Supporting information

Intriguing C–H···Cu interactions in bis-(phenanthroline)Cu(I) redox mediators for dye-sensitized solar cells

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Experimental Section: Synthesis and characterization of both ligands and complexes. X-ray structure determination of compounds **2**-**4**

Figure S1: Normalized visible absorption spectra for complexes **(1**-**5)** in acetonitrile.

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

Table S2. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **(2)**.

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

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **(2).**

Table S5. Hydrogen coordinates and isotropic displacement parameters for **(2).**

Table S6. Crystal data and structure refinement details for **(3).**

Table S7. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **(3)**.

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

Table S9. Anisotropic displacement parameters ($Å^2$ x 10^3) for **(3).**

Table S10. Hydrogen coordinates and isotropic displacement parameters for **(3).**

Table S11. Crystal data and structure refinement details for **(4).**

Table S12. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **(4)**.

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

Table S14. Anisotropic displacement parameters ($Å^2$ x 10^3) for **(4).**

Table S15. Hydrogen coordinates and isotropic displacement parameters for **(4).**

Theoretical Section: DFT method used and Cartesian coordinates of the complexes.

Experimental section

1. General comments

All reagents and solvents were purchased from Sigma-Aldrich and were used without further purification. Reactions requiring anhydrous conditions were performed under argon. Thin layer chromatography (TLC) was carried out with pre-coated Merck F254 silica gel plates or alumina. Chromatographic purification of phenanthroline ligands was performed using neutral alumina (Brokmann II)

^{1}H NMR and proton decoupled ^{13}C NMR spectra were recorded at 400 MHz (T = 300 K) on a Bruker Avance-400 instrument. Chemical shifts (δ) for ^{1}H spectra are expressed in ppm relative to internal Me_4Si as standard. Signals were abbreviated as s, singlet; d, doublet; dd, double doublet. Elemental analyses were performed using an Exeter Analytical E-440 analyser.

2. Synthesis of ligands- General Procedure

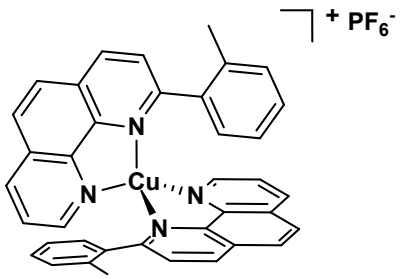
To a stirred suspension of the appropiate phenanthroline in dry toluene cooled to 0°C, the organolithium-derivative solution was slowly added dropwise via syringe. The resulting deep-red solution was stirred at room temperature overnight and then quenched with water. The layers were separated and the aqueous phase was extracted with dichloromethane. The combined exctracts were stirred with an excess of activated manganese dioxide (previously heated under vacuum at 160°C for 4-5 h) for 18 h, until the intense yellow color of the solution has discharged.

The mixture was filtered through a pad of Celite and the solvent evaporated under reduced pressure to give the crude product which was purified by chromatography on a neutral alumina.

3. Synthesis of complexes- General Procedure

The appropriate phenanthroline ligand and the Cu(I) precursor $[Cu(CH_3CN)_4][PF_6]$ were dissolved in dry CH_2Cl_2 (or dry DMF) in two separate Schlenk vessels, both kept under Ar atmosphere. The ligand solution was then slowly added via syringe to the copper solution which instantaneously turned to red. The mixture was stirred for 1 hour at 40°C and then the solvent was removed and the residue recrystallized from CH_3CN / iPr_2O or $MeOH/Et_2O$.

Synthesis of [Cu(2-(2-Tolyl)-1,10-phenanthroline)$_2$]PF$_6$ (2)



2-Tolyllithium. To a solution of 2-bromotoluene (2.32 mL, 19.2 mmol) in 65 mL of dry ether at -78 °C was slowly added *t*-BuLi (1.7 M in pentane, 20 mL, 34.8 mmol) under argon, and the solution was stirred for 10 min at -78°C. The reaction mixture was warmed to room temperature gradually over 30 min and than was concentred to about 15-20 mL and used in the next step without purification.

2-(2-Tolyl)-phenanthroline ligand was prepared following the general procedure previously reported using 1,10-phenanthroline (570 mg g, 3.16 mmol) in 70mL of dry toluene and the 2-tolyllithium solution. Reoxidation was achieved treating with activated manganese dioxide (8.8 g, 101 mmol). The product was isolated after a quick chromatographic separation on neutral alumina using first toluene/CH_2Cl_2 7:3 and then toluene/CH_2Cl_2 1:1 as eluent. The pure product was obtained in 30% yield as orange solid.

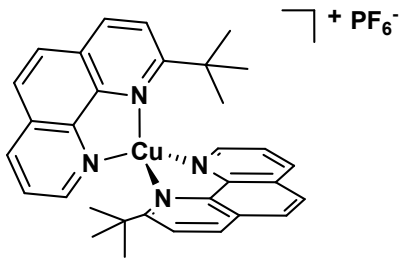
^{1}H NMR (400 MHz, CD_2Cl_2) δ 9.18 (d, J =4.25, 1H), 8.36 (d, J =8.24 Hz, 1H), 8.33 (d, J =8.10 Hz,1H), 7.91 (d, J =8.78, 1H), 7.87 (d, J =8.78 Hz, 1H), 7.81 (d, J =8.24 Hz, 1H), 7.67 (dd, J =8.10, 4.3 Hz, 1H), 7.60 (d, J =4.3 Hz, 1H), 7.43-7.39 (m, 3H), 2.51(s, 3H)

Elemental analysis: Calcd. (%) for $C_{19}H_{14}N_2$: C, 84.42; H, 5.22; N, 10.36; found: C, 84.44; H, 5.21; N, 10.37

The **complex (2**) was prepared following the general procedure using 2-(2-tolyl)-phenanthroline (300.1 mg, 1.11 mmol) and [Cu(CH_3CN)$_4$][PF_6] (206.5 mg, 0.56 mmol) in 6+11.5 mL of dry CH_2Cl_2. The product was obtained as red crystals (340 mg, 82%) after crystallization from CH_2Cl_2/iPr_2O

^{1}H-NMR (400 MHz, CD_2Cl_2) δ 8.93 (d, J =4.39 Hz, 2H), 8.55-8.51 (m, 4H) 8.10(d, J =8.78 Hz, 2H), 8.01 (d, J =8.78 Hz, 2H), 7.88 (dd, J =8.10, 4.3 Hz, 2H), 7.74 (d, J =8.16 Hz, 2H), 6.56 (d, J =7.40 Hz, 2H), 6.42 (t, J =7.39 Hz, 2H), 6.35 (d, J =7.49 Hz, 2H), 6.06 (t, J =7.39 Hz, 2H), 1.85(s, 6H). ^{13}C-NMR 100MHz,CD_2Cl_2) δ 157.92, 148.63, 143.61, 143.07, 138.70, 136.58, 134.67, 129.42, 128.71,127.76, 127.64, 126.56, 125.62, 125.14, 123.90, 19.98. Elemental analysis: Calcd. (%) for $C_{38}H_{28}CuF_6N_4P$ (749.17): C, 60.92; H, 3.77; N, 7.48; found: C, 61.01; H, 3.77; N, 7.47.

Synthesis of [Cu(2-tert-butyl-1,10-phenanthroline)$_2$]PF$_6$ (3)



2-terbutyl-phenanthroline ligand was prepared following the general procedure using 1,10-phenanthroline (360.6 mg, 2.00 mmol) and terbutyl lithium solution 1.7 M in pentane (1.8 mL, 3.06 mmol) in 60 mL of dry toluene. Reoxidation was achieved with activated manganese dioxide (5.5602 g, 63.9 mmol). The crude product was purified by chromatography.

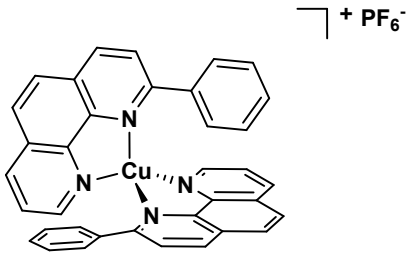
^{1}H NMR (400 MHz, CD_2Cl_2) δ 9.20 (dd, J =4.27, J =1.62 Hz, 1H), 8.31 (dd, J =8.02, 1.62 Hz, 1H), 8.24 (d, J =8.50 Hz, 1H), 7.84-7.78 (m, 3H), 7.66 (dd, J =8.02 Hz, J =4.27 Hz, 1H), 1.61 (s, 9H).

Elemental analysis: Calcd. (%) for $C_{16}H_{16}N_2$: C, 81.32; H, 6.82; N, 11.85; found: C, 81.29; H, 6.81; N, 11.89.

The **complex (3)** was prepared following the general procedure using 2-terbutyl-1,10-phenanthroline (31.5 mg, 0.149 mmol) and [Cu(CH_3CN)$_4$][PF_6] (27.6 mg, 0.074 mmol) in 0.6+0.3 mL of dry CH_2Cl_2. The product was obtained as a red-orange powder (0.049 mmol, 66%) after crystallization from CH_3CN/iPr_2O.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.84 (dd, J =4.27, J =1.41 Hz, 1H), 8.62 (dd, J =8.58, 1.41 Hz, 1H), 8.57 (d, J =8.58 Hz, 1H), 8.13-8.05 (m, 3H), 7.86 (dd, J =8.58 Hz, J =4.73 Hz, 1H), 1.32 (s, 9H). ^{13}C-NMR 100MHz,CD_2Cl_2) δ 172.8, 158.6, 149.9, 138.6, 137.4, 136.4 136.0, 130.2, 128.3, 127.4 126.7, 121.5, 117.5, 32.9, 30.1 Elemental analysis: Calcd. (%) for $C_{32}H_{32}CuF_6N_4P$ (681.13): C, 56.43; H, 4.74; N, 8.23; found: C, 56.49; H, 4.72; N, 8.20.

Synthesis of [Cu(2-phenyl-1,10-phenanthroline)$_2$]PF$_6$ (4)



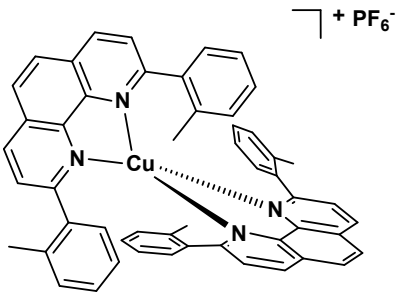
2-phenyl-phenanthroline ligand was prepared following the general procedure previously reported using 1,10-phenanthroline (360.5 mg, 2.00 mmol) and phenyl lithium solution (1.2 mL, 2.16 mmol) in 60 mL of dry toluene. Reoxidation was achieved treating with activated manganese dioxide (5.5 g, 64.1 mmol). The product was isolated after a quick chromatographic separation as a bright yellow dense liquid, which had been induced to crystallize as a light pink powder.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 9.28 (dd, J =4.3, 1.4 Hz, 1H), 8.37 (d, J =7.5 Hz, 2H), 8.35 (d, J =8.4 Hz,1H), 8.29 (dd, J =8.0, 1.4 Hz, 1H), 8.14 (d, J =8.4 Hz, 1H), 7.86 (d, J =8.8 Hz, 1H), 7.81 (d,J =8.8Hz, 1H), 7.67 (dd, J =8.0, 4.3 Hz, 1H), 7.58 (t, J =7.5 Hz, 2H), 7.50 (t, J =7.5 Hz, 1H).

The **complex (4**) was prepared following the general procedure using 2-phenyl-1,10-phenanthroline (66.1 mg, 0.26 mmol) and $[Cu(CH_3CN)_4][PF_6]$ (48.0 mg, 0.13 mmol) in 0.6+1.2 mL of dry CH_2Cl_2. The product was obtained as little dark-Bordeaux rhomboid platelets (0.091 mmol, 70%) after crystallization from CH_3CN/iPr_2O.

^{1}H-NMR (400 MHz, CD_2Cl_2) δ 9.06 (dd, J =4.3 Hz, J= 1.4 Hz 2H), 8.65 (d, J =8.45 Hz, 2H), 8.47 (d, J =8.45 Hz, 2H), 8.09 (d, J =8.08 Hz, 2H), 8.04 (d, J =8.08 Hz, 2H), 7.96 (dd, J =8.0, 1.4 Hz, 2H), 7.85 (d, J =8.08 Hz, 2H), 7.23 (d, J =7.4 Hz, 4H), 6.66 (t, J =7.4 Hz, 2H), 6.38 (t, J =7.4 Hz, 4H). ^{13}C-NMR 100MHz,CD_2Cl_2) δ 158.20, 148.83, 143.71, 143.13, 138.68, 136.64, 134.77, 129.40, 128.55,127.76, 127.68, 126.59, 125.66, 125.14, 124.01. Elemental analysis: Calcd. (%) for $C_{36}H_{24}CuF_6N_4P$ (721.11): C, 59.96; H, 3.35; N, 7.77; found: C, 60.03; H, 3.34; N, 7.80.

Synthesis of [Cu(2,9-diTolyl-1,10-phenanthroline)$_2$]PF$_6$ (5)



2,9–ditolyl-1,10-phenanthroline ligand was prepared following the general procedure previously reported using 1,10-phenanthroline (400 mg) in 40 mL of dry toluene and a strong excess of the 2-tolyllithium solution previously prepared (mmol). Reoxidation was achieved treating with activated manganese dioxide (12 g). The product was isolated after chromatographic separation on neutral alumina using toluene/ CH_2Cl_2 7:3. The pure product was obtained in 20% yield as

orange solid. ^{1}H-NMR (400 MHz, CD_2Cl_2) δ 8.38 (d, J =8.26 Hz, 2H), 7.92 (s, 2H) 7.82 (d, J =8.26 Hz, 2H), 7.62-7.60 (m, 2H), 7.39-7.34 (m, 6H), 2.56(s, 6H).

The **complex 5** was prepared following the general procedure using 2,9-di-tolyl-1,10-phenanthroline (96.6 mg, 0.27 mmol) and $[Cu(CH_3CN)_4][PF_6]$ (50.0 mg, 0.13 mmol) in 2.5 mL of dry CH_2Cl_2. The pure product was obtained after recrystallization from CH_2Cl_2/Et_2O as red solid.

^{1}H-NMR (400 MHz, CD_2Cl_2) δ 8.53 (d, J =8.10 Hz, 4H), 8.11 (s, 4H) 7.77 (d, J =8.10 Hz, 4H), 6.94 (d, J =8.00 Hz, 4H), 6.82 (d, J =8.00, 4.3 Hz, 4H), 6.77 (t, J =8.00 Hz, 4H), 6.05 (t, J =8.0 Hz, 4H), 1.57(s, 12H).
^{13}CNMR(100MHz,CD_2Cl_2) δ 157.36, 145.67, 143.73, 140.24, 138.79, 136.44, 134.40, 129.83, 128.67, 128.20127.72, 127.43, 126.76, 126.55, 123.93, 19.79.

Elemental analysis: Calcd. (%) for $C_{52}H_{40}CuF_6N_4P$: C, 67.20; H, 4.34; N, 6.03; found: C, 67.50; H, 4.36; N, 6.05.

4. X-ray structure determination of complexes (2)-(4)

A summary of the crystal data and refinement details for complexes **(2)-(4)** is given in the supplementary Tables S1, S6, S11, respectively. Intensity data for all compounds were collected at room temperature on a Bruker APEX II CCD diffractometer using graphite-monochromatized Mo-*K*α radiation (λ = 0.71073 Å). Datasets were corrected for Lorentz-polarization effects and for absorption (*SADABS* [1]). All structures were solved by direct methods (*SIR-97* [2]) and completed by iterative cycles of full-matrix least squares refinement on $F_o^2$and *ΔF* synthesis using the *SHELXL-2017* [3] program (*WinGX* suite) [4]. Hydrogen atoms were allowed to ride on their carbon atoms.

In compound **(2)** the asymmetric unit contains two independent molecules, slightly differing in the conformational parameters of a phenyl ring. The high values of R and Rw for compound **2** are due to low quality of the crystals used, in spite of the several attempts to obtain more suitable crystals. The presence in the final Difference Fourier maps of significant electron density residuals, is related to clathrated solvent molecules disordered about a symmetry inversion centre. This disorder was partly accounted for by refining a fraction of a methanol molecule, close to this centre, but several electron density residuals are still present and could not be rationalized, with a satisfactory model of disorder. Moreover the PF_6^- anions are affected by high thermal motion, which may be interpreted as another situation of partial disorder due to slight rotation about the P atoms. Any attempt to split the fluorine atoms did not give a satisfactory model of disorder.

In **(4)** the fluorine atoms of the PF_6^- anion are heavily disordered, the model of disorder consisting of two PF_6^- anion slightly rotated about the P atom with occupancy 0.56 and 0.44.Crystallographic data for compounds **(2)-(4)** have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1564905-1564907. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk.

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[3] G.M. Sheldrick, *Acta Crystallogr.* **A64** (2008), 112-122.

[4] L. J. Farrugia, *J. Appl. Crystallogr*. **32** (1999) 837.

Figure S1. Normalized visible absorption spectra for complexes **1**-**5** in acetonitrile.

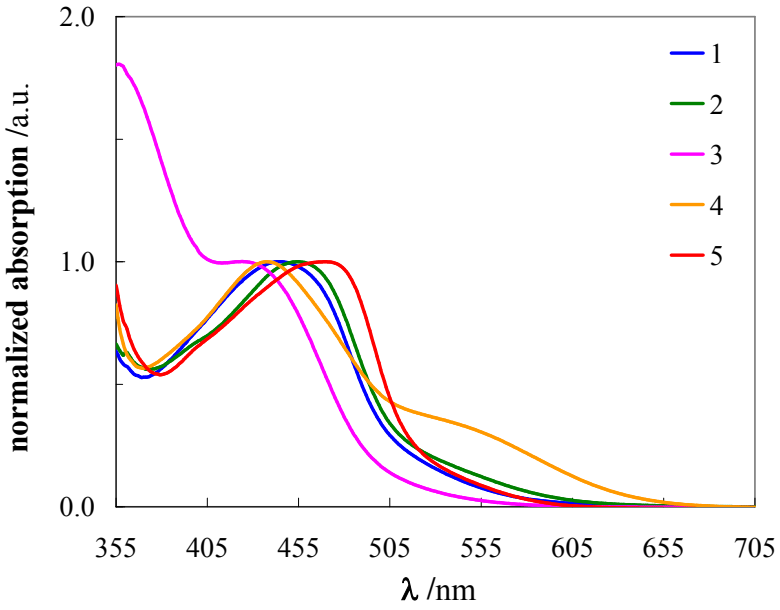

Table S1. Crystal data and structure refinement details for **(2).**

Empirical formula	C38.25 H29.50 Cu F6 N4 O0.25 P
Formula weight	757.67
Temperature	294(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 14.2112(8) A alpha = 108.740(10) deg.
	b = 15.8165(8) A beta = 100.180(10) deg.
	c = 16.8488(9) A gamma = 98.380(10) deg.
Volume	3445.6(4) A^3
Z, Calculated density	4, 1.461 Mg/m^3
Absorption coefficient	0.748 mm^-1
F(000)	1548
Crystal size	0.25 x 0.07 x 0.04 mm
Theta range for data collection	1.314 to 30.143 deg.
Limiting indices	-20<=h<=20, -22<=k<=22, -23<=l<=23
Reflections collected / unique	35745 / 19938 [R(int) = 0.0375]
Completeness to theta = 25.242	99.7 %
Absorption correction	Empirical
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	19938 / 0 / 919
Goodness-of-fit on F^2	0.962
Final R indices [I>2sigma(I)]	R1 = 0.0694, wR2 = 0.2136
R indices (all data)	R1 = 0.1191, wR2 = 0.2443
Extinction coefficient	n/a
Largest diff. peak and hole	1.131 and -0.378 e.A^-3

Table S2. 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 Uij tensor.

	x	y	z	U(eq)
C(1)	755(3)	-3384(2)	-189(2)	58(1)
C(2)	681(3)	-3749(3)	454(3)	69(1)
C(3)	1511(3)	-3756(3)	986(3)	73(1)
C(4)	2417(3)	-3416(3)	878(2)	64(1)
C(5)	2432(2)	-3062(2)	216(2)	49(1)
C(6)	3358(2)	-2700(2)	80(2)	54(1)
C(7)	4228(3)	-2722(3)	590(3)	71(1)
C(8)	4193(4)	-3072(4)	1276(3)	87(1)
C(9)	3309(4)	-3406(3)	1409(3)	80(1)
C(10)	5096(3)	-2407(4)	390(4)	97(2)
C(11)	5052(3)	-2073(4)	-263(3)	90(1)
C(12)	4153(3)	-2061(3)	-756(3)	63(1)
C(13)	4077(2)	-1701(3)	-1464(3)	63(1)
C(14)	4091(3)	-783(3)	-1297(3)	79(1)
C(15)	4007(4)	-455(4)	-1971(5)	95(2)
C(16)	3905(4)	-997(5)	-2773(4)	101(2)
C(17)	3903(4)	-1927(4)	-2962(3)	93(1)
C(18)	3987(3)	-2283(3)	-2299(3)	77(1)
C(19)	3983(5)	-3277(4)	-2509(4)	106(2)
C(20)	1358(3)	-3288(3)	-3060(2)	67(1)
C(21)	1208(4)	-3246(4)	-3897(3)	86(1)
C(22)	1189(4)	-2463(4)	-4007(3)	84(1)
C(23)	1305(3)	-1669(3)	-3294(3)	67(1)
C(24)	1464(2)	-1749(2)	-2473(2)	51(1)
C(25)	1614(2)	-955(2)	-1717(2)	53(1)

C(26)	1631(3)	-90(3)	-1794(3)	69(1)
C(27)	1458(4)	-37(4)	-2633(4)	88(1)
C(28)	1310(4)	-771(4)	-3330(4)	88(1)
C(29)	1853(4)	651(3)	-1030(3)	84(1)
C(30)	2016(4)	539(3)	-258(3)	84(1)
C(31)	1955(3)	-345(2)	-216(2)	66(1)
C(32)	2165(4)	-518(3)	604(3)	80(1)
C(33)	3140(4)	-233(4)	1126(3)	100(2)
C(34)	3355(5)	-482(5)	1849(4)	128(2)
C(35)	2616(5)	-936(4)	2051(3)	105(2)
C(36)	1659(5)	-1210(4)	1612(3)	99(2)
C(37)	1428(4)	-981(3)	816(3)	80(1)
C(38)	454(4)	-1194(3)	378(3)	93(1)
C(39)	697(3)	4275(2)	6984(2)	58(1)
C(40)	674(3)	4570(3)	7851(2)	67(1)
C(41)	1517(3)	4800(2)	8464(2)	64(1)
C(42)	2404(3)	4739(2)	8229(2)	53(1)
C(43)	2369(2)	4431(2)	7338(2)	45(1)
C(44)	3254(2)	4329(2)	7053(2)	46(1)
C(45)	4153(3)	4550(2)	7664(2)	57(1)
C(46)	4158(3)	4878(3)	8569(2)	69(1)
C(47)	3326(3)	4957(3)	8827(2)	68(1)
C(48)	4981(3)	4421(3)	7343(3)	69(1)
C(49)	4897(3)	4076(3)	6479(3)	68(1)
C(50)	3976(2)	3893(2)	5901(2)	53(1)
C(51)	3873(2)	3567(3)	4953(2)	62(1)
C(52)	3962(3)	2686(4)	4521(3)	87(1)
C(53)	3858(4)	2381(5)	3639(4)	109(2)
C(54)	3646(4)	2951(5)	3190(3)	105(2)

C(55)	3564(3)	3821(5)	3609(3)	89(2)
C(56)	3683(3)	4151(3)	4497(3)	69(1)
C(57)	3635(3)	5110(4)	4947(3)	82(1)
C(58)	1276(3)	4317(3)	4036(2)	62(1)
C(59)	1146(3)	4213(3)	3168(3)	74(1)
C(60)	1052(3)	3374(3)	2571(2)	71(1)
C(61)	1090(3)	2637(3)	2828(2)	62(1)
C(62)	1227(2)	2789(2)	3726(2)	50(1)
C(63)	1294(2)	2043(2)	4023(2)	53(1)
C(64)	1234(3)	1165(3)	3436(2)	72(1)
C(65)	1099(4)	1034(4)	2540(3)	94(2)
C(66)	1015(3)	1742(4)	2254(2)	81(1)
C(67)	1318(5)	485(3)	3771(3)	101(2)
C(68)	1433(5)	660(3)	4643(3)	96(2)
C(69)	1471(3)	1550(3)	5190(2)	72(1)
C(70)	1504(5)	1820(3)	6143(3)	103(2)
C(71)	597(6)	1944(4)	6385(3)	128(2)
C(72)	626(8)	2255(5)	7265(5)	158(3)
C(73)	1519(9)	2406(4)	7783(5)	160(3)
C(74)	2435(9)	2331(5)	7684(5)	161(3)
C(75)	2318(7)	1978(4)	6731(5)	136(2)
C(76)	3177(7)	1853(6)	6512(5)	145(3)
N(1)	1600(2)	-3047(2)	-316(2)	49(1)
N(2)	3322(2)	-2374(2)	-577(2)	51(1)
N(3)	1493(2)	-2557(2)	-2360(2)	51(1)
N(4)	1756(2)	-1077(2)	-950(2)	52(1)
N(5)	1516(2)	4203(2)	6719(2)	48(1)
N(6)	3177(2)	4019(2)	6192(2)	47(1)
N(7)	1315(2)	3625(2)	4314(2)	49(1)

N(8)	1407(2)	2233(2)	4883(2)	54(1)
F(1)	3178(6)	3400(6)	1308(4)	263(3)
F(2)	1767(4)	3820(5)	-24(3)	211(3)
F(3)	2134(6)	4240(3)	1357(4)	235(3)
F(4)	2799(3)	2882(3)	-91(2)	142(1)
F(5)	1668(4)	2802(3)	647(3)	185(2)
F(6)	3236(4)	4352(3)	625(3)	189(2)
F(7)	1736(4)	-3426(3)	4191(3)	192(2)
F(8)	3045(6)	-2312(5)	3477(4)	247(3)
F(9)	2756(4)	-3711(4)	3336(3)	188(2)
F(10)	2120(7)	-2005(4)	4415(5)	269(4)
F(11)	3187(5)	-2685(6)	4638(4)	269(4)
F(12)	1607(5)	-3060(7)	3044(3)	270(4)
P(1)	2467(1)	3577(1)	641(1)	69(1)
P(2)	2421(1)	-2826(1)	3865(1)	100(1)
Cu(1)	1881(1)	-2408(1)	-1121(1)	53(1)
Cu(2)	1698(1)	3644(1)	5524(1)	54(1)
O(100)	4260(10)	284(6)	4396(7)	154(5)
C(100)	4907(12)	-194(16)	4072(9)	176(9)

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

C(1)-N(1)	1.323(4)
C(1)-C(2)	1.394(5)
C(1)-H(1)	0.9300
C(2)-C(3)	1.353(6)
C(2)-H(2)	0.9300
C(3)-C(4)	1.388(6)
C(3)-H(3)	0.9300
C(4)-C(5)	1.400(5)
C(4)-C(9)	1.412(6)
C(5)-N(1)	1.360(4)
C(5)-C(6)	1.444(5)
C(6)-N(2)	1.360(4)
C(6)-C(7)	1.387(5)
C(7)-C(10)	1.400(6)
C(7)-C(8)	1.438(6)
C(8)-C(9)	1.374(6)
C(8)-H(8)	0.9300
C(9)-H(9)	0.9300
C(10)-C(11)	1.361(7)
C(10)-H(10)	0.9300
C(11)-C(12)	1.401(6)
C(11)-H(11)	0.9300
C(12)-N(2)	1.336(4)
C(12)-C(13)	1.473(5)
C(13)-C(18)	1.382(6)
C(13)-C(14)	1.384(6)
C(14)-C(15)	1.387(7)

C(14)-H(14)	0.9300
C(15)-C(16)	1.317(8)
C(15)-H(15)	0.9300
C(16)-C(17)	1.401(8)
C(16)-H(16)	0.9300
C(17)-C(18)	1.397(6)
C(17)-H(17)	0.9300
C(18)-C(19)	1.496(7)
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-N(3)	1.320(4)
C(20)-C(21)	1.413(6)
C(20)-H(20)	0.9300
C(21)-C(22)	1.313(7)
C(21)-H(21)	0.9300
C(22)-C(23)	1.395(6)
C(22)-H(22)	0.9300
C(23)-C(24)	1.410(5)
C(23)-C(28)	1.441(6)
C(24)-N(3)	1.357(4)
C(24)-C(25)	1.430(5)
C(25)-N(4)	1.352(4)
C(25)-C(26)	1.412(5)
C(26)-C(29)	1.382(6)
C(26)-C(27)	1.424(6)
C(27)-C(28)	1.317(7)
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300

C(29)-C(30)	1.353(6)
C(29)-H(29)	0.9300
C(30)-C(31)	1.413(5)
C(30)-H(30)	0.9300
C(31)-N(4)	1.345(4)
C(31)-C(32)	1.481(6)
C(32)-C(37)	1.356(7)
C(32)-C(33)	1.424(7)
C(33)-C(34)	1.394(8)
C(33)-H(33)	0.9300
C(34)-C(35)	1.342(9)
C(34)-H(34)	0.9300
C(35)-C(36)	1.360(8)
C(35)-H(35)	0.9300
C(36)-C(37)	1.492(7)
C(36)-H(36)	0.9300
C(37)-C(38)	1.385(7)
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600
C(39)-N(5)	1.325(4)
C(39)-C(40)	1.393(5)
C(39)-H(39)	0.9300
C(40)-C(41)	1.352(6)
C(40)-H(40)	0.9300
C(41)-C(42)	1.394(5)
C(41)-H(41)	0.9300
C(42)-C(43)	1.411(4)
C(42)-C(47)	1.424(5)

C(43)-N(5)	1.369(4)
C(43)-C(44)	1.436(4)
C(44)-N(6)	1.352(4)
C(44)-C(45)	1.409(4)
C(45)-C(48)	1.395(5)
C(45)-C(46)	1.441(5)
C(46)-C(47)	1.339(6)
C(46)-H(46)	0.9300
C(47)-H(47)	0.9300
C(48)-C(49)	1.355(5)
C(48)-H(48)	0.9300
C(49)-C(50)	1.416(5)
C(49)-H(49)	0.9300
C(50)-N(6)	1.329(4)
C(50)-C(51)	1.485(5)
C(51)-C(52)	1.386(6)
C(51)-C(56)	1.405(6)
C(52)-C(53)	1.379(7)
C(52)-H(52)	0.9300
C(53)-C(54)	1.385(8)
C(53)-H(53)	0.9300
C(54)-C(55)	1.362(8)
C(54)-H(54)	0.9300
C(55)-C(56)	1.386(6)
C(55)-H(55)	0.9300
C(56)-C(57)	1.480(7)
C(57)-H(57A)	0.9600
C(57)-H(57B)	0.9600
C(57)-H(57C)	0.9600

C(58)-N(7)	1.325(4)
C(58)-C(59)	1.393(5)
C(58)-H(58)	0.9300
C(59)-C(60)	1.354(6)
C(59)-H(59)	0.9300
C(60)-C(61)	1.372(6)
C(60)-H(60)	0.9300
C(61)-C(66)	1.411(6)
C(61)-C(62)	1.427(4)
C(62)-N(7)	1.347(4)
C(62)-C(63)	1.430(5)
C(63)-N(8)	1.356(4)
C(63)-C(64)	1.403(5)
C(64)-C(67)	1.376(6)
C(64)-C(65)	1.429(6)
C(65)-C(66)	1.367(7)
C(65)-H(65)	0.9300
C(66)-H(66)	0.9300
C(67)-C(68)	1.379(6)
C(67)-H(67)	0.9300
C(68)-C(69)	1.400(6)
C(68)-H(68)	0.9300
C(69)-N(8)	1.346(4)
C(69)-C(70)	1.514(6)
C(70)-C(75)	1.318(9)
C(70)-C(71)	1.439(9)
C(71)-C(72)	1.396(8)
C(71)-H(71)	0.9300
C(72)-C(73)	1.346(11)

C(72)-H(72)	0.9300
C(73)-C(74)	1.359(11)
C(73)-H(73)	0.9300
C(74)-C(75)	1.489(10)
C(74)-H(74)	0.9300
C(75)-C(76)	1.360(10)
C(76)-H(76A)	0.9600
C(76)-H(76B)	0.9600
C(76)-H(76C)	0.9600
N(1)-Cu(1)	1.992(3)
N(2)-Cu(1)	2.075(3)
N(3)-Cu(1)	1.990(3)
N(4)-Cu(1)	2.070(3)
N(5)-Cu(2)	2.002(2)
N(6)-Cu(2)	2.100(3)
N(7)-Cu(2)	2.004(3)
N(8)-Cu(2)	2.084(3)
F(1)-P(1)	1.498(5)
F(2)-P(1)	1.545(4)
F(3)-P(1)	1.521(4)
F(4)-P(1)	1.560(3)
F(5)-P(1)	1.547(4)
F(6)-P(1)	1.530(4)
F(7)-P(2)	1.550(4)
F(8)-P(2)	1.487(5)
F(9)-P(2)	1.589(5)
F(10)-P(2)	1.503(5)
F(11)-P(2)	1.474(5)
F(12)-P(2)	1.539(5)

O(100)-C(100)	1.35(2)

N(1)-C(1)-C(2)	123.5(3)
N(1)-C(1)-H(1)	118.2
C(2)-C(1)-H(1)	118.3
C(3)-C(2)-C(1)	118.9(4)
C(3)-C(2)-H(2)	120.5
C(1)-C(2)-H(2)	120.5
C(2)-C(3)-C(4)	120.0(4)
C(2)-C(3)-H(3)	120.1
C(4)-C(3)-H(3)	119.9
C(3)-C(4)-C(5)	117.7(4)
C(3)-C(4)-C(9)	122.7(4)
C(5)-C(4)-C(9)	119.6(4)
N(1)-C(5)-C(4)	122.6(3)
N(1)-C(5)-C(6)	117.7(3)
C(4)-C(5)-C(6)	119.7(3)
N(2)-C(6)-C(7)	123.2(3)
N(2)-C(6)-C(5)	116.8(3)
C(7)-C(6)-C(5)	120.0(3)
C(6)-C(7)-C(10)	116.9(4)
C(6)-C(7)-C(8)	119.1(4)
C(10)-C(7)-C(8)	123.9(4)
C(9)-C(8)-C(7)	120.5(4)
C(9)-C(8)-H(8)	119.6
C(7)-C(8)-H(8)	119.8
C(8)-C(9)-C(4)	121.0(4)
C(8)-C(9)-H(9)	119.7
C(4)-C(9)-H(9)	119.3

C(11)-C(10)-C(7)	119.5(4)
C(11)-C(10)-H(10)	120.2
C(7)-C(10)-H(10)	120.3
C(10)-C(11)-C(12)	121.3(4)
C(10)-C(11)-H(11)	119.4
C(12)-C(11)-H(11)	119.3
N(2)-C(12)-C(11)	119.5(4)
N(2)-C(12)-C(13)	117.6(3)
C(11)-C(12)-C(13)	122.9(3)
C(18)-C(13)-C(14)	119.9(4)
C(18)-C(13)-C(12)	120.0(4)
C(14)-C(13)-C(12)	120.1(4)
C(13)-C(14)-C(15)	119.6(5)
C(13)-C(14)-H(14)	120.2
C(15)-C(14)-H(14)	120.2
C(16)-C(15)-C(14)	121.6(5)
C(16)-C(15)-H(15)	119.0
C(14)-C(15)-H(15)	119.3
C(15)-C(16)-C(17)	120.1(5)
C(15)-C(16)-H(16)	120.0
C(17)-C(16)-H(16)	119.8
C(18)-C(17)-C(16)	119.8(5)
C(18)-C(17)-H(17)	120.1
C(16)-C(17)-H(17)	120.1
C(13)-C(18)-C(17)	118.9(4)
C(13)-C(18)-C(19)	121.8(4)
C(17)-C(18)-C(19)	119.3(5)
C(18)-C(19)-H(19A)	109.6
C(18)-C(19)-H(19B)	109.4

H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
N(3)-C(20)-C(21)	122.5(4)
N(3)-C(20)-H(20)	118.7
C(21)-C(20)-H(20)	118.8
C(22)-C(21)-C(20)	120.3(4)
C(22)-C(21)-H(21)	119.8
C(20)-C(21)-H(21)	119.8
C(21)-C(22)-C(23)	119.9(4)
C(21)-C(22)-H(22)	120.2
C(23)-C(22)-H(22)	120.0
C(22)-C(23)-C(24)	117.4(4)
C(22)-C(23)-C(28)	125.0(4)
C(24)-C(23)-C(28)	117.5(4)
N(3)-C(24)-C(23)	122.7(3)
N(3)-C(24)-C(25)	117.3(3)
C(23)-C(24)-C(25)	120.0(3)
N(4)-C(25)-C(26)	123.1(3)
N(4)-C(25)-C(24)	117.1(3)
C(26)-C(25)-C(24)	119.8(3)
C(29)-C(26)-C(25)	116.2(4)
C(29)-C(26)-C(27)	125.0(4)
C(25)-C(26)-C(27)	118.7(4)
C(28)-C(27)-C(26)	121.4(4)
C(28)-C(27)-H(27)	119.5
C(26)-C(27)-H(27)	119.2
C(27)-C(28)-C(23)	122.6(4)

C(27)-C(28)-H(28)	118.5
C(23)-C(28)-H(28)	118.9
C(30)-C(29)-C(26)	121.1(4)
C(30)-C(29)-H(29)	119.4
C(26)-C(29)-H(29)	119.5
C(29)-C(30)-C(31)	120.5(4)
C(29)-C(30)-H(30)	119.8
C(31)-C(30)-H(30)	119.7
N(4)-C(31)-C(30)	119.6(4)
N(4)-C(31)-C(32)	116.7(3)
C(30)-C(31)-C(32)	123.5(4)
C(37)-C(32)-C(33)	121.9(5)
C(37)-C(32)-C(31)	118.7(4)
C(33)-C(32)-C(31)	119.4(4)
C(34)-C(33)-C(32)	119.2(6)
C(34)-C(33)-H(33)	120.5
C(32)-C(33)-H(33)	120.4
C(35)-C(34)-C(33)	118.0(6)
C(35)-C(34)-H(34)	121.0
C(33)-C(34)-H(34)	120.9
C(34)-C(35)-C(36)	127.1(6)
C(34)-C(35)-H(35)	116.5
C(36)-C(35)-H(35)	116.5
C(35)-C(36)-C(37)	115.3(6)
C(35)-C(36)-H(36)	122.3
C(37)-C(36)-H(36)	122.3
C(32)-C(37)-C(38)	124.0(5)
C(32)-C(37)-C(36)	118.4(5)
C(38)-C(37)-C(36)	117.4(5)

C(37)-C(38)-H(38A)	109.7
C(37)-C(38)-H(38B)	109.4
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.3
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
N(5)-C(39)-C(40)	123.1(3)
N(5)-C(39)-H(39)	118.5
C(40)-C(39)-H(39)	118.5
C(41)-C(40)-C(39)	119.7(4)
C(41)-C(40)-H(40)	120.2
C(39)-C(40)-H(40)	120.1
C(40)-C(41)-C(42)	120.2(3)
C(40)-C(41)-H(41)	119.9
C(42)-C(41)-H(41)	119.9
C(41)-C(42)-C(43)	116.9(3)
C(41)-C(42)-C(47)	124.2(3)
C(43)-C(42)-C(47)	118.9(3)
N(5)-C(43)-C(42)	122.8(3)
N(5)-C(43)-C(44)	117.6(3)
C(42)-C(43)-C(44)	119.6(3)
N(6)-C(44)-C(45)	122.9(3)
N(6)-C(44)-C(43)	117.2(3)
C(45)-C(44)-C(43)	119.9(3)
C(48)-C(45)-C(44)	116.9(3)
C(48)-C(45)-C(46)	124.5(3)
C(44)-C(45)-C(46)	118.7(3)
C(47)-C(46)-C(45)	121.0(3)
C(47)-C(46)-H(46)	119.6

C(45)-C(46)-H(46)	119.5
C(46)-C(47)-C(42)	122.0(3)
C(46)-C(47)-H(47)	119.0
C(42)-C(47)-H(47)	119.0
C(49)-C(48)-C(45)	120.1(3)
C(49)-C(48)-H(48)	120.0
C(45)-C(48)-H(48)	119.9
C(48)-C(49)-C(50)	120.0(3)
C(48)-C(49)-H(49)	120.0
C(50)-C(49)-H(49)	120.0
N(6)-C(50)-C(49)	120.9(3)
N(6)-C(50)-C(51)	118.0(3)
C(49)-C(50)-C(51)	121.2(3)
C(52)-C(51)-C(56)	120.2(4)
C(52)-C(51)-C(50)	119.9(4)
C(56)-C(51)-C(50)	119.9(4)
C(53)-C(52)-C(51)	119.8(5)
C(53)-C(52)-H(52)	120.0
C(51)-C(52)-H(52)	120.2
C(52)-C(53)-C(54)	119.8(5)
C(52)-C(53)-H(53)	120.1
C(54)-C(53)-H(53)	120.2
C(55)-C(54)-C(53)	120.9(5)
C(55)-C(54)-H(54)	119.7
C(53)-C(54)-H(54)	119.4
C(54)-C(55)-C(56)	120.6(5)
C(54)-C(55)-H(55)	119.7
C(56)-C(55)-H(55)	119.7
C(55)-C(56)-C(51)	118.7(5)

C(55)-C(56)-C(57)	119.9(4)
C(51)-C(56)-C(57)	121.4(4)
C(56)-C(57)-H(57A)	109.5
C(56)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
C(56)-C(57)-H(57C)	109.4
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
N(7)-C(58)-C(59)	122.9(4)
N(7)-C(58)-H(58)	118.6
C(59)-C(58)-H(58)	118.5
C(60)-C(59)-C(58)	119.6(4)
C(60)-C(59)-H(59)	120.3
C(58)-C(59)-H(59)	120.2
C(59)-C(60)-C(61)	119.6(3)
C(59)-C(60)-H(60)	120.2
C(61)-C(60)-H(60)	120.2
C(60)-C(61)-C(66)	123.5(4)
C(60)-C(61)-C(62)	118.1(4)
C(66)-C(61)-C(62)	118.4(4)
N(7)-C(62)-C(61)	121.8(3)
N(7)-C(62)-C(63)	118.4(3)
C(61)-C(62)-C(63)	119.8(3)
N(8)-C(63)-C(64)	123.0(3)
N(8)-C(63)-C(62)	116.7(3)
C(64)-C(63)-C(62)	120.3(3)
C(67)-C(64)-C(63)	116.9(4)
C(67)-C(64)-C(65)	124.4(4)
C(63)-C(64)-C(65)	118.6(4)

C(66)-C(65)-C(64)	121.1(4)
C(66)-C(65)-H(65)	119.4
C(64)-C(65)-H(65)	119.5
C(65)-C(66)-C(61)	121.7(4)
C(65)-C(66)-H(66)	119.1
C(61)-C(66)-H(66)	119.1
C(64)-C(67)-C(68)	121.2(4)
C(64)-C(67)-H(67)	119.4
C(68)-C(67)-H(67)	119.5
C(67)-C(68)-C(69)	118.8(4)
C(67)-C(68)-H(68)	120.6
C(69)-C(68)-H(68)	120.5
N(8)-C(69)-C(68)	121.4(4)
N(8)-C(69)-C(70)	114.1(3)
C(68)-C(69)-C(70)	124.4(4)
C(75)-C(70)-C(71)	121.1(7)
C(75)-C(70)-C(69)	122.7(7)
C(71)-C(70)-C(69)	116.2(5)
C(72)-C(71)-C(70)	117.1(7)
C(72)-C(71)-H(71)	121.5
C(70)-C(71)-H(71)	121.4
C(73)-C(72)-C(71)	114.5(9)
C(73)-C(72)-H(72)	123.6
C(71)-C(72)-H(72)	121.9
C(72)-C(73)-C(74)	137.0(9)
C(72)-C(73)-H(73)	112.6
C(74)-C(73)-H(73)	110.4
C(73)-C(74)-C(75)	104.1(9)
C(73)-C(74)-H(74)	129.5

C(75)-C(74)-H(74)	126.4
C(76)-C(75)-C(70)	121.7(8)
C(76)-C(75)-C(74)	112.2(8)
C(70)-C(75)-C(74)	126.1(9)
C(75)-C(76)-H(76A)	107.7
C(75)-C(76)-H(76B)	111.2
H(76A)-C(76)-H(76B)	109.5
C(75)-C(76)-H(76C)	109.5
H(76A)-C(76)-H(76C)	109.5
H(76B)-C(76)-H(76C)	109.5
C(1)-N(1)-C(5)	117.3(3)
C(1)-N(1)-Cu(1)	130.3(2)
C(5)-N(1)-Cu(1)	112.2(2)
C(12)-N(2)-C(6)	119.6(3)
C(12)-N(2)-Cu(1)	130.2(2)
C(6)-N(2)-Cu(1)	110.1(2)
C(20)-N(3)-C(24)	117.1(3)
C(20)-N(3)-Cu(1)	130.1(3)
C(24)-N(3)-Cu(1)	112.4(2)
C(31)-N(4)-C(25)	119.4(3)
C(31)-N(4)-Cu(1)	129.4(2)
C(25)-N(4)-Cu(1)	110.1(2)
C(39)-N(5)-C(43)	117.4(3)
C(39)-N(5)-Cu(2)	129.5(2)
C(43)-N(5)-Cu(2)	112.5(2)
C(50)-N(6)-C(44)	119.1(3)
C(50)-N(6)-Cu(2)	130.1(2)
C(44)-N(6)-Cu(2)	110.2(2)
C(58)-N(7)-C(62)	118.0(3)

C(58)-N(7)-Cu(2)	129.4(2)
C(62)-N(7)-Cu(2)	111.8(2)
C(69)-N(8)-C(63)	118.7(3)
C(69)-N(8)-Cu(2)	130.7(2)
C(63)-N(8)-Cu(2)	109.7(2)
F(1)-P(1)-F(3)	89.5(4)
F(1)-P(1)-F(6)	91.5(4)
F(3)-P(1)-F(6)	91.2(3)
F(1)-P(1)-F(2)	176.6(5)
F(3)-P(1)-F(2)	88.8(4)
F(6)-P(1)-F(2)	85.5(4)
F(1)-P(1)-F(5)	89.8(4)
F(3)-P(1)-F(5)	88.3(3)
F(6)-P(1)-F(5)	178.6(4)
F(2)-P(1)-F(5)	93.2(4)
F(1)-P(1)-F(4)	90.2(4)
F(3)-P(1)-F(4)	179.1(3)
F(6)-P(1)-F(4)	89.7(3)
F(2)-P(1)-F(4)	91.5(3)
F(5)-P(1)-F(4)	90.8(2)
F(11)-P(2)-F(8)	96.1(5)
F(11)-P(2)-F(10)	86.1(5)
F(8)-P(2)-F(10)	95.4(4)
F(11)-P(2)-F(12)	175.2(5)
F(8)-P(2)-F(12)	86.8(4)
F(10)-P(2)-F(12)	97.5(5)
F(11)-P(2)-F(7)	87.4(4)
F(8)-P(2)-F(7)	175.1(3)
F(10)-P(2)-F(7)	88.2(3)

F(12)-P(2)-F(7)	89.4(4)
F(11)-P(2)-F(9)	90.9(4)
F(8)-P(2)-F(9)	87.0(3)
F(10)-P(2)-F(9)	176.3(3)
F(12)-P(2)-F(9)	85.5(4)
F(7)-P(2)-F(9)	89.6(3)
N(3)-Cu(1)-N(1)	140.46(11)
N(3)-Cu(1)-N(4)	82.18(11)
N(1)-Cu(1)-N(4)	124.39(10)
N(3)-Cu(1)-N(2)	119.44(11)
N(1)-Cu(1)-N(2)	82.74(11)
N(4)-Cu(1)-N(2)	107.80(11)
N(5)-Cu(2)-N(7)	143.38(11)
N(5)-Cu(2)-N(8)	122.21(11)
N(7)-Cu(2)-N(8)	81.90(11)
N(5)-Cu(2)-N(6)	81.82(10)
N(7)-Cu(2)-N(6)	120.50(10)
N(8)-Cu(2)-N(6)	105.80(11)

Table S4. Anisotropic displacement parameters (Å^2 x 10^3) for **(2)**. The anisotropic displacement factor exponent takes the form: -2 π2 [h^2 a*^{2} U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	55(2)	54(2)	70(2)	26(2)	22(2)	14(2)
C(2)	72(2)	75(2)	81(3)	42(2)	38(2)	18(2)
C(3)	92(3)	75(3)	77(3)	45(2)	43(2)	29(2)
C(4)	80(3)	60(2)	64(2)	31(2)	26(2)	25(2)
C(5)	57(2)	46(2)	52(2)	20(1)	20(1)	20(1)
C(6)	55(2)	50(2)	59(2)	18(2)	16(2)	18(1)
C(7)	60(2)	81(3)	75(3)	32(2)	12(2)	19(2)
C(8)	80(3)	113(4)	74(3)	47(3)	0(2)	32(3)
C(9)	90(3)	95(3)	74(3)	48(2)	22(2)	35(3)
C(10)	53(2)	142(5)	107(4)	64(4)	10(2)	23(3)
C(11)	48(2)	125(4)	107(4)	57(3)	21(2)	15(2)
C(12)	49(2)	62(2)	81(3)	26(2)	22(2)	13(2)
C(13)	42(2)	72(2)	83(3)	35(2)	25(2)	7(2)
C(14)	60(2)	77(3)	109(3)	43(3)	29(2)	9(2)
C(15)	72(3)	90(3)	151(5)	75(4)	37(3)	14(2)
C(16)	78(3)	134(5)	131(5)	90(4)	45(3)	20(3)
C(17)	84(3)	117(4)	94(3)	51(3)	42(3)	17(3)
C(18)	66(2)	83(3)	93(3)	40(3)	38(2)	12(2)
C(19)	143(5)	89(3)	101(4)	34(3)	61(4)	34(3)
C(20)	71(2)	59(2)	62(2)	11(2)	22(2)	7(2)
C(21)	97(3)	88(3)	57(2)	4(2)	25(2)	14(3)
C(22)	90(3)	105(4)	55(2)	30(2)	21(2)	11(3)
C(23)	60(2)	86(3)	62(2)	40(2)	17(2)	7(2)
C(24)	43(2)	56(2)	58(2)	26(2)	16(1)	6(1)

C(25)	51(2)	50(2)	67(2)	30(2)	17(2)	12(1)
C(26)	73(2)	56(2)	95(3)	42(2)	27(2)	18(2)
C(27)	98(3)	84(3)	111(4)	69(3)	32(3)	22(3)
C(28)	97(3)	99(4)	87(3)	60(3)	21(3)	20(3)
C(29)	104(3)	48(2)	110(4)	37(2)	31(3)	21(2)
C(30)	104(4)	46(2)	98(3)	13(2)	35(3)	19(2)
C(31)	78(3)	53(2)	66(2)	14(2)	25(2)	18(2)
C(32)	106(4)	53(2)	72(3)	8(2)	32(2)	15(2)
C(33)	101(4)	118(4)	68(3)	22(3)	4(3)	26(3)
C(34)	106(5)	138(6)	105(5)	18(4)	1(4)	16(4)
C(35)	115(5)	113(4)	67(3)	13(3)	14(3)	20(4)
C(36)	141(5)	73(3)	85(3)	15(3)	45(3)	36(3)
C(37)	87(3)	72(3)	72(3)	7(2)	24(2)	27(2)
C(38)	104(4)	77(3)	101(4)	27(3)	48(3)	13(3)
C(39)	59(2)	58(2)	58(2)	19(2)	19(2)	10(2)
C(40)	78(3)	62(2)	64(2)	19(2)	36(2)	14(2)
C(41)	98(3)	50(2)	47(2)	14(2)	33(2)	15(2)
C(42)	73(2)	42(2)	39(2)	12(1)	12(1)	4(1)
C(43)	55(2)	36(1)	42(2)	14(1)	11(1)	2(1)
C(44)	50(2)	42(2)	42(2)	16(1)	5(1)	2(1)
C(45)	58(2)	53(2)	54(2)	22(2)	0(2)	3(2)
C(46)	79(3)	68(2)	47(2)	20(2)	-11(2)	6(2)
C(47)	96(3)	62(2)	40(2)	18(2)	7(2)	7(2)
C(48)	50(2)	83(3)	68(2)	37(2)	-6(2)	1(2)
C(49)	44(2)	92(3)	76(3)	42(2)	16(2)	14(2)
C(50)	47(2)	62(2)	55(2)	27(2)	15(1)	7(1)
C(51)	43(2)	88(3)	57(2)	26(2)	18(2)	12(2)
C(52)	81(3)	111(4)	76(3)	28(3)	33(2)	36(3)
C(53)	96(4)	125(5)	94(4)	7(4)	44(3)	37(3)

C(54)	72(3)	169(6)	64(3)	30(4)	25(2)	8(3)
C(55)	56(2)	146(5)	67(3)	43(3)	22(2)	7(3)
C(56)	43(2)	108(3)	64(2)	45(2)	14(2)	5(2)
C(57)	67(3)	102(3)	86(3)	52(3)	14(2)	7(2)
C(58)	56(2)	78(2)	60(2)	31(2)	14(2)	19(2)
C(59)	68(2)	104(3)	67(2)	53(3)	14(2)	22(2)
C(60)	59(2)	116(4)	45(2)	40(2)	9(2)	16(2)
C(61)	53(2)	89(3)	38(2)	18(2)	11(1)	10(2)
C(62)	37(2)	69(2)	39(2)	16(1)	8(1)	4(1)
C(63)	51(2)	59(2)	40(2)	12(1)	9(1)	5(1)
C(64)	87(3)	66(2)	51(2)	6(2)	16(2)	17(2)
C(65)	122(4)	90(3)	44(2)	-9(2)	19(2)	21(3)
C(66)	86(3)	104(3)	36(2)	9(2)	11(2)	15(2)
C(67)	152(5)	57(3)	77(3)	1(2)	29(3)	21(3)
C(68)	154(5)	54(2)	69(3)	19(2)	10(3)	17(3)
C(69)	103(3)	53(2)	51(2)	18(2)	5(2)	4(2)
C(70)	184(5)	45(3)	61(3)	27(2)	-9(3)	-7(3)
C(71)	265(7)	71(3)	83(3)	35(3)	102(4)	50(4)
C(72)	288(9)	93(5)	129(6)	58(4)	95(6)	59(5)
C(73)	270(9)	69(4)	108(5)	50(4)	-38(6)	-3(5)
C(74)	274(10)	74(4)	102(5)	46(4)	-17(6)	-18(5)
C(75)	203(7)	76(4)	107(5)	51(4)	-17(5)	-17(4)
C(76)	155(7)	142(6)	139(6)	76(5)	4(5)	15(5)
N(1)	53(2)	44(1)	55(2)	19(1)	21(1)	14(1)
N(2)	49(2)	50(2)	60(2)	21(1)	18(1)	12(1)
N(3)	49(2)	49(1)	53(2)	15(1)	15(1)	5(1)
N(4)	56(2)	43(1)	59(2)	19(1)	20(1)	12(1)
N(5)	51(2)	45(1)	45(1)	13(1)	15(1)	6(1)
N(6)	48(1)	50(1)	42(1)	17(1)	9(1)	6(1)

N(7)	42(1)	62(2)	42(1)	19(1)	9(1)	10(1)
N(8)	61(2)	52(2)	41(1)	13(1)	8(1)	3(1)
F(1)	291(8)	375(10)	143(4)	141(5)	-21(4)	107(7)
F(2)	182(5)	337(8)	157(4)	120(5)	17(3)	142(5)
F(3)	460(10)	99(3)	196(4)	36(3)	235(6)	60(4)
F(4)	133(3)	149(3)	135(3)	15(2)	65(2)	46(2)
F(5)	191(4)	101(3)	231(5)	4(3)	125(4)	-27(3)
F(6)	210(5)	164(4)	165(4)	49(3)	73(3)	-57(3)
F(7)	221(5)	163(4)	155(4)	8(3)	112(4)	-42(3)
F(8)	328(9)	213(6)	196(5)	71(4)	142(6)	-45(5)
F(9)	203(5)	216(5)	168(4)	54(4)	98(4)	80(4)
F(10)	480(12)	164(5)	262(7)	96(5)	249(8)	134(6)
F(11)	224(6)	366(11)	156(5)	84(6)	-57(4)	20(7)
F(12)	190(5)	482(13)	124(4)	92(6)	0(3)	116(7)
P(1)	81(1)	70(1)	51(1)	19(1)	17(1)	7(1)
P(2)	95(1)	127(1)	76(1)	39(1)	25(1)	8(1)
Cu(1)	58(1)	52(1)	60(1)	28(1)	19(1)	16(1)
Cu(2)	58(1)	60(1)	37(1)	11(1)	8(1)	1(1)
O(100)	203(12)	72(5)	132(8)	13(5)	-50(7)	24(6)
C(100)	134(12)	280(20)	102(10)	131(13)	-24(8)	-89(13)

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

	x	y	z	U(eq)
H(1)	180	-3378	-549	69
H(2)	70	-3983	517	83
H(3)	1474	-3988	1424	87
H(8)	4772	-3072	1632	104
H(9)	3299	-3630	1856	96
H(10)	5697	-2426	700	116
H(11)	5630	-1848	-385	108
H(14)	4156	-389	-736	95
H(15)	4023	164	-1853	115
H(16)	3835	-763	-3215	122
H(17)	3846	-2307	-3527	112
H(19A)	4578	-3343	-2186	127
H(19B)	3937	-3560	-3115	127
H(19C)	3433	-3565	-2360	127
H(20)	1363	-3852	-3000	80
H(21)	1122	-3776	-4374	104
H(22)	1098	-2437	-4558	101
H(27)	1448	527	-2691	106
H(28)	1205	-707	-3866	105
H(29)	1891	1237	-1047	101
H(30)	2169	1047	249	101
H(33)	3626	115	987	120
H(34)	3993	-337	2182	153
H(35)	2775	-1080	2545	126
H(36)	1183	-1518	1795	119

H(38A)	250	-643	371	112
H(38B)	59	-1487	663	112
H(38C)	377	-1599	-204	112
H(39)	110	4120	6571	70
H(40)	82	4610	8008	80
H(41)	1504	4999	9044	77
H(46)	4748	5037	8978	83
H(47)	3351	5161	9415	82
H(48)	5593	4572	7721	82
H(49)	5444	3958	6267	81
H(52)	4092	2301	4825	104
H(53)	3930	1794	3348	131
H(54)	3558	2738	2593	126
H(55)	3428	4196	3297	107
H(57A)	3499	5401	4532	99
H(57B)	4251	5432	5348	99
H(57C)	3125	5121	5253	99
H(58)	1338	4897	4437	75
H(59)	1123	4716	3000	89
H(60)	963	3298	1990	85
H(65)	1068	457	2145	113
H(66)	905	1631	1665	97
H(67)	1297	-103	3403	121
H(68)	1485	196	4863	115
H(71)	17	1821	5972	154
H(72)	74	2351	7477	189
H(73)	1504	2617	8362	192
H(74)	3005	2469	8113	193
H(76A)	3054	1315	6004	174

H(76B)	3614	1780	6978	174
H(76C)	3471	2375	6398	174

Table S6. Crystal data and structure refinement details for **(3).**

Empirical formula	C32 H32 Cu F6 N4 P	
Formula weight	681.12	
Temperature	294(2) K	
Wavelength	0.71073 A	
Crystal system, space group	Triclinic, P -1	
Unit cell dimensions	a = 8.7383(7) A	alpha = 91.870(10) deg.
	b = 12.8143(10) A	beta = 98.400(10) deg.
	c = 14.3893(12) A	gamma = 105.650(10) deg.
Volume	1530.5(2) A^3	
Z, Calculated density	2, 1.478 Mg/m^3	
Absorption coefficient	0.832 mm^-1	
F(000)	700	
Crystal size	0.15 x 0.04 x 0.02 mm	
Theta range for data collection	2.107 to 23.681 deg.	
Limiting indices	-9<=h<=9, -14<=k<=14, -16<=l<=16	
Reflections collected / unique	8940 / 4623 [R(int) = 0.0161]	
Completeness to theta = 23.681	99.9 %	
Absorption correction	Empirical	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4623 / 0 / 397	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0390, wR2 = 0.1052	
R indices (all data)	R1 = 0.0485, wR2 = 0.1103	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.488 and -0.274 e.A^-3	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **(3**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	12145(4)	2711(3)	4225(2)	63(1)
C(2)	13380(4)	2508(3)	4852(2)	69(1)
C(3)	13396(4)	1466(3)	4966(2)	64(1)
C(4)	12153(4)	615(3)	4480(2)	50(1)
C(5)	12095(4)	-499(3)	4559(2)	61(1)
C(6)	10888(5)	-1288(3)	4073(2)	61(1)
C(7)	9583(4)	-1049(2)	3480(2)	49(1)
C(8)	9567(3)	38(2)	3396(2)	39(1)
C(9)	10916(3)	880(2)	3882(2)	41(1)
C(10)	8271(5)	-1839(3)	2989(3)	62(1)
C(11)	7009(4)	-1552(3)	2504(2)	60(1)
C(12)	7026(3)	-456(2)	2483(2)	44(1)
C(13)	5555(4)	-123(3)	2018(2)	53(1)
C(14)	4962(5)	436(4)	2786(3)	86(1)
C(15)	6000(4)	653(3)	1265(2)	66(1)
C(16)	4199(5)	-1092(3)	1548(3)	92(1)
C(17)	7583(4)	3519(3)	3816(2)	62(1)
C(18)	6777(5)	4303(3)	3885(3)	72(1)
C(19)	6376(4)	4800(3)	3105(3)	65(1)
C(20)	6834(3)	4543(2)	2256(2)	47(1)
C(21)	6459(4)	5031(3)	1408(3)	58(1)
C(22)	6945(4)	4773(3)	616(3)	60(1)
C(23)	7907(3)	4026(2)	593(2)	46(1)
C(24)	8310(3)	3530(2)	1413(2)	36(1)
C(25)	7699(3)	3769(2)	2251(2)	38(1)
C(26)	8514(4)	3784(3)	-202(2)	57(1)
C(27)	9530(4)	3153(3)	-147(2)	56(1)

C(28)	9973(3)	2718(2)	708(2)	41(1)
C(29)	11272(4)	2120(2)	824(2)	51(1)
C(30)	11932(5)	2005(3)	-96(3)	80(1)
C(31)	12650(4)	2780(3)	1579(3)	70(1)
C(32)	10597(5)	977(3)	1124(3)	64(1)
N(1)	10942(3)	1927(2)	3746(2)	46(1)
N(2)	8313(3)	330(2)	2893(2)	39(1)
N(3)	8030(3)	3236(2)	3022(2)	45(1)
N(4)	9303(3)	2871(2)	1462(1)	36(1)
F(1)	13363(3)	5447(2)	3802(2)	84(1)
F(2)	11304(3)	6694(2)	2494(2)	97(1)
F(3)	13635(3)	6302(2)	2489(2)	94(1)
F(4)	10978(3)	5833(3)	3792(2)	118(1)
F(5)	13163(3)	7130(2)	3777(2)	111(1)
F(6)	11461(4)	4985(2)	2524(2)	128(1)
P	12295(1)	6055(1)	3140(1)	47(1)
Cu	9174(1)	2127(1)	2800(1)	53(1)

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

C(1)-N(1)	1.328(4)
C(1)-C(2)	1.389(5)
C(2)-C(3)	1.354(5)
C(3)-C(4)	1.396(5)
C(4)-C(9)	1.403(4)
C(4)-C(5)	1.423(5)
C(5)-C(6)	1.337(5)
C(6)-C(7)	1.430(4)
C(7)-C(10)	1.389(5)
C(7)-C(8)	1.404(4)

C(8)-N(2)	1.368(3)
C(8)-C(9)	1.438(4)
C(9)-N(1)	1.357(4)
C(10)-C(11)	1.360(5)
C(11)-C(12)	1.402(4)
C(12)-N(2)	1.335(4)
C(12)-C(13)	1.532(4)
C(13)-C(15)	1.515(4)
C(13)-C(16)	1.523(5)
C(13)-C(14)	1.523(5)
C(17)-N(3)	1.330(4)
C(17)-C(18)	1.382(5)
C(18)-C(19)	1.357(5)
C(19)-C(20)	1.396(5)
C(20)-C(25)	1.400(4)
C(20)-C(21)	1.424(4)
C(21)-C(22)	1.335(5)
C(22)-C(23)	1.436(4)
C(23)-C(26)	1.389(4)
C(23)-C(24)	1.403(4)
C(24)-N(4)	1.361(3)
C(24)-C(25)	1.444(4)
C(25)-N(3)	1.359(3)
C(26)-C(27)	1.349(5)
C(27)-C(28)	1.413(4)
C(28)-N(4)	1.339(3)
C(28)-C(29)	1.525(4)
C(29)-C(32)	1.525(4)
C(29)-C(31)	1.535(5)
C(29)-C(30)	1.538(4)
N(1)-Cu	1.981(2)
N(2)-Cu	2.236(2)

N(3)-Cu	1.988(2)
N(4)-Cu	2.180(2)
F(1)-P	1.602(2)
F(2)-P	1.576(2)
F(3)-P	1.577(2)
F(4)-P	1.563(2)
F(5)-P	1.570(2)
F(6)-P	1.546(2)

N(1)-C(1)-C(2)	123.1(3)
C(3)-C(2)-C(1)	119.0(3)
C(2)-C(3)-C(4)	119.9(3)
C(3)-C(4)-C(9)	117.9(3)
C(3)-C(4)-C(5)	123.1(3)
C(9)-C(4)-C(5)	119.0(3)
C(6)-C(5)-C(4)	121.0(3)
C(5)-C(6)-C(7)	121.4(3)
C(10)-C(7)-C(8)	116.7(3)
C(10)-C(7)-C(6)	123.6(3)
C(8)-C(7)-C(6)	119.7(3)
N(2)-C(8)-C(7)	123.1(3)
N(2)-C(8)-C(9)	118.6(2)
C(7)-C(8)-C(9)	118.3(3)
N(1)-C(9)-C(4)	121.7(3)
N(1)-C(9)-C(8)	117.9(2)
C(4)-C(9)-C(8)	120.4(3)
C(11)-C(10)-C(7)	120.2(3)
C(10)-C(11)-C(12)	120.5(3)
N(2)-C(12)-C(11)	120.9(3)
N(2)-C(12)-C(13)	117.9(2)
C(11)-C(12)-C(13)	121.2(3)
C(15)-C(13)-C(16)	107.3(3)

C(15)-C(13)-C(14)	109.7(3)
C(16)-C(13)-C(14)	109.3(3)
C(15)-C(13)-C(12)	110.7(3)
C(16)-C(13)-C(12)	112.4(3)
C(14)-C(13)-C(12)	107.4(3)
N(3)-C(17)-C(18)	123.4(3)
C(19)-C(18)-C(17)	119.2(3)
C(18)-C(19)-C(20)	119.7(3)
C(19)-C(20)-C(25)	117.7(3)
C(19)-C(20)-C(21)	123.0(3)
C(25)-C(20)-C(21)	119.4(3)
C(22)-C(21)-C(20)	120.9(3)
C(21)-C(22)-C(23)	121.5(3)
C(26)-C(23)-C(24)	117.1(3)
C(26)-C(23)-C(22)	123.3(3)
C(24)-C(23)-C(22)	119.6(3)
N(4)-C(24)-C(23)	122.9(3)
N(4)-C(24)-C(25)	118.7(2)
C(23)-C(24)-C(25)	118.3(2)
N(3)-C(25)-C(20)	122.4(3)
N(3)-C(25)-C(24)	117.4(2)
C(20)-C(25)-C(24)	120.2(2)
C(27)-C(26)-C(23)	119.9(3)
C(26)-C(27)-C(28)	121.0(3)
N(4)-C(28)-C(27)	120.0(3)
N(4)-C(28)-C(29)	117.8(2)
C(27)-C(28)-C(29)	122.1(3)
C(28)-C(29)-C(32)	110.5(3)
C(28)-C(29)-C(31)	107.5(2)
C(32)-C(29)-C(31)	110.3(3)
C(28)-C(29)-C(30)	112.1(3)
C(32)-C(29)-C(30)	107.5(3)

C(31)-C(29)-C(30)	109.0(3)
C(1)-N(1)-C(9)	118.3(3)
C(1)-N(1)-Cu	126.3(2)
C(9)-N(1)-Cu	115.43(18)
C(12)-N(2)-C(8)	118.4(2)
C(12)-N(2)-Cu	134.69(18)
C(8)-N(2)-Cu	106.20(16)
C(17)-N(3)-C(25)	117.5(3)
C(17)-N(3)-Cu	128.6(2)
C(25)-N(3)-Cu	113.96(18)
C(28)-N(4)-C(24)	118.8(2)
C(28)-N(4)-Cu	133.98(18)
C(24)-N(4)-Cu	106.75(16)
F(6)-P-F(4)	92.36(18)
F(6)-P-F(5)	178.88(17)
F(4)-P-F(5)	87.70(18)
F(6)-P-F(2)	91.34(17)
F(4)-P-F(2)	89.79(15)
F(5)-P-F(2)	89.78(14)
F(6)-P-F(3)	88.69(17)
F(4)-P-F(3)	178.90(17)
F(5)-P-F(3)	91.26(17)
F(2)-P-F(3)	89.88(13)
F(6)-P-F(1)	90.53(16)
F(4)-P-F(1)	91.46(14)
F(5)-P-F(1)	88.36(13)
F(2)-P-F(1)	177.71(15)
F(3)-P-F(1)	88.83(12)
N(1)-Cu-N(3)	121.64(10)
N(1)-Cu-N(4)	129.13(9)
N(3)-Cu-N(4)	81.59(9)
N(1)-Cu-N(2)	80.40(9)

N(3)-Cu-N(2)	128.00(9)
N(4)-Cu-N(2)	122.76(8)

Table S9. Anisotropic displacement parameters (Å^2 x 10^3) for **(3)**. The anisotropic displacement factor exponent takes the form: -2 π2 [h^2 a*^{2} U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	65(2)	55(2)	56(2)	9(2)	-5(2)	3(2)
C(2)	53(2)	81(3)	53(2)	6(2)	-11(2)	-2(2)
C(3)	47(2)	99(3)	46(2)	18(2)	0(2)	24(2)
C(4)	47(2)	73(2)	38(2)	18(2)	13(1)	26(2)
C(5)	65(2)	85(3)	53(2)	25(2)	17(2)	48(2)
C(6)	78(2)	62(2)	64(2)	24(2)	26(2)	47(2)
C(7)	64(2)	45(2)	48(2)	14(1)	24(2)	25(2)
C(8)	46(2)	42(2)	35(1)	12(1)	15(1)	18(1)
C(9)	43(2)	49(2)	34(1)	11(1)	10(1)	18(1)
C(10)	86(3)	38(2)	70(2)	11(2)	23(2)	23(2)
C(11)	70(2)	41(2)	61(2)	4(2)	11(2)	2(2)
C(12)	48(2)	42(2)	39(2)	9(1)	11(1)	4(1)
C(13)	46(2)	57(2)	48(2)	14(1)	0(1)	3(2)
C(14)	65(2)	135(4)	71(3)	19(2)	10(2)	50(3)
C(15)	60(2)	65(2)	60(2)	22(2)	-7(2)	3(2)
C(16)	64(2)	72(3)	113(3)	30(2)	-20(2)	-13(2)
C(17)	84(2)	66(2)	45(2)	12(2)	22(2)	30(2)
C(18)	90(3)	76(2)	66(2)	4(2)	36(2)	35(2)
C(19)	62(2)	59(2)	85(3)	8(2)	29(2)	29(2)
C(20)	37(2)	43(2)	63(2)	9(1)	8(1)	11(1)
C(21)	46(2)	52(2)	81(2)	20(2)	5(2)	22(2)
C(22)	55(2)	60(2)	64(2)	28(2)	-5(2)	19(2)
C(23)	42(2)	44(2)	43(2)	13(1)	-3(1)	4(1)
C(24)	34(1)	32(1)	37(1)	7(1)	0(1)	2(1)
C(25)	34(1)	35(1)	42(2)	7(1)	4(1)	5(1)
C(26)	65(2)	62(2)	37(2)	18(2)	0(2)	12(2)
C(27)	71(2)	58(2)	34(2)	5(1)	14(2)	8(2)

C(28)	48(2)	33(2)	38(2)	1(1)	9(1)	1(1)
C(29)	61(2)	39(2)	55(2)	2(1)	24(2)	12(1)
C(30)	107(3)	66(2)	85(3)	17(2)	56(2)	33(2)
C(31)	51(2)	69(2)	93(3)	1(2)	8(2)	23(2)
C(32)	84(2)	45(2)	70(2)	8(2)	31(2)	22(2)
N(1)	49(1)	43(1)	43(1)	9(1)	-1(1)	10(1)
N(2)	43(1)	38(1)	35(1)	11(1)	8(1)	11(1)
N(3)	54(2)	47(1)	37(1)	8(1)	11(1)	19(1)
N(4)	41(1)	29(1)	33(1)	4(1)	3(1)	6(1)
F(1)	111(2)	89(2)	72(1)	28(1)	22(1)	57(1)
F(2)	98(2)	145(2)	69(1)	17(1)	-2(1)	75(2)
F(3)	85(2)	113(2)	107(2)	52(2)	50(1)	45(1)
F(4)	97(2)	171(3)	105(2)	38(2)	58(2)	46(2)
F(5)	102(2)	77(2)	138(2)	-49(2)	-44(2)	39(1)
F(6)	121(2)	85(2)	147(3)	-53(2)	-6(2)	-5(2)
P	48(1)	47(1)	44(1)	0(1)	6(1)	10(1)
Cu	68(1)	51(1)	47(1)	11(1)	-1(1)	29(1)

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

	x	y	z	U(eq)
H(1)	12161	3430	4137	75
H(2)	14185	3080	5188	82
H(3)	14233	1318	5368	76
H(5)	12910	-681	4954	73
H(6)	10897	-2009	4122	73
H(10)	8255	-2568	2993	75
H(11)	6129	-2086	2183	72
H(14A)	5638	1167	2927	103
H(14B)	5001	45	3343	103
H(14C)	3874	448	2572	103
H(15A)	6741	1320	1553	79
H(15B)	5047	800	943	79
H(15C)	6495	331	823	79
H(16A)	3292	-848	1287	111
H(16B)	3888	-1601	2008	111
H(16C)	4562	-1437	1055	111
H(17)	7825	3171	4353	74
H(18)	6513	4487	4460	87
H(19)	5799	5310	3136	78
H(21)	5869	5536	1407	70
H(22)	6653	5083	66	72
H(26)	8220	4057	-772	68
H(27)	9945	3003	-679	67
H(30A)	11091	1938	-623	95
H(30B)	12314	1370	-102	95
H(30C)	12803	2637	-139	95
H(31A)	13350	3346	1295	84

H(31B)	13249	2310	1859	84
H(31C)	12215	3095	2057	84
H(32A)	10213	1022	1712	76
H(32B)	11430	613	1198	76
H(32C)	9725	577	651	76

Table S11. Crystal data and structure refinement details for **(4).**

Empirical formula	C36 H24 Cu F6 N4 P
Formula weight	721.10
Temperature	294(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 9.9803(4) A alpha = 76.620(10) deg.
	b = 11.7805(5) A beta = 88.060(10) deg.
	c = 13.9367(6) A gamma = 76.880(10) deg.
Volume	1552.19(14) A^3
Z, Calculated density	2, 1.543 Mg/m^3
Absorption coefficient	0.825 mm^-1
F(000)	732
Crystal size	0.23 x 0.05 x 0.03 mm
Theta range for data collection	1.502 to 32.379 deg.
Limiting indices	-14<=h<=14, -16<=k<=17, -20<=l<=20
Reflections collected / unique	15192 / 9967 [R(int) = 0.0147]
Completeness to theta = 25.000	100.0 %
Absorption correction	Empirical
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9967 / 0 / 488
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0442, wR2 = 0.1192
R indices (all data)	R1 = 0.0698, wR2 = 0.1369
Extinction coefficient	n/a
Largest diff. peak and hole	0.453 and -0.387 e.A^-3

Table S12 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **(4)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	8914(2)	-1041(2)	1498(2)	61(1)
C(2)	8383(3)	-1445(3)	753(2)	75(1)
C(3)	7936(2)	-668(3)	-103(2)	77(1)
C(4)	7988(2)	535(3)	-250(2)	66(1)
C(5)	7479(3)	1431(4)	-1116(2)	84(1)
C(6)	7500(3)	2576(3)	-1201(2)	86(1)
C(7)	8069(2)	2962(2)	-433(2)	68(1)
C(8)	8635(2)	2095(2)	421(1)	52(1)
C(9)	8553(2)	877(2)	527(1)	51(1)
C(10)	8074(3)	4148(3)	-454(2)	78(1)
C(11)	8630(2)	4422(2)	307(2)	72(1)
C(12)	9269(2)	3504(2)	1112(2)	54(1)
C(13)	10027(2)	3756(2)	1902(2)	57(1)
C(14)	11357(2)	3100(2)	2163(2)	60(1)
C(15)	12087(3)	3333(2)	2891(2)	74(1)
C(16)	11486(4)	4207(3)	3377(3)	93(1)
C(17)	10160(4)	4851(3)	3131(3)	100(1)
C(18)	9434(3)	4645(2)	2387(2)	80(1)
C(19)	12135(2)	-10(2)	3614(2)	64(1)
C(20)	13021(3)	23(3)	4358(2)	77(1)
C(21)	12541(3)	689(3)	5018(2)	77(1)
C(22)	11168(3)	1317(2)	4962(2)	66(1)
C(23)	10582(4)	2047(3)	5625(2)	83(1)
C(24)	9269(4)	2655(3)	5528(2)	88(1)
C(25)	8387(3)	2612(2)	4747(2)	69(1)
C(26)	8925(2)	1883(2)	4090(1)	53(1)
C(27)	10337(2)	1234(2)	4195(1)	51(1)

C(28)	7023(3)	3268(3)	4576(2)	85(1)
C(29)	6290(3)	3196(2)	3802(2)	79(1)
C(30)	6884(2)	2443(2)	3175(2)	58(1)
C(31)	6112(2)	2359(2)	2315(2)	57(1)
C(32)	5967(2)	1265(2)	2179(2)	62(1)
C(33)	5292(2)	1193(3)	1353(2)	74(1)
C(34)	4773(2)	2218(3)	642(2)	83(1)
C(35)	4897(3)	3303(3)	777(2)	84(1)
C(36)	5543(2)	3389(2)	1611(2)	71(1)
N(1)	8997(2)	91(2)	1397(1)	49(1)
N(2)	9255(2)	2363(1)	1163(1)	46(1)
N(3)	10833(2)	587(1)	3517(1)	51(1)
N(4)	8174(2)	1786(1)	3331(1)	48(1)
F(1')	5758(7)	-2535(11)	4184(5)	125(3)
F(1)	4214(4)	-2577(6)	3193(3)	91(2)
F(2')	5906(8)	-3130(11)	2106(5)	135(3)
F(2)	7408(5)	-3052(6)	2953(6)	125(3)
F(3)	6063(7)	-3649(9)	4113(4)	158(3)
F(3')	7137(12)	-2401(17)	2927(5)	196(6)
F(4')	4515(14)	-3345(16)	3277(8)	191(5)
F(4)	5512(5)	-1968(7)	2002(4)	126(2)
F(5')	4973(16)	-1633(9)	2735(11)	234(7)
F(5)	5827(7)	-3869(6)	2550(7)	143(3)
F(6')	6581(18)	-4025(7)	3650(9)	238(7)
F(6)	5852(7)	-1704(6)	3423(9)	159(4)
P	5816(1)	-2837(1)	3093(1)	67(1)
Cu	9503(1)	873(1)	2405(1)	50(1)

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

C(1)-N(1)	1.329(3)
C(1)-C(2)	1.402(3)
C(2)-C(3)	1.343(4)
C(3)-C(4)	1.396(4)
C(4)-C(9)	1.414(3)
C(4)-C(5)	1.428(4)
C(5)-C(6)	1.331(4)
C(6)-C(7)	1.435(4)
C(7)-C(10)	1.392(4)
C(7)-C(8)	1.414(3)
C(8)-N(2)	1.355(2)
C(8)-C(9)	1.428(3)
C(9)-N(1)	1.363(2)
C(10)-C(11)	1.348(4)
C(11)-C(12)	1.417(3)
C(12)-N(2)	1.333(3)
C(12)-C(13)	1.477(3)
C(13)-C(18)	1.386(3)
C(13)-C(14)	1.390(3)
C(14)-C(15)	1.379(3)
C(15)-C(16)	1.377(4)
C(16)-C(17)	1.378(5)
C(17)-C(18)	1.381(4)
C(19)-N(3)	1.324(3)
C(19)-C(20)	1.398(3)
C(20)-C(21)	1.351(4)
C(21)-C(22)	1.397(4)
C(22)-C(27)	1.410(3)
C(22)-C(23)	1.428(4)

C(23)-C(24)	1.337(5)
C(24)-C(25)	1.440(4)
C(25)-C(28)	1.402(4)
C(25)-C(26)	1.409(3)
C(26)-N(4)	1.357(2)
C(26)-C(27)	1.437(3)
C(27)-N(3)	1.360(3)
C(28)-C(29)	1.353(4)
C(29)-C(30)	1.409(3)
C(30)-N(4)	1.339(3)
C(30)-C(31)	1.481(3)
C(31)-C(32)	1.384(3)
C(31)-C(36)	1.389(3)
C(32)-C(33)	1.382(3)
C(33)-C(34)	1.380(4)
C(34)-C(35)	1.367(4)
C(35)-C(36)	1.383(4)
N(1)-Cu	1.9837(15)
N(2)-Cu	2.1363(15)
N(3)-Cu	1.9934(15)
N(4)-Cu	2.1124(15)
F(1')-F(6)	1.283(9)
F(1')-F(3)	1.304(9)
F(1')-P	1.637(5)
F(1)-F(4')	0.868(15)
F(1)-F(5')	1.497(17)
F(1)-P	1.566(4)
F(2')-F(5)	0.962(9)
F(2')-F(4)	1.311(10)
F(2')-P	1.489(6)
F(2)-F(3')	0.746(19)
F(2)-P	1.564(5)

F(2)-F(6')	1.673(16)
F(3)-F(6')	0.940(10)
F(3)-P	1.511(5)
F(3')-P	1.513(7)
F(3')-F(6)	1.587(15)
F(4')-P	1.539(8)
F(4')-F(5)	1.719(13)
F(4)-F(5')	1.241(12)
F(4)-P	1.619(4)
F(5')-F(6)	1.297(10)
F(5')-P	1.459(7)
F(5)-P	1.572(5)
F(5)-F(6')	1.684(14)
F(6')-P	1.482(7)
F(6)-P	1.518(4)

N(1)-C(1)-C(2)	122.7(2)
C(3)-C(2)-C(1)	119.5(2)
C(2)-C(3)-C(4)	120.5(2)
C(3)-C(4)-C(9)	117.0(2)
C(3)-C(4)-C(5)	124.3(2)
C(9)-C(4)-C(5)	118.6(3)
C(6)-C(5)-C(4)	121.8(2)
C(5)-C(6)-C(7)	121.4(2)
C(10)-C(7)-C(8)	116.9(2)
C(10)-C(7)-C(6)	124.4(2)
C(8)-C(7)-C(6)	118.6(3)
N(2)-C(8)-C(7)	122.9(2)
N(2)-C(8)-C(9)	117.41(16)
C(7)-C(8)-C(9)	119.68(19)
N(1)-C(9)-C(4)	122.4(2)
N(1)-C(9)-C(8)	117.85(16)

C(4)-C(9)-C(8)	119.73(19)
C(11)-C(10)-C(7)	120.0(2)
C(10)-C(11)-C(12)	120.5(2)
N(2)-C(12)-C(11)	120.8(2)
N(2)-C(12)-C(13)	117.21(17)
C(11)-C(12)-C(13)	121.9(2)
C(18)-C(13)-C(14)	119.1(2)
C(18)-C(13)-C(12)	121.1(2)
C(14)-C(13)-C(12)	119.8(2)
C(15)-C(14)-C(13)	120.6(2)
C(16)-C(15)-C(14)	119.9(3)
C(15)-C(16)-C(17)	119.8(3)
C(16)-C(17)-C(18)	120.6(3)
C(17)-C(18)-C(13)	119.9(3)
N(3)-C(19)-C(20)	123.2(2)
C(21)-C(20)-C(19)	119.2(3)
C(20)-C(21)-C(22)	120.0(2)
C(21)-C(22)-C(27)	117.5(2)
C(21)-C(22)-C(23)	123.6(2)
C(27)-C(22)-C(23)	118.9(3)
C(24)-C(23)-C(22)	121.4(2)
C(23)-C(24)-C(25)	121.6(2)
C(28)-C(25)-C(26)	117.0(2)
C(28)-C(25)-C(24)	124.5(2)
C(26)-C(25)-C(24)	118.5(3)
N(4)-C(26)-C(25)	122.8(2)
N(4)-C(26)-C(27)	117.50(17)
C(25)-C(26)-C(27)	119.7(2)
N(3)-C(27)-C(22)	122.3(2)
N(3)-C(27)-C(26)	117.82(16)
C(22)-C(27)-C(26)	119.8(2)
C(29)-C(28)-C(25)	120.1(2)

C(28)-C(29)-C(30)	120.2(3)
N(4)-C(30)-C(29)	121.1(2)
N(4)-C(30)-C(31)	117.58(18)
C(29)-C(30)-C(31)	121.3(2)
C(32)-C(31)-C(36)	118.7(2)
C(32)-C(31)-C(30)	121.35(19)
C(36)-C(31)-C(30)	120.0(2)
C(33)-C(32)-C(31)	120.8(2)
C(34)-C(33)-C(32)	120.0(3)
C(35)-C(34)-C(33)	119.5(3)
C(34)-C(35)-C(36)	121.0(2)
C(35)-C(36)-C(31)	120.0(3)
C(1)-N(1)-C(9)	117.88(17)
C(1)-N(1)-Cu	128.68(14)
C(9)-N(1)-Cu	113.09(13)
C(12)-N(2)-C(8)	118.64(17)
C(12)-N(2)-Cu	130.29(13)
C(8)-N(2)-Cu	108.36(12)
C(19)-N(3)-C(27)	117.74(17)
C(19)-N(3)-Cu	129.29(14)
C(27)-N(3)-Cu	112.41(13)
C(30)-N(4)-C(26)	118.81(17)
C(30)-N(4)-Cu	130.67(14)
C(26)-N(4)-Cu	108.84(13)
F(6)-F(1')-F(3)	119.5(5)
F(6)-F(1')-P	61.2(3)
F(3)-F(1')-P	60.6(3)
F(4')-F(1)-F(5')	126.5(10)
F(4')-F(1)-P	72.1(7)
F(5')-F(1)-P	56.8(4)
F(5)-F(2')-F(4)	141.0(9)
F(5)-F(2')-P	76.4(6)

F(4)-F(2')-P	70.3(4)
F(3')-F(2)-P	72.2(8)
F(3')-F(2)-F(6')	118.3(10)
P-F(2)-F(6')	54.4(5)
F(6')-F(3)-F(1')	131.7(11)
F(6')-F(3)-P	70.0(6)
F(1')-F(3)-P	70.7(4)
F(2)-F(3')-P	79.8(9)
F(2)-F(3')-F(6)	131.8(11)
P-F(3')-F(6)	58.6(4)
F(1)-F(4')-P	75.5(7)
F(1)-F(4')-F(5)	118.6(10)
P-F(4')-F(5)	57.4(4)
F(5')-F(4)-F(2')	115.5(7)
F(5')-F(4)-P	59.6(4)
F(2')-F(4)-P	60.0(3)
F(4)-F(5')-F(6)	113.6(12)
F(4)-F(5')-P	73.2(5)
F(6)-F(5')-P	66.5(4)
F(4)-F(5')-F(1)	103.9(8)
F(6)-F(5')-F(1)	102.8(10)
P-F(5')-F(1)	64.0(5)
F(2')-F(5)-P	67.0(5)
F(2')-F(5)-F(6')	111.0(8)
P-F(5)-F(6')	54.0(3)
F(2')-F(5)-F(4')	100.2(8)
P-F(5)-F(4')	55.5(3)
F(6')-F(5)-F(4')	75.0(7)
F(3)-F(6')-P	73.4(6)
F(3)-F(6')-F(2)	108.1(12)
P-F(6')-F(2)	59.1(4)
F(3)-F(6')-F(5)	117.7(13)

P-F(6')-F(5)	59.1(4)
F(2)-F(6')-F(5)	80.8(5)
F(1')-F(6)-F(5')	111.7(10)
F(1')-F(6)-P	70.9(3)
F(5')-F(6)-P	61.8(4)
F(1')-F(6)-F(3')	98.9(6)
F(5')-F(6)-F(3')	95.4(8)
P-F(6)-F(3')	58.3(4)
F(5')-P-F(6')	168.7(8)
F(5')-P-F(2')	94.2(5)
F(6')-P-F(2')	96.6(6)
F(5')-P-F(3)	132.1(7)
F(6')-P-F(3)	36.6(4)
F(2')-P-F(3)	130.4(6)
F(5')-P-F(3')	92.3(10)
F(6')-P-F(3')	90.7(8)
F(2')-P-F(3')	91.1(5)
F(3)-P-F(3')	101.9(5)
F(5')-P-F(6)	51.6(4)
F(6')-P-F(6)	121.0(6)
F(2')-P-F(6)	132.6(6)
F(3)-P-F(6)	95.1(5)
F(3')-P-F(6)	63.2(6)
F(5')-P-F(4')	90.5(8)
F(6')-P-F(4')	86.6(8)
F(2')-P-F(4')	88.6(4)
F(3)-P-F(4')	76.3(6)
F(3')-P-F(4')	177.2(8)
F(6)-P-F(4')	118.9(6)
F(5')-P-F(2)	118.6(8)
F(6')-P-F(2)	66.6(7)
F(2')-P-F(2)	80.4(4)

F(3)-P-F(2)	89.2(4)
F(3')-P-F(2)	28.0(7)
F(6)-P-F(2)	88.8(3)
F(4')-P-F(2)	149.3(7)
F(5')-P-F(1)	59.2(7)
F(6')-P-F(1)	115.8(7)
F(2')-P-F(1)	98.5(3)
F(3)-P-F(1)	93.2(3)
F(3')-P-F(1)	150.3(8)
F(6)-P-F(1)	90.4(4)
F(4')-P-F(1)	32.4(6)
F(2)-P-F(1)	177.6(4)
F(5')-P-F(5)	121.8(5)
F(6')-P-F(5)	66.9(6)
F(2')-P-F(5)	36.5(3)
F(3)-P-F(5)	95.3(5)
F(3')-P-F(5)	111.1(7)
F(6)-P-F(5)	169.1(5)
F(4')-P-F(5)	67.1(5)
F(2)-P-F(5)	87.9(3)
F(1)-P-F(5)	92.5(3)
F(5')-P-F(4)	47.2(5)
F(6')-P-F(4)	144.0(6)
F(2')-P-F(4)	49.7(4)
F(3)-P-F(4)	178.6(3)
F(3')-P-F(4)	79.5(4)
F(6)-P-F(4)	85.2(5)
F(4')-P-F(4)	102.4(6)
F(2)-P-F(4)	92.2(3)
F(1)-P-F(4)	85.5(2)
F(5)-P-F(4)	84.5(4)
F(5')-P-F(1')	87.0(6)

F(6')-P-F(1')	82.2(5)
F(2')-P-F(1')	178.5(5)
F(3)-P-F(1')	48.8(4)
F(3')-P-F(1')	88.0(4)
F(6)-P-F(1')	47.8(3)
F(4')-P-F(1')	92.3(4)
F(2)-P-F(1')	98.3(4)
F(1)-P-F(1')	82.9(3)
F(5)-P-F(1')	143.1(5)
F(4)-P-F(1')	131.2(5)
N(1)-Cu-N(3)	141.33(7)
N(1)-Cu-N(4)	127.71(6)
N(3)-Cu-N(4)	82.12(7)
N(1)-Cu-N(2)	81.47(6)
N(3)-Cu-N(2)	124.02(6)
N(4)-Cu-N(2)	95.67(6)

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

	U11	U22	U33	U23	U13	U12
C(1)	65(1)	73(1)	58(1)	-28(1)	13(1)	-29(1)
C(2)	73(2)	94(2)	82(2)	-49(2)	16(1)	-41(1)
C(3)	58(1)	124(2)	72(2)	-58(2)	7(1)	-34(1)
C(4)	44(1)	112(2)	51(1)	-37(1)	-1(1)	-16(1)
C(5)	60(1)	142(3)	50(1)	-35(2)	-15(1)	-10(2)
C(6)	63(1)	134(3)	46(1)	-7(1)	-15(1)	-3(2)
C(7)	45(1)	99(2)	48(1)	1(1)	-4(1)	-6(1)
C(8)	34(1)	74(1)	41(1)	-8(1)	-1(1)	-7(1)
C(9)	36(1)	80(1)	40(1)	-20(1)	1(1)	-13(1)
C(10)	56(1)	86(2)	67(1)	19(1)	-6(1)	-5(1)

C(11)	56(1)	62(1)	85(2)	11(1)	1(1)	-12(1)
C(12)	40(1)	55(1)	62(1)	-3(1)	8(1)	-10(1)
C(13)	54(1)	48(1)	69(1)	-9(1)	11(1)	-21(1)
C(14)	55(1)	58(1)	68(1)	-10(1)	5(1)	-19(1)
C(15)	65(1)	73(1)	85(2)	-9(1)	-2(1)	-29(1)
C(16)	101(2)	92(2)	105(2)	-36(2)	-6(2)	-47(2)
C(17)	106(2)	84(2)	131(3)	-59(2)	11(2)	-31(2)
C(18)	69(2)	63(1)	113(2)	-32(1)	7(1)	-16(1)
C(19)	65(1)	65(1)	60(1)	-13(1)	-17(1)	-9(1)
C(20)	70(2)	87(2)	72(2)	-5(1)	-27(1)	-20(1)
C(21)	89(2)	94(2)	56(1)	-5(1)	-26(1)	-43(2)
C(22)	95(2)	74(1)	42(1)	-11(1)	-7(1)	-47(1)
C(23)	118(2)	102(2)	52(1)	-29(1)	-2(1)	-59(2)
C(24)	136(3)	100(2)	60(1)	-47(1)	25(2)	-63(2)
C(25)	96(2)	69(1)	57(1)	-30(1)	23(1)	-37(1)
C(26)	72(1)	53(1)	42(1)	-15(1)	11(1)	-29(1)
C(27)	69(1)	54(1)	38(1)	-9(1)	-2(1)	-29(1)
C(28)	107(2)	78(2)	84(2)	-46(1)	39(2)	-28(2)
C(29)	75(2)	76(2)	90(2)	-36(1)	25(1)	-11(1)
C(30)	59(1)	54(1)	63(1)	-15(1)	17(1)	-16(1)
C(31)	41(1)	62(1)	65(1)	-10(1)	11(1)	-9(1)
C(32)	51(1)	67(1)	65(1)	-11(1)	0(1)	-13(1)
C(33)	53(1)	87(2)	85(2)	-21(1)	-1(1)	-20(1)
C(34)	48(1)	120(2)	75(2)	-11(2)	-9(1)	-20(1)
C(35)	51(1)	93(2)	88(2)	10(2)	-7(1)	-6(1)
C(36)	50(1)	66(1)	89(2)	-4(1)	5(1)	-8(1)
N(1)	47(1)	64(1)	42(1)	-19(1)	2(1)	-18(1)
N(2)	38(1)	56(1)	43(1)	-7(1)	2(1)	-9(1)
N(3)	60(1)	51(1)	42(1)	-10(1)	-10(1)	-15(1)
N(4)	56(1)	49(1)	44(1)	-14(1)	7(1)	-18(1)
F(1')	120(4)	183(8)	99(4)	-73(5)	6(3)	-46(5)
F(1)	55(2)	136(4)	67(2)	-12(2)	-7(1)	0(2)

F(2')	144(5)	207(11)	78(3)	-63(5)	14(3)	-57(7)
F(2)	52(2)	139(4)	191(6)	-79(5)	-13(2)	10(3)
F(3)	147(5)	190(8)	78(3)	29(4)	-13(3)	21(4)
F(3')	174(9)	363(16)	88(4)	17(7)	-12(5)	-201(11)
F(4')	177(10)	319(14)	146(7)	-87(9)	51(7)	-174(10)
F(4)	104(3)	156(5)	94(3)	33(3)	-17(2)	-41(3)
F(5')	298(14)	131(7)	224(12)	-55(7)	-123(12)	83(8)
F(5)	155(5)	111(4)	197(8)	-87(4)	0(5)	-42(3)
F(6')	389(18)	90(4)	160(9)	17(5)	3(10)	50(7)
F(6)	151(5)	115(4)	236(10)	-105(6)	-53(6)	-11(3)
P	59(1)	67(1)	74(1)	-19(1)	-8(1)	-10(1)
Cu	55(1)	58(1)	38(1)	-15(1)	-6(1)	-13(**1)**

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

	x	y	z	U(eq)
H(1)	9220	-1588	2087	74
H(2)	8342	-2244	850	90
H(3)	7588	-933	-600	92
H(5)	7124	1210	-1636	100
H(6)	7138	3137	-1770	103
H(10)	7694	4752	-994	93
H(11)	8594	5218	304	87
H(14)	11760	2498	1845	72
H(15)	12984	2900	3052	88
H(16)	11973	4363	3871	112
H(17)	9749	5431	3470	120
H(18)	8551	5100	2211	96
H(19)	12477	-473	3165	76
H(20)	13930	-407	4397	93
H(21)	13124	729	5510	93
H(23)	11124	2101	6135	99
H(24)	8917	3117	5976	106
H(28)	6621	3753	4996	110
H(29)	5391	3644	3683	103
H(32)	6329	570	2650	81
H(33)	5187	455	1276	96
H(34)	4343	2171	75	108
H(35)	4541	3994	300	109
H(36)	5596	4135	1701	93