C(40)-H(40A)	103.0
C(26)-C(28)-H(28A)	109.5	C(39)-C(40)-H(40A)	106.2
C(26)-C(28)-H(28B)	109.5	C(41)-C(40)-H(40A)	105.2
H(28A)-C(28)-H(28B)	109.5	C(42)-C(40)-H(40B)	93.9
C(26)-C(28)-H(28C)	109.5	C(43)-C(40)-H(40B)	35.9
H(28A)-C(28)-H(28C)	109.5	C(39)-C(40)-H(40B)	98.4
H(28B)-C(28)-H(28C)	109.5	C(41)-C(40)-H(40B)	96.8
C(30)-C(29)-P(1)	118.3(4)	H(40A)-C(40)-H(40B)	138.8
C(30)-C(29)-H(29A)	107.7	C(40)-C(41)-H(41A)	109.5
P(1)-C(29)-H(29A)	107.7	C(40)-C(41)-H(41B)	109.5
C(30)-C(29)-H(29B)	107.7	H(41A)-C(41)-H(41B)	109.5
P(1)-C(29)-H(29B)	107.7	C(40)-C(41)-H(41C)	109.5
H(29A)-C(29)-H(29B)	107.1	H(41A)-C(41)-H(41C)	109.5
C(31)-C(30)-C(29)	113.9(6)	H(41B)-C(41)-H(41C)	109.5
C(31)-C(30)-C(32)	108.5(7)	C(40)-C(42)-H(40A)	58.1
C(29)-C(30)-C(32)	109.9(6)	C(40)-C(42)-H(42A)	112.8
C(31)-C(30)-H(30)	108.0	H(40A)-C(42)-H(42A)	143.9
C(29)-C(30)-H(30)	108.3	C(40)-C(42)-H(42B)	112.3
C(32)-C(30)-H(30)	108.2	H(40A)-C(42)-H(42B)	105.7
C(30)-C(31)-H(31A)	109.5	H(42A)-C(42)-H(42B)	109.6
C(30)-C(31)-H(31B)	109.5	C(40)-C(42)-H(42C)	109.0
H(31A)-C(31)-H(31B)	109.5	H(40A)-C(42)-H(42C)	55.0
C(30)-C(31)-H(31C)	109.5	H(42A)-C(42)-H(42C)	106.8
H(31A)-C(31)-H(31C)	109.5	H(42B)-C(42)-H(42C)	106.0
H(31B)-C(31)-H(31C)	109.5	C(40)-C(42)-H(43C)	106.7
C(30)-C(32)-H(32A)	109.5	H(40A)-C(42)-H(43C)	144.7
C(30)-C(32)-H(32B)	109.5	H(42A)-C(42)-H(43C)	7.4
H(32A)-C(32)-H(32B)	109.5	H(42B)-C(42)-H(43C)	109.5
C(30)-C(32)-H(32C)	109.5	H(42C)-C(42)-H(43C)	113.5
H(32A)-C(32)-H(32C)	109.5	C(40)-C(42)-H(40B)	39.1
H(32B)-C(32)-H(32C)	109.5	H(40A)-C(42)-H(40B)	96.9
C(37)-C(33)-P(2)	121.1(5)	H(42A)-C(42)-H(40B)	79.1
C(37)-C(33)-H(33A)	107.1	H(42B)-C(42)-H(40B)	108.3
P(2)-C(33)-H(33A)	107.1	H(42C)-C(42)-H(40B)	140.7
C(37)-C(33)-H(33B)	107.1	H(43C)-C(42)-H(40B)	72.0
P(2)-C(33)-H(33B)	107.1	C(48)-C(44)-C(45)	28.9(5)
H(33A)-C(33)-H(33B)	106.8	C(48)-C(44)-P(3)	120.3(5)
C(38)-C(37)-C(33)	127.5(8)	C(45)-C(44)-P(3)	114.9(5)
C(38)-C(37)-C(36)	112.8(8)	C(48)-C(44)-H(44A)	82.5
C(33)-C(37)-C(36)	110.5(7)	C(45)-C(44)-H(44A)	110.4
C(38)-C(37)-H(37)	100.5	P(3)-C(44)-H(44A)	109.2
C(33)-C(37)-H(37)	99.9	C(48)-C(44)-H(44B)	124.8
C(36)-C(37)-H(37)	99.8	C(45)-C(44)-H(44B)	108.4
C(40)-C(39)-P(2)	116.9(4)	P(3)-C(44)-H(44B)	108.7
C(40)-C(39)-H(39A)	108.1	H(44A)-C(44)-H(44B)	104.8
P(2)-C(39)-H(39A)	108.1	C(48)-C(44)-H(44C)	107.8

C(45)-C(44)-H(44C)	131.7	H(46A)-C(46)-H(49B)	117.2
P(3)-C(44)-H(44C)	107.2	H(46B)-C(46)-H(49B)	128.9
H(44A)-C(44)-H(44C)	29.6	H(46C)-C(46)-H(49B)	36.1
H(44B)-C(44)-H(44C)	77.9	H(48)-C(46)-H(49B)	122.1
C(48)-C(44)-H(44D)	108.4	C(45)-C(46)-H(49C)	82.0
C(45)-C(44)-H(44D)	85.0	H(46A)-C(46)-H(49C)	152.1
P(3)-C(44)-H(44D)	107.8	H(46B)-C(46)-H(49C)	42.9
H(44A)-C(44)-H(44D)	127.8	H(46C)-C(46)-H(49C)	88.2
H(44B)-C(44)-H(44D)	27.3	H(48)-C(46)-H(49C)	124.5
H(44C)-C(44)-H(44D)	104.1	H(49B)-C(46)-H(49C)	89.9
C(48)-C(47)-C(45)	28.5(5)	C(44)-C(48)-C(49)	111.2(13)
C(48)-C(47)-H(47A)	81.8	C(44)-C(48)-C(47)	112.4(7)
C(45)-C(47)-H(47A)	110.2	C(49)-C(48)-C(47)	97.6(12)
C(48)-C(47)-H(47B)	124.9	C(44)-C(48)-H(48)	111.6
C(45)-C(47)-H(47B)	111.4	C(49)-C(48)-H(48)	111.7
H(47A)-C(47)-H(47B)	107.3	C(47)-C(48)-H(48)	111.7
C(48)-C(47)-H(47C)	119.0	C(48)-C(49)-H(45)	80.0
C(45)-C(47)-H(47C)	111.2	C(48)-C(49)-H(46B)	86.5
H(47A)-C(47)-H(47C)	106.3	H(45)-C(49)-H(46B)	140.1
H(47B)-C(47)-H(47C)	110.3	C(48)-C(49)-H(46C)	111.1
C(40)-C(43)-H(42A)	89.9	H(45)-C(49)-H(46C)	147.2
C(40)-C(43)-H(43A)	109.5	H(46B)-C(49)-H(46C)	72.6
H(42A)-C(43)-H(43A)	130.4	C(48)-C(49)-H(49A)	105.6
C(40)-C(43)-H(43B)	110.4	H(45)-C(49)-H(49A)	26.4
H(42A)-C(43)-H(43B)	106.7	H(46B)-C(49)-H(49A)	135.1
H(43A)-C(43)-H(43B)	108.0	H(46C)-C(49)-H(49A)	135.4
C(40)-C(43)-H(43C)	111.2	C(48)-C(49)-H(49B)	106.4
H(42A)-C(43)-H(43C)	24.8	H(45)-C(49)-H(49B)	112.6
H(43A)-C(43)-H(43C)	109.0	H(46B)-C(49)-H(49B)	107.2
H(43B)-C(43)-H(43C)	108.6	H(46C)-C(49)-H(49B)	35.3
C(40)-C(43)-H(40B)	41.7	H(49A)-C(49)-H(49B)	110.2
H(42A)-C(43)-H(40B)	127.2	C(48)-C(49)-H(49C)	106.7
H(43A)-C(43)-H(40B)	70.6	H(45)-C(49)-H(49C)	126.3
H(43B)-C(43)-H(40B)	109.4	H(46B)-C(49)-H(49C)	26.4
H(43C)-C(43)-H(40B)	139.8	H(46C)-C(49)-H(49C)	81.4
C(46)-C(45)-C(47)	109.0(9)	H(49A)-C(49)-H(49C)	111.5
C(46)-C(45)-C(44)	114.7(11)	H(49B)-C(49)-H(49C)	115.8
C(47)-C(45)-C(44)	101.6(8)	C(51)-C(50)-C(52)	39.6(6)
C(46)-C(45)-H(45)	112.0	C(51)-C(50)-P(3)	122.0(5)
C(47)-C(45)-H(45)	108.7	C(52)-C(50)-P(3)	117.6(6)
C(44)-C(45)-H(45)	110.2	C(51)-C(50)-H(50C)	128.0
C(46)-C(45)-H(49A)	90.6	C(52)-C(50)-H(50C)	107.0
C(47)-C(45)-H(49A)	121.6	P(3)-C(50)-H(50C)	108.4
C(44)-C(45)-H(49A)	119.4	C(51)-C(50)-H(50D)	70.9
H(45)-C(45)-H(49A)	21.7	C(52)-C(50)-H(50D)	108.9
C(45)-C(46)-H(46A)	110.9	P(3)-C(50)-H(50D)	108.9
C(45)-C(46)-H(46B)	109.0	H(50C)-C(50)-H(50D)	105.3
H(46A)-C(46)-H(46B)	109.5	C(51)-C(50)-H(50A)	106.4
C(45)-C(46)-H(46C)	108.6	C(52)-C(50)-H(50A)	71.3
H(46A)-C(46)-H(46C)	109.5	P(3)-C(50)-H(50A)	107.8
H(46B)-C(46)-H(46C)	109.5	H(50C)-C(50)-H(50A)	41.4
C(45)-C(46)-H(48)	68.7	H(50D)-C(50)-H(50A)	137.3
H(46A)-C(46)-H(48)	47.5	C(51)-C(50)-H(50B)	107.6
H(46B)-C(46)-H(48)	104.1	C(52)-C(50)-H(50B)	134.3
H(46C)-C(46)-H(48)	144.9	P(3)-C(50)-H(50B)	107.1
C(45)-C(46)-H(49B)	73.1	H(50C)-C(50)-H(50B)	64.8

H(50D)-C(50)-H(50B)	43.3	C(56)-C(55)-H(55A)	107.9
H(50A)-C(50)-H(50B)	104.7	P(4)-C(55)-H(55A)	107.9
C(50)-C(51)-C(53)	116.1(8)	C(56)-C(55)-H(55B)	107.9
C(50)-C(51)-C(54)	107.7(7)	P(4)-C(55)-H(55B)	107.9
C(53)-C(51)-C(54)	104.4(8)	H(55A)-C(55)-H(55B)	107.2
C(50)-C(51)-H(50D)	39.8	C(57)-C(56)-C(58)	110.2(5)
C(53)-C(51)-H(50D)	148.4	C(57)-C(56)-C(55)	114.7(5)
C(54)-C(51)-H(50D)	103.6	C(58)-C(56)-C(55)	108.1(5)
C(50)-C(51)-H(51)	108.5	C(57)-C(56)-H(56)	107(4)
C(53)-C(51)-H(51)	111.1	C(58)-C(56)-H(56)	110(4)
C(54)-C(51)-H(51)	108.6	C(55)-C(56)-H(56)	107(4)
H(50D)-C(51)-H(51)	72.8	C(56)-C(57)-H(57A)	109.5
C(50)-C(51)-H(53A)	140.2	C(56)-C(57)-H(57B)	109.5
C(53)-C(51)-H(53A)	37.9	H(57A)-C(57)-H(57B)	109.5
C(54)-C(51)-H(53A)	108.6	C(56)-C(57)-H(57C)	109.5
H(50D)-C(51)-H(53A)	139.7	H(57A)-C(57)-H(57C)	109.5
H(51)-C(51)-H(53A)	74.4	H(57B)-C(57)-H(57C)	109.5
C(53)-C(52)-C(50)	122.2(11)	C(56)-C(58)-H(58A)	109.5
C(53)-C(52)-C(54)	108.0(10)	C(56)-C(58)-H(58B)	109.5
C(50)-C(52)-C(54)	96.3(10)	H(58A)-C(58)-H(58B)	109.5
C(53)-C(52)-H(52)	108.4	C(56)-C(58)-H(58C)	109.5
C(50)-C(52)-H(52)	110.4	H(58A)-C(58)-H(58C)	109.5
C(54)-C(52)-H(52)	110.7	H(58B)-C(58)-H(58C)	109.5
C(53)-C(52)-H(50A)	150.4	C(60)-C(59)-P(4)	117.6(4)
C(50)-C(52)-H(50A)	36.9	C(60)-C(59)-H(59A)	107.9
C(54)-C(52)-H(50A)	97.1	P(4)-C(59)-H(59A)	107.9
H(52)-C(52)-H(50A)	75.8	C(60)-C(59)-H(59B)	107.9
C(52)-C(53)-C(51)	41.9(8)	P(4)-C(59)-H(59B)	107.9
C(52)-C(53)-H(53A)	112.3	H(59A)-C(59)-H(59B)	107.2
C(51)-C(53)-H(53A)	71.3	C(64)-C(60)-C(59)	114.6(7)
C(52)-C(53)-H(53B)	112.0	C(64)-C(60)-C(63)	109.8(6)
C(51)-C(53)-H(53B)	134.9	C(59)-C(60)-C(63)	108.7(5)
H(53A)-C(53)-H(53B)	107.9	C(64)-C(60)-H(60B)	111(4)
C(52)-C(53)-H(53C)	111.2	C(59)-C(60)-H(60B)	123(4)
C(51)-C(53)-H(53C)	116.8	C(63)-C(60)-H(60B)	84(4)
H(53A)-C(53)-H(53C)	106.2	C(60)-C(63)-H(63A)	109.5
H(53B)-C(53)-H(53C)	106.8	C(60)-C(63)-H(63B)	109.5
C(51)-C(54)-C(52)	36.5(6)	H(63A)-C(63)-H(63B)	109.5
C(51)-C(54)-H(54A)	98.6	C(60)-C(63)-H(63C)	109.5
C(52)-C(54)-H(54A)	111.4	H(63A)-C(63)-H(63C)	109.5
C(51)-C(54)-H(54B)	83.7	H(63B)-C(63)-H(63C)	109.5
C(52)-C(54)-H(54B)	110.3	C(60)-C(64)-H(64A)	109.5
H(54A)-C(54)-H(54B)	108.7	C(60)-C(64)-H(64B)	109.5
C(51)-C(54)-H(54C)	144.0	H(64A)-C(64)-H(64B)	109.5
C(52)-C(54)-H(54C)	109.5	C(60)-C(64)-H(64C)	109.5
H(54A)-C(54)-H(54C)	108.8	H(64A)-C(64)-H(64C)	109.5
H(54B)-C(54)-H(54C)	108.1	H(64B)-C(64)-H(64C)	109.5
C(56)-C(55)-P(4)	117.8(4)		

Table 7. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **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)	14(1)	17(1)	23(1)	-2(1)	-1(1)	-3(1)
Cu(2)	19(1)	17(1)	16(1)	5(1)	2(1)	0(1)
N(2)	17(2)	20(2)	16(2)	3(2)	-4(2)	-6(2)
N(1)	16(2)	14(2)	14(2)	3(1)	-4(2)	0(2)
P(1)	16(1)	25(1)	18(1)	-3(1)	4(1)	-5(1)
P(2)	14(1)	20(1)	20(1)	7(1)	0(1)	-3(1)
P(3)	24(1)	14(1)	15(1)	1(1)	-2(1)	0(1)
P(4)	15(1)	14(1)	31(1)	-2(1)	-5(1)	1(1)
C(1)	17(2)	21(2)	27(3)	1(2)	-1(2)	-7(2)
C(2)	19(2)	15(2)	27(3)	-3(2)	2(2)	-4(2)
C(3)	21(2)	31(3)	28(3)	-7(2)	8(2)	-10(2)
C(4)	38(3)	41(3)	38(3)	-13(3)	5(3)	-28(3)
C(5)	52(4)	56(4)	27(3)	-13(3)	5(3)	-34(3)
C(6)	39(3)	43(3)	24(3)	-5(2)	11(2)	-24(3)
C(7)	19(2)	19(2)	17(2)	2(2)	-5(2)	-4(2)
C(8)	18(2)	14(2)	19(2)	0(2)	-1(2)	-3(2)
C(9)	25(2)	17(2)	23(2)	5(2)	-3(2)	-7(2)
C(10)	34(3)	20(2)	22(2)	5(2)	-6(2)	-1(2)
C(11)	28(3)	34(3)	27(3)	9(2)	-14(2)	2(2)
C(12)	18(2)	36(3)	35(3)	10(3)	-8(2)	-8(2)
C(13)	21(2)	18(2)	19(2)	2(2)	2(2)	-2(2)
C(14)	17(2)	16(2)	20(2)	5(2)	-3(2)	-2(2)
C(15)	20(2)	18(2)	21(2)	2(2)	4(2)	-2(2)
C(16)	35(3)	26(3)	14(2)	4(2)	4(2)	-4(2)
C(17)	46(3)	23(3)	22(3)	14(2)	1(2)	-4(2)
C(18)	39(3)	18(2)	27(3)	4(2)	-1(2)	-3(2)
C(19)	16(2)	16(2)	13(2)	4(2)	-1(2)	-1(2)
C(20)	17(2)	17(2)	22(2)	2(2)	-1(2)	-1(2)
C(21)	19(2)	16(2)	34(3)	0(2)	-7(2)	-1(2)
C(22)	22(2)	21(2)	27(3)	-2(2)	-5(2)	-8(2)
C(23)	16(2)	26(2)	16(2)	0(2)	-1(2)	0(2)
C(24)	19(2)	18(2)	18(2)	1(2)	1(2)	2(2)
C(25)	16(2)	39(3)	30(3)	-12(2)	8(2)	-5(2)
C(26)	19(3)	33(3)	49(4)	-14(3)	5(2)	1(2)
C(27)	61(5)	37(4)	72(5)	-9(4)	-21(4)	16(3)
C(28)	68(6)	61(5)	102(7)	-24(5)	36(5)	20(4)
C(29)	22(3)	34(3)	31(3)	10(2)	7(2)	-6(2)
C(30)	23(3)	69(5)	45(4)	26(3)	-3(3)	-18(3)
C(31)	47(4)	170(10)	23(4)	-6(5)	-7(3)	-12(5)
C(32)	71(6)	106(7)	93(7)	78(6)	-20(5)	-42(5)
C(33)	21(3)	32(3)	43(3)	7(2)	-5(2)	-14(2)
C(36)	60(5)	85(6)	82(6)	18(5)	-47(5)	-41(5)
C(37)	36(4)	63(5)	107(7)	0(5)	-38(4)	-11(4)
C(38)	30(5)	168(12)	190(13)	-76(10)	-55(6)	33(6)
C(39)	17(2)	33(3)	24(3)	16(2)	5(2)	4(2)
C(40)	34(3)	90(6)	33(3)	-21(4)	20(3)	-23(4)
C(41)	39(4)	107(7)	41(4)	-29(4)	25(3)	-15(4)
C(42)	33(11)	23(10)	54(14)	-16(9)	1(9)	-2(8)
C(44)	50(1)	17(1)	21(2)	-3(2)	-5(2)	7(2)
C(47)	27(4)	33(4)	204(12)	21(5)	32(5)	11(3)

C(43)	28(4)	35(4)	22(4)	-2(3)	3(3)	-4(3)
C(45)	18(5)	38(7)	17(8)	3(5)	-6(4)	5(4)
C(46)	68(1)	21(1)	45(9)	-2(5)	24(7)	3(5)
C(48)	36(7)	22(6)	10(8)	4(5)	-10(5)	-8(4)
C(49)	22(6)	54(11)	60(12)	-38(10)	-3(6)	-19(6)
C(50)	35(3)	22(3)	26(3)	6(2)	-5(2)	-8(2)
C(51)	25(5)	30(6)	50(6)	-27(5)	-4(4)	10(4)
C(52)	26(8)	20(8)	45(9)	-10(6)	-4(6)	-4(6)
C(53)	63(5)	89(6)	32(4)	-18(4)	-15(3)	-17(4)
C(54)	109(8)	157(11)	110(8)	-103(8)	42(7)	-97(8)
C(55)	27(3)	17(2)	33(3)	-1(2)	-9(2)	4(2)
C(56)	49(4)	21(3)	48(4)	-3(3)	-26(3)	6(3)
C(57)	34(3)	38(4)	89(6)	2(4)	-29(4)	13(3)
C(58)	79(5)	30(3)	51(4)	7(3)	-28(4)	14(3)
C(59)	23(3)	17(2)	42(3)	-3(2)	4(2)	4(2)
C(60)	63(4)	29(3)	60(4)	11(3)	40(4)	13(3)
C(63)	78(6)	56(5)	49(4)	-1(4)	3(4)	-5(4)
C(64)	66(5)	64(5)	51(5)	-2(4)	1(4)	-8(4)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **2**.

	x	y	z	U(eq)
H(3)	2625	8628	6430	32
H(4)	2776	8935	7359	47
H(5)	2137	8505	8059	54
H(6)	1353	7832	7830	42
H(9)	-128	6089	7927	26
H(10)	736	5656	8361	30
H(11)	1723	6001	8093	36
H(12)	1837	6758	7408	36
H(15)	63	7502	4563	24
H(16)	-12	8351	3962	30
H(17)	-97	9361	4325	37
H(18)	-73	9515	5287	33
H(21)	-277	5424	5396	28
H(22)	-1283	5583	5067	28
H(23)	-1646	6606	4966	23
H(24)	-1046	7441	5242	22
H(25A)	2591	7452	5236	34
H(25B)	2881	7644	5827	34
H(26)	2200(30)	6520(30)	5700(30)	41
H(27A)	3084	6860	6535	85
H(27B)	2745	6198	6505	85
H(27C)	2351	6814	6630	85
H(28A)	3037	6499	5058	116
H(28B)	3122	5979	5533	116
H(28C)	3514	6611	5562	116
H(29A)	1715	8886	5721	35
H(29B)	2339	8645	5438	35
H(30)	1162	8487	4921	55
H(31A)	2357	8398	4428	120
H(31B)	1719	8351	4088	120
H(31C)	1897	7825	4535	120
H(32A)	2024	9467	4683	135
H(32B)	1395	9567	5027	135
H(32C)	1369	9372	4379	135
H(33A)	-594	6155	6671	39
H(33B)	-876	6134	7287	39
H(36A)	-1472	5610	6325	113
H(36B)	-2153	5895	6395	113
H(36C)	-1804	5600	6925	113
H(37)	-1364	6613	6325	83
H(38A)	-2283	6826	6641	194
H(38B)	-1745	7318	6774	194
H(38C)	-1993	6865	7258	194
H(39A)	-1212	7403	7697	30
H(39B)	-741	7004	8068	30
H(41A)	-764	8458	8765	94
H(41B)	-863	7727	8860	94
H(41C)	-1351	8115	8495	94
H(40A)	-638	8286	7790	75
H(42A)	166	8273	7801	55

H(42B)	-290	8725	8140	55
H(42C)	-468	8503	7520	55
H(47A)	-1823	9405	6813	132
H(47B)	-2244	9308	6267	132
H(47C)	-1728	9844	6277	132
H(44A)	-736	9294	6806	106
H(44B)	-616	9635	6220	106
H(43A)	323	7621	8264	42
H(43B)	201	8319	8473	42
H(43C)	342	8185	7825	42
H(40B)	-161	7756	8252	34
H(45)	-1331	8965	5737	29
H(46A)	-1616	8289	6737	67
H(46B)	-1130	8015	6293	67
H(46C)	-1836	8127	6112	67
H(44C)	-604	9478	6736	54
H(44D)	-719	9518	6078	54
H(48)	-1316	8711	6835	27
H(49A)	-1348	8753	5633	68
H(49B)	-1878	8430	6003	68
H(49C)	-1187	8158	6010	68
H(50C)	991	9158	6111	34
H(50D)	493	9700	6193	34
H(51)	304	10094	6697	42
H(52)	1187	9074	7065	36
H(50A)	1029	9059	6393	36
H(50B)	671	9520	5983	36
H(53A)	295	9911	7347	92
H(53B)	771	9549	7746	92
H(53C)	221	9177	7444	92
H(54A)	1201	10405	7083	188
H(54B)	1166	10231	6431	188
H(54C)	1737	9994	6802	188
H(55A)	405	5656	6486	31
H(55B)	569	5189	5988	31
H(56)	1500(30)	5750(30)	6690(30)	47
H(57A)	2166	4950	6363	80
H(57B)	1968	5419	5872	80
H(57C)	1649	4748	5917	80
H(58A)	996	4517	6796	80
H(58B)	831	5083	7208	80
H(58C)	1520	4808	7192	80
H(59A)	1508	5766	5114	32
H(59B)	855	5434	5022	32
H(63A)	1065	5960	3635	91
H(63B)	873	5377	4016	91
H(63C)	1573	5623	4019	91
H(64A)	1260	7037	4768	90
H(64B)	1230	6987	4099	90
H(64C)	1783	6660	4434	90
H(60B)	520(40)	6250(40)	4270(30)	72