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Bis[μ-bis(diphenylphosphino)amine-κ^2P:P']bis[(1,10-phenanthroline-κ^2N,N')-copper(I)] bis(tetrafluoridoborate) dichloromethane solvate

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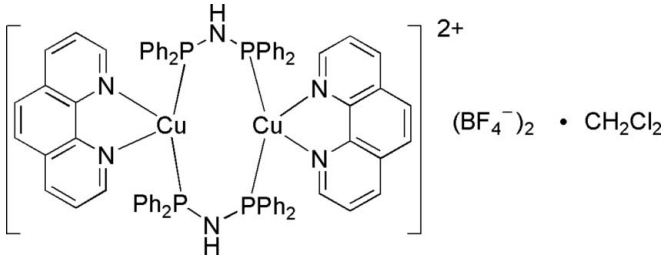
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.009 Å; disorder in solvent or counterion; R factor = 0.049; wR factor = 0.194; data-to-parameter ratio = 13.3.

In the title compound, $[Cu_2(C_{25}H_{21}NP_2)_2(C_{12}H_8N_2)_2](BF_4)_2\cdot CH_2Cl_2$, two Cu^I atoms are bridged by two bis(diphenylphosphino)amine (dppa) ligands to form an eight-membered $Cu_2P_4N_2$ ring with crystallographic twofold rotation symmetry. The coordination polyhedron of each Cu^I atom is distorted tetrahedral. Four F atoms are disordered equally over two sites.

Related literature

For related literature concerning diphosphinoamine complexes, see: Ahuja *et al.* (2007); İrişli & Şen (2005); Liu *et al.* (2002); Sekabunga *et al.* (2002).



Experimental

Crystal data

$[Cu_2(C_{25}H_{21}NP_2)_2(C_{12}H_8N_2)_2](BF_4)_2\cdot CH_2Cl_2$
M_r = 1514.76
Orthorhombic, *Pbcn*
a = 19.8730 (15) Å
b = 17.4039 (13) Å
c = 21.0008 (16) Å
V = 7263.5 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.81 mm^{-1}
T = 294 (2) K
0.26 × 0.18 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.833, T_{max} = 0.919
34870 measured reflections
6356 independent reflections
4243 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.195
S = 1.01
6356 reflections
478 parameters
93 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	2.135 (4)	Cu1—P1	2.2687 (12)
Cu1—N3	2.088 (4)	Cu1—P2	2.2272 (13)
P1—Cu1—N2	98.96 (11)	P2—Cu1—N2	105.24 (11)
P1—Cu1—N3	98.69 (11)	P2—Cu1—N3	122.16 (11)
P1—Cu1—P2	135.28 (5)	N2—Cu1—N3	79.47 (15)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2209).

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supplementary materials

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Bis[μ-bis(diphenylphosphino)amine-κ^2P:P']bis[(1,10-phenanthroline-κ^2N,N')copper(I)] bis(tetrafluoridoborate) dichloromethane solvate

J. Mo, H.-Y. Qian, X.-D. Du and W. Chen

Comment

Diphosphinoamine ligands can bind to metals in monodentate, bidentate, chelating and bridging modes and their complexes find application in diverse areas such as supramolecular design, photophysics and catalysis (Liu *et al.*, 2002; İrişli & Şen, 2005; Ahuja *et al.*, 2007; Sekabunga *et al.*, 2002). The title compound is a new Cu^I complex with bis(diphenylphosphino)amine (dppa).

The compound consists of $[Cu_2(phen)_2(dppa)_2]^{2+}$ cations (phen is 1,10-phenanthroline) located on 2-fold rotation axes. The two Cu^I atoms are bridged by two dppa ligands to form an eight-membered $Cu_2P_4N_2$ ring. The distance between the two metal centres is 3.616 (4) Å, which is too long for any significant metal–metal bonding interaction. Each Cu^I atom adopts a distorted tetrahedral coordination geometry, with the angles around Cu^I ranging from 79.5 (2) ° for N2—Cu1—N3 to 135.28 (5) ° for P1—Cu1—P2A (where the suffix A denotes the symmetry operator $-x$, y, $1/2-z$).

Experimental

$[Cu(CH_3CN)_4](BF_4)$ (0.372 g, 1.0 mmol) was dissolved in CH_2Cl_2 (15 ml) under nitrogen, and a solution of dppa (0.385 g, 1.0 mmol) and phen (0.18 g, 1.0 mmol) in CH_2Cl_2 (10 ml) was added at room temperature. The filtrate was kept under a diethyl ether atmosphere for three weeks, during which time yellow block-shaped crystals were formed.

Refinement

H atoms were placed geometrically and allowed to ride during refinement with C—H = 0.93 Å or 0.97 Å for the CH_2Cl_2 molecule and with $U_{iso}(H) = 1.2U_{eq}(C)$. The tetrafluoroborate anion is modelled as disordered over two orientations with equal site occupancies. All B—F distances were restrained to be 1.38 (1) Å, and the F···F distances within each component were restrained to be equal with an effective standard uncertainty of 0.02 Å (SADI instruction in *SHELXL*). The C—Cl distances in the CH_2Cl_2 molecule were restrained to be 1.74 (1) Å.

Figures

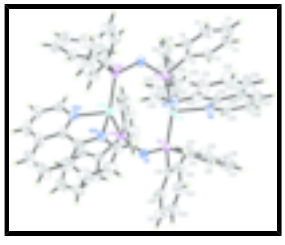


Fig. 1. Molecular structure of the title compound with displacement ellipsoids drawn at the 40% probability level for non-H atoms. The suffix A denotes the symmetry operator $-x$, y, $1/2-z$. The BF_4^- anions and CH_2Cl_2 solvent molecule are omitted.

Bis[μ-bis(diphenylphosphino)amine-κ^2*P*:*P*']bis[(1,10-\ phenanthroline-κ^2*N*,*N*')copper(I)] bis(tetrafluoridoborate) dichloromethane solvate

Crystal data

$[Cu_2(C_{25}H_{21}N_1P_2)_2(C_{12}H_8N_2)_2](BF_4)_2{\cdot}CH_2Cl_2$	F_{000} = 3088
M_r = 1514.76	D_x = 1.385 Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2n 2ab	Cell parameters from 9095 reflections
a = 19.8730 (15) Å	θ = 2.3–25.5º
b = 17.4039 (13) Å	μ = 0.81 mm^{-1}
c = 21.0008 (16) Å	*T* = 294 (2) K
V = 7263.5 (9) Å^3	Block, yellow
Z = 4	0.26 × 0.18 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer	6356 independent reflections
Radiation source: fine-focus sealed tube	4243 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.046
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	*h* = −23→23
T_{min} = 0.833, T_{max} = 0.919	*k* = −20→17
34870 measured reflections	*l* = −24→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.049	H-atom parameters constrained
$wR(F^2)$ = 0.195	$w = 1/[\sigma^2(F_o^2) + (0.1181P)^2 + 8.285P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
6356 reflections	$\Delta\rho_{max}$ = 0.96 e Å^{-3}
478 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
93 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

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

Refinement. 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 $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.02403 (3)	0.72312 (3)	0.33303 (2)	0.0378 (2)	
P1	0.10615 (5)	0.64958 (6)	0.28923 (5)	0.0348 (3)	
P2	−0.08734 (6)	0.71415 (6)	0.34225 (5)	0.0333 (3)	
N2	0.0610 (2)	0.7281 (2)	0.42839 (17)	0.0428 (9)	
N3	0.07362 (19)	0.8288 (2)	0.33142 (17)	0.0410 (9)	
C1	0.1811 (2)	0.6657 (3)	0.3371 (2)	0.0381 (10)	
C2	0.1936 (3)	0.6201 (3)	0.3902 (2)	0.0523 (12)	
H2	0.1665	0.5775	0.3980	0.063*	
C3	0.2450 (3)	0.6370 (4)	0.4311 (3)	0.0688 (16)	
H3	0.2527	0.6055	0.4662	0.083*	
C4	0.2851 (4)	0.6993 (4)	0.4213 (3)	0.084 (2)	
H4	0.3196	0.7108	0.4495	0.101*	
C5	0.2737 (3)	0.7454 (4)	0.3686 (3)	0.0790 (19)	
H5	0.3013	0.7876	0.3611	0.095*	
C6	0.2215 (3)	0.7291 (3)	0.3270 (3)	0.0553 (13)	
H6	0.2137	0.7609	0.2922	0.066*	
C7	0.1003 (2)	0.5451 (3)	0.2906 (2)	0.0424 (11)	
C8	0.1512 (3)	0.4987 (3)	0.2659 (3)	0.0644 (15)	
H8	0.1893	0.5210	0.2479	0.077*	
C9	0.1450 (4)	0.4195 (4)	0.2682 (3)	0.083 (2)	
H9	0.1789	0.3886	0.2515	0.100*	
C10	0.0898 (5)	0.3868 (4)	0.2948 (4)	0.088 (2)	
H10	0.0858	0.3336	0.2958	0.106*	
C11	0.0402 (4)	0.4314 (4)	0.3200 (4)	0.080 (2)	
H11	0.0028	0.4084	0.3385	0.096*	
C12	0.0453 (3)	0.5111 (3)	0.3183 (3)	0.0554 (13)	
H12	0.0115	0.5413	0.3359	0.067*	
N1	−0.13374 (19)	0.6728 (2)	0.28423 (17)	0.0402 (9)	
C13	−0.1069 (2)	0.6535 (3)	0.4112 (2)	0.0401 (10)	
C14	−0.1192 (3)	0.5761 (3)	0.4043 (3)	0.0598 (14)	
H14	−0.1212	0.5540	0.3641	0.072*	
C15	−0.1285 (4)	0.5311 (4)	0.4590 (4)	0.085 (2)	
H15	−0.1377	0.4789	0.4549	0.102*	

C16	−0.1244 (4)	0.5631 (4)	0.5182 (3)	0.087 (2)	
H16	−0.1304	0.5327	0.5541	0.104*	
C17	−0.1116 (3)	0.6393 (4)	0.5247 (3)	0.0733 (17)	
H17	−0.1082	0.6609	0.5651	0.088*	
C18	−0.1037 (3)	0.6842 (3)	0.4720 (2)	0.0558 (13)	
H18	−0.0959	0.7365	0.4770	0.067*	
C19	−0.1318 (2)	0.8025 (3)	0.3631 (2)	0.0379 (10)	
C20	−0.2006 (3)	0.8095 (3)	0.3566 (3)	0.0542 (13)	
H20	−0.2255	0.7681	0.3415	0.065*	
C21	−0.2330 (3)	0.8772 (3)	0.3720 (3)	0.0657 (15)	
H21	−0.2795	0.8812	0.3675	0.079*	
C22	−0.1963 (3)	0.9387 (3)	0.3940 (3)	0.0690 (16)	
H22	−0.2178	0.9846	0.4037	0.083*	
C23	−0.1283 (3)	0.9323 (3)	0.4016 (3)	0.0708 (17)	
H23	−0.1035	0.9738	0.4168	0.085*	
C24	−0.0962 (3)	0.8639 (3)	0.3866 (3)	0.0537 (13)	
H24	−0.0499	0.8595	0.3924	0.064*	
C25	0.0563 (3)	0.6769 (3)	0.4752 (2)	0.0530 (12)	
H25	0.0308	0.6328	0.4686	0.064*	
C26	0.0880 (3)	0.6868 (4)	0.5337 (3)	0.0669 (16)	
H26	0.0825	0.6505	0.5658	0.080*	
C27	0.1265 (4)	0.7492 (4)	0.5435 (3)	0.0778 (19)	
H27	0.1476	0.7559	0.5826	0.093*	
C28	0.1353 (3)	0.8041 (3)	0.4956 (3)	0.0648 (15)	
C29	0.1773 (4)	0.8697 (4)	0.5002 (3)	0.088 (2)	
H29	0.2003	0.8787	0.5380	0.106*	
C30	0.1850 (4)	0.9189 (4)	0.4521 (4)	0.091 (2)	
H30	0.2133	0.9609	0.4569	0.109*	
C31	0.1503 (3)	0.9080 (3)	0.3931 (3)	0.0663 (15)	
C32	0.1572 (4)	0.9563 (4)	0.3403 (3)	0.0786 (19)	
H32	0.1848	0.9994	0.3428	0.094*	
C33	0.1238 (3)	0.9406 (3)	0.2854 (3)	0.0710 (17)	
H33	0.1282	0.9725	0.2501	0.085*	
C34	0.0835 (3)	0.8769 (3)	0.2829 (3)	0.0526 (12)	
H34	0.0615	0.8664	0.2448	0.063*	
C35	0.1080 (2)	0.8435 (3)	0.3865 (2)	0.0453 (11)	
C36	0.1003 (3)	0.7908 (3)	0.4380 (2)	0.0452 (11)	
B1	0.1709 (3)	0.1415 (3)	0.2016 (3)	0.0675 (19)	
F1	0.1630 (2)	0.2187 (2)	0.2035 (2)	0.0981 (13)	
F2	0.1308 (7)	0.1095 (8)	0.1551 (7)	0.106 (6)	0.50
F3	0.2349 (5)	0.1189 (8)	0.1952 (6)	0.124 (6)	0.50
F4	0.1463 (7)	0.1148 (7)	0.2595 (5)	0.132 (5)	0.50
F4'	0.1836 (6)	0.1066 (6)	0.2591 (4)	0.106 (4)	0.50
F3'	0.2306 (4)	0.1295 (6)	0.1665 (5)	0.079 (3)	0.50
F2'	0.1202 (7)	0.1039 (9)	0.1708 (8)	0.116 (7)	0.50
C38	0.9690 (8)	0.1159 (5)	0.1366 (5)	0.101 (5)	0.50
H38A	0.9298	0.1019	0.1615	0.122*	0.50
H38B	1.0087	0.0972	0.1587	0.122*	0.50
Cl1	0.9641 (3)	0.0732 (5)	0.0619 (3)	0.163 (2)	0.50

Cl2	0.9731 (2)	0.2138 (2)	0.1298 (4)	0.139 (2)	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0379 (3)	0.0375 (4)	0.0380 (3)	−0.0015 (2)	0.0012 (2)	−0.0012 (2)
P1	0.0355 (6)	0.0346 (6)	0.0343 (6)	0.0007 (5)	0.0006 (5)	0.0041 (5)
P2	0.0365 (6)	0.0327 (6)	0.0308 (6)	−0.0001 (5)	0.0019 (4)	−0.0031 (4)
N2	0.042 (2)	0.051 (2)	0.0350 (19)	0.0004 (19)	0.0016 (17)	−0.0008 (17)
N3	0.044 (2)	0.037 (2)	0.042 (2)	−0.0030 (17)	0.0016 (16)	−0.0014 (17)
C1	0.034 (2)	0.039 (2)	0.041 (2)	0.0019 (19)	0.0031 (18)	−0.0007 (19)
C2	0.055 (3)	0.049 (3)	0.053 (3)	0.000 (2)	−0.009 (2)	0.009 (2)
C3	0.075 (4)	0.071 (4)	0.060 (3)	0.010 (3)	−0.027 (3)	0.008 (3)
C4	0.071 (4)	0.104 (5)	0.078 (4)	−0.011 (4)	−0.031 (3)	−0.003 (4)
C5	0.067 (4)	0.090 (5)	0.080 (4)	−0.033 (4)	−0.016 (3)	0.005 (4)
C6	0.046 (3)	0.064 (4)	0.056 (3)	−0.007 (3)	−0.003 (2)	0.005 (3)
C7	0.055 (3)	0.033 (2)	0.038 (2)	0.000 (2)	−0.009 (2)	0.0076 (19)
C8	0.077 (4)	0.050 (3)	0.066 (3)	0.014 (3)	0.008 (3)	0.009 (3)
C9	0.127 (6)	0.052 (4)	0.071 (4)	0.023 (4)	−0.001 (4)	0.004 (3)
C10	0.141 (7)	0.043 (4)	0.080 (5)	−0.011 (4)	−0.035 (5)	0.012 (3)
C11	0.092 (5)	0.062 (4)	0.086 (5)	−0.031 (4)	−0.025 (4)	0.027 (4)
C12	0.058 (3)	0.051 (3)	0.057 (3)	−0.011 (3)	−0.008 (3)	0.012 (3)
N1	0.044 (2)	0.041 (2)	0.0348 (19)	−0.0029 (17)	0.0031 (16)	−0.0101 (16)
C13	0.034 (2)	0.041 (3)	0.045 (3)	0.0016 (19)	0.0036 (19)	0.006 (2)
C14	0.072 (4)	0.043 (3)	0.064 (3)	−0.007 (3)	−0.003 (3)	0.005 (3)
C15	0.100 (5)	0.049 (4)	0.105 (6)	−0.012 (3)	−0.005 (4)	0.030 (4)
C16	0.103 (5)	0.091 (5)	0.066 (4)	−0.003 (4)	0.008 (4)	0.041 (4)
C17	0.090 (5)	0.083 (5)	0.047 (3)	0.006 (4)	0.016 (3)	0.015 (3)
C18	0.070 (3)	0.056 (3)	0.042 (3)	0.007 (3)	0.009 (2)	0.006 (2)
C19	0.046 (3)	0.035 (2)	0.032 (2)	0.001 (2)	0.0057 (19)	0.0000 (18)
C20	0.055 (3)	0.046 (3)	0.062 (3)	0.003 (2)	0.002 (3)	−0.011 (3)
C21	0.056 (3)	0.070 (4)	0.071 (4)	0.021 (3)	0.006 (3)	−0.007 (3)
C22	0.085 (5)	0.045 (3)	0.077 (4)	0.019 (3)	0.010 (3)	−0.008 (3)
C23	0.079 (4)	0.046 (3)	0.088 (4)	−0.005 (3)	0.009 (3)	−0.024 (3)
C24	0.052 (3)	0.046 (3)	0.063 (3)	−0.003 (2)	0.004 (2)	−0.014 (2)
C25	0.053 (3)	0.059 (3)	0.047 (3)	0.009 (3)	0.004 (2)	0.007 (2)
C26	0.086 (4)	0.071 (4)	0.044 (3)	0.011 (3)	−0.002 (3)	0.002 (3)
C27	0.103 (5)	0.088 (5)	0.042 (3)	0.020 (4)	−0.016 (3)	−0.009 (3)
C28	0.075 (4)	0.064 (4)	0.056 (3)	0.007 (3)	−0.017 (3)	−0.019 (3)
C29	0.112 (6)	0.075 (4)	0.077 (4)	−0.008 (4)	−0.044 (4)	−0.021 (4)
C30	0.105 (6)	0.066 (4)	0.101 (5)	−0.030 (4)	−0.034 (4)	−0.016 (4)
C31	0.073 (4)	0.054 (3)	0.072 (4)	−0.012 (3)	−0.009 (3)	−0.011 (3)
C32	0.096 (5)	0.051 (4)	0.088 (5)	−0.026 (3)	0.001 (4)	−0.003 (3)
C33	0.083 (4)	0.050 (3)	0.079 (4)	−0.016 (3)	0.002 (3)	0.010 (3)
C34	0.060 (3)	0.045 (3)	0.053 (3)	−0.002 (2)	0.005 (2)	−0.001 (2)
C35	0.045 (3)	0.040 (3)	0.051 (3)	−0.002 (2)	−0.001 (2)	−0.010 (2)
C36	0.054 (3)	0.044 (3)	0.038 (2)	0.004 (2)	−0.002 (2)	−0.008 (2)
B1	0.068 (5)	0.064 (5)	0.071 (5)	−0.015 (4)	−0.010 (4)	0.015 (4)

F1	0.112 (3)	0.073 (3)	0.110 (3)	−0.003 (2)	−0.003 (2)	0.004 (2)
F2	0.090 (8)	0.116 (9)	0.113 (8)	−0.001 (6)	−0.029 (6)	−0.023 (6)
F3	0.086 (7)	0.134 (8)	0.151 (10)	0.002 (6)	−0.035 (6)	−0.025 (7)
F4	0.156 (9)	0.128 (8)	0.113 (7)	−0.030 (7)	0.039 (7)	0.033 (6)
F4'	0.129 (7)	0.097 (6)	0.091 (6)	−0.035 (6)	−0.028 (5)	0.033 (5)
F3'	0.046 (5)	0.091 (6)	0.100 (7)	−0.016 (4)	−0.012 (4)	−0.006 (5)
F2'	0.064 (7)	0.144 (13)	0.139 (12)	−0.038 (7)	−0.028 (7)	−0.034 (9)
C38	0.090 (11)	0.079 (10)	0.135 (14)	−0.024 (8)	−0.022 (9)	0.037 (10)
Cl1	0.129 (4)	0.217 (6)	0.143 (4)	−0.018 (4)	−0.006 (3)	−0.062 (4)
Cl2	0.101 (3)	0.079 (3)	0.238 (6)	0.010 (2)	0.051 (3)	0.018 (3)

Geometric parameters (Å, °)

Cu1—N2	2.135 (4)	C17—C18	1.364 (7)
Cu1—N3	2.088 (4)	C17—H17	0.930
Cu1—P1	2.2687 (12)	C18—H18	0.930
Cu1—P2	2.2272 (13)	C19—C24	1.373 (7)
P1—N1^{i}	1.686 (4)	C19—C20	1.380 (7)
P1—C1	1.818 (4)	C20—C21	1.382 (7)
P1—C7	1.822 (5)	C20—H20	0.930
P2—N1	1.689 (4)	C21—C22	1.374 (9)
P2—C19	1.826 (4)	C21—H21	0.930
P2—C13	1.833 (4)	C22—C23	1.366 (9)
N2—C25	1.329 (6)	C22—H22	0.930
N2—C36	1.358 (6)	C23—C24	1.388 (8)
N3—C34	1.332 (6)	C23—H23	0.930
N3—C35	1.368 (6)	C24—H24	0.930
C1—C6	1.380 (7)	C25—C26	1.391 (7)
C1—C2	1.392 (6)	C25—H25	0.930
C2—C3	1.367 (7)	C26—C27	1.345 (9)
C2—H2	0.930	C26—H26	0.930
C3—C4	1.362 (9)	C27—C28	1.399 (9)
C3—H3	0.930	C27—H27	0.930
C4—C5	1.384 (9)	C28—C36	1.415 (7)
C4—H4	0.930	C28—C29	1.417 (9)
C5—C6	1.385 (8)	C29—C30	1.333 (10)
C5—H5	0.930	C29—H29	0.930
C6—H6	0.930	C30—C31	1.431 (9)
C7—C12	1.372 (7)	C30—H30	0.930
C7—C8	1.394 (7)	C31—C32	1.398 (9)
C8—C9	1.385 (8)	C31—C35	1.408 (7)
C8—H8	0.930	C32—C33	1.360 (9)
C9—C10	1.357 (11)	C32—H32	0.930
C9—H9	0.930	C33—C34	1.369 (8)
C10—C11	1.360 (11)	C33—H33	0.930
C10—H10	0.930	C34—H34	0.930
C11—C12	1.392 (9)	C35—C36	1.426 (7)
C11—H11	0.930	B1—F1	1.353 (6)
C12—H12	0.930	B1—F2	1.379 (9)

N1—P1^{i}	1.686 (4)	B1—F3	1.339 (9)
C13—C14	1.377 (7)	B1—F4	1.389 (8)
C13—C18	1.385 (7)	B1—F2'	1.366 (8)
C14—C15	1.402 (8)	B1—F4'	1.374 (8)
C14—H14	0.930	B1—F3'	1.414 (8)
C15—C16	1.366 (10)	C38—Cl2	1.711 (9)
C15—H15	0.930	C38—Cl1	1.739 (10)
C16—C17	1.357 (10)	C38—H38A	0.970
C16—H16	0.930	C38—H38B	0.970
P1—Cu1—N2	98.96 (11)	C17—C18—C13	121.5 (5)
P1—Cu1—N3	98.69 (11)	C17—C18—H18	119.2
P1—Cu1—P2	135.28 (5)	C13—C18—H18	119.2
P2—Cu1—N2	105.24 (11)	C24—C19—C20	118.5 (4)
P2—Cu1—N3	122.16 (11)	C24—C19—P2	119.4 (4)
N2—Cu1—N3	79.47 (15)	C20—C19—P2	122.0 (4)
N1^{i}—P1—C1	101.66 (19)	C19—C20—C21	121.0 (5)
N1^{i}—P1—C7	105.9 (2)	C19—C20—H20	119.5
C1—P1—C7	101.4 (2)	C21—C20—H20	119.5
N1^{i}—P1—Cu1	117.99 (14)	C22—C21—C20	119.6 (5)
C1—P1—Cu1	106.13 (14)	C22—C21—H21	120.2
C7—P1—Cu1	120.71 (17)	C20—C21—H21	120.2
N1—P2—C19	105.5 (2)	C23—C22—C21	120.2 (5)
N1—P2—C13	102.1 (2)	C23—C22—H22	119.9
C19—P2—C13	101.1 (2)	C21—C22—H22	119.9
N1—P2—Cu1	120.64 (14)	C22—C23—C24	119.8 (5)
C19—P2—Cu1	116.27 (15)	C22—C23—H23	120.1
C13—P2—Cu1	108.62 (15)	C24—C23—H23	120.1
C25—N2—C36	117.9 (4)	C19—C24—C23	120.9 (5)
C25—N2—Cu1	130.0 (3)	C19—C24—H24	119.6
C36—N2—Cu1	111.7 (3)	C23—C24—H24	119.6
C34—N3—C35	117.1 (4)	N2—C25—C26	122.7 (5)
C34—N3—Cu1	129.4 (3)	N2—C25—H25	118.7
C35—N3—Cu1	112.8 (3)	C26—C25—H25	118.7
C6—C1—C2	118.3 (4)	C27—C26—C25	119.5 (6)
C6—C1—P1	121.1 (4)	C27—C26—H26	120.3
C2—C1—P1	120.0 (4)	C25—C26—H26	120.3
C3—C2—C1	121.0 (5)	C26—C27—C28	120.9 (5)
C3—C2—H2	119.5	C26—C27—H27	119.6
C1—C2—H2	119.5	C28—C27—H27	119.6
C4—C3—C2	120.8 (6)	C27—C28—C36	116.2 (6)
C4—C3—H3	119.6	C27—C28—C29	125.1 (6)
C2—C3—H3	119.6	C36—C28—C29	118.6 (6)
C3—C4—C5	119.2 (6)	C30—C29—C28	122.2 (6)
C3—C4—H4	120.4	C30—C29—H29	118.9
C5—C4—H4	120.4	C28—C29—H29	118.9
C4—C5—C6	120.4 (6)	C29—C30—C31	121.1 (6)
C4—C5—H5	119.8	C29—C30—H30	119.5
C6—C5—H5	119.8	C31—C30—H30	119.5

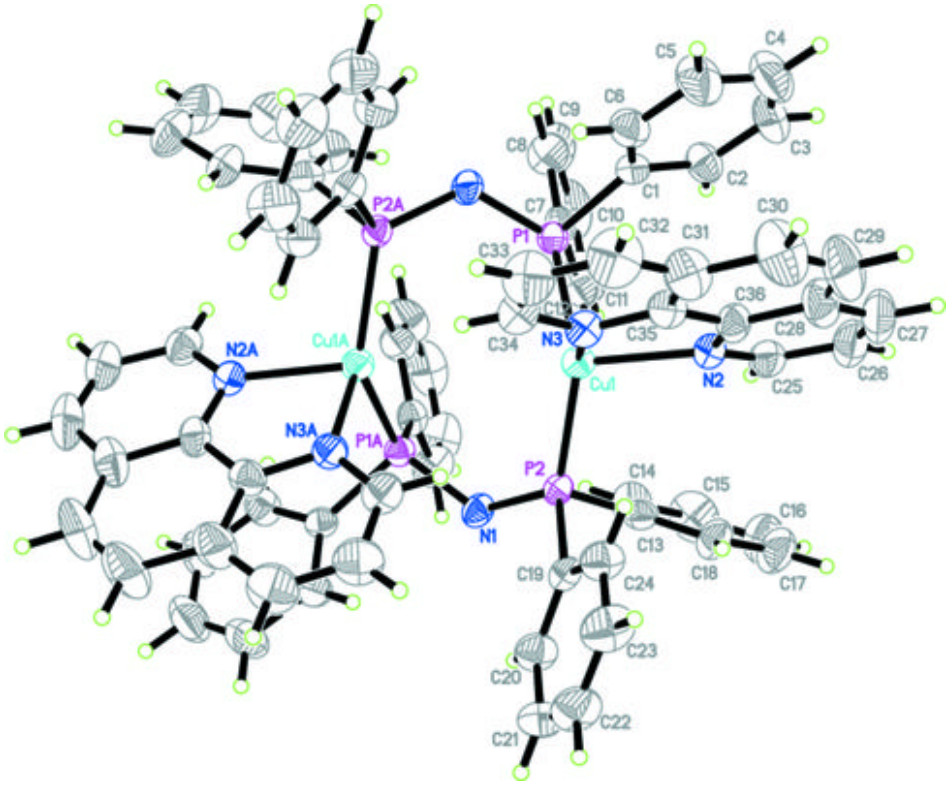
C1—C6—C5	120.3 (5)	C32—C31—C35	117.4 (5)
C1—C6—H6	119.9	C32—C31—C30	124.0 (6)
C5—C6—H6	119.9	C35—C31—C30	118.5 (6)
C12—C7—C8	119.1 (5)	C33—C32—C31	120.2 (6)
C12—C7—P1	119.2 (4)	C33—C32—H32	119.9
C8—C7—P1	121.7 (4)	C31—C32—H32	119.9
C9—C8—C7	119.9 (6)	C32—C33—C34	118.7 (6)
C9—C8—H8	120.0	C32—C33—H33	120.6
C7—C8—H8	120.0	C34—C33—H33	120.6
C10—C9—C8	120.3 (7)	N3—C34—C33	124.5 (5)
C10—C9—H9	119.9	N3—C34—H34	117.7
C8—C9—H9	119.9	C33—C34—H34	117.7
C9—C10—C11	120.4 (6)	N3—C35—C31	122.0 (5)
C9—C10—H10	119.8	N3—C35—C36	117.8 (4)
C11—C10—H10	119.8	C31—C35—C36	120.2 (5)
C10—C11—C12	120.4 (7)	N2—C36—C28	122.8 (5)
C10—C11—H11	119.8	N2—C36—C35	117.8 (4)
C12—C11—H11	119.8	C28—C36—C35	119.3 (5)
C7—C12—C11	120.0 (6)	F3—B1—F1	113.9 (8)
C7—C12—H12	120.0	F3—B1—F2	111.0 (8)
C11—C12—H12	120.0	F1—B1—F2	110.8 (8)
P1^{i}—N1—P2	125.8 (2)	F3—B1—F4	108.9 (8)
C14—C13—C18	118.8 (5)	F1—B1—F4	105.4 (7)
C14—C13—P2	121.2 (4)	F2—B1—F4	106.4 (9)
C18—C13—P2	119.8 (4)	F1—B1—F2'	113.8 (8)
C13—C14—C15	119.0 (6)	F1—B1—F4'	115.7 (7)
C13—C14—H14	120.5	F2'—B1—F4'	109.9 (8)
C15—C14—H14	120.5	F1—B1—F3'	105.1 (6)
C16—C15—C14	120.6 (6)	F2'—B1—F3'	107.5 (9)
C16—C15—H15	119.7	F4'—B1—F3'	103.8 (7)
C14—C15—H15	119.7	Cl2—C38—Cl1	110.7 (7)
C17—C16—C15	120.2 (6)	Cl2—C38—H38A	109.5
C17—C16—H16	119.9	Cl1—C38—H38A	109.5
C15—C16—H16	119.9	Cl2—C38—H38B	109.5
C16—C17—C18	119.9 (6)	Cl1—C38—H38B	109.5
C16—C17—H17	120.1	H38A—C38—H38B	108.1
C18—C17—H17	120.1		
N3—Cu1—P1—N1^{i}	−58.92 (19)	Cu1—P2—C13—C14	−95.0 (4)
N2—Cu1—P1—N1^{i}	−139.54 (19)	N1—P2—C13—C18	−152.1 (4)
P2—Cu1—P1—N1^{i}	97.95 (17)	C19—P2—C13—C18	−43.4 (4)
N3—Cu1—P1—C1	54.15 (18)	Cu1—P2—C13—C18	79.4 (4)
N2—Cu1—P1—C1	−26.47 (19)	C18—C13—C14—C15	0.5 (8)
P2—Cu1—P1—C1	−148.98 (15)	P2—C13—C14—C15	174.9 (5)
N3—Cu1—P1—C7	168.4 (2)	C13—C14—C15—C16	−1.1 (10)
N2—Cu1—P1—C7	87.8 (2)	C14—C15—C16—C17	0.4 (12)
P2—Cu1—P1—C7	−34.70 (19)	C15—C16—C17—C18	0.8 (11)
N3—Cu1—P2—N1	118.7 (2)	C16—C17—C18—C13	−1.5 (9)
N2—Cu1—P2—N1	−154.27 (19)	C14—C13—C18—C17	0.8 (8)

P1—Cu1—P2—N1	−33.96 (18)	P2—C13—C18—C17	−173.7 (5)
N3—Cu1—P2—C19	−11.0 (2)	N1—P2—C19—C24	−151.9 (4)
N2—Cu1—P2—C19	76.01 (19)	C13—P2—C19—C24	102.1 (4)
P1—Cu1—P2—C19	−163.68 (16)	Cu1—P2—C19—C24	−15.3 (4)
N3—Cu1—P2—C13	−124.1 (2)	N1—P2—C19—C20	28.6 (4)
N2—Cu1—P2—C13	−37.12 (19)	C13—P2—C19—C20	−77.4 (4)
P1—Cu1—P2—C13	83.19 (17)	Cu1—P2—C19—C20	165.3 (4)
N3—Cu1—N2—C25	−177.5 (4)	C24—C19—C20—C21	1.2 (8)
P2—Cu1—N2—C25	61.8 (4)	P2—C19—C20—C21	−179.3 (4)
P1—Cu1—N2—C25	−80.3 (4)	C19—C20—C21—C22	0.3 (9)
N3—Cu1—N2—C36	−4.7 (3)	C20—C21—C22—C23	−1.2 (9)
P2—Cu1—N2—C36	−125.4 (3)	C21—C22—C23—C24	0.6 (10)
P1—Cu1—N2—C36	92.6 (3)	C20—C19—C24—C23	−1.9 (8)
N2—Cu1—N3—C34	175.7 (4)	P2—C19—C24—C23	178.6 (4)
P2—Cu1—N3—C34	−82.9 (4)	C22—C23—C24—C19	1.0 (9)
P1—Cu1—N3—C34	78.1 (4)	C36—N2—C25—C26	2.4 (7)
N2—Cu1—N3—C35	5.7 (3)	Cu1—N2—C25—C26	174.9 (4)
P2—Cu1—N3—C35	107.2 (3)	N2—C25—C26—C27	−1.8 (9)
P1—Cu1—N3—C35	−91.9 (3)	C25—C26—C27—C28	−0.2 (10)
$N1^{i}$—P1—C1—C6	41.9 (4)	C26—C27—C28—C36	1.4 (9)
C7—P1—C1—C6	151.0 (4)	C26—C27—C28—C29	−176.8 (7)
Cu1—P1—C1—C6	−82.1 (4)	C27—C28—C29—C30	178.1 (7)
$N1^{i}$—P1—C1—C2	−147.0 (4)	C36—C28—C29—C30	−0.1 (11)
C7—P1—C1—C2	−37.9 (4)	C28—C29—C30—C31	0.6 (12)
Cu1—P1—C1—C2	89.0 (4)	C29—C30—C31—C32	−178.5 (8)
C6—C1—C2—C3	−0.7 (8)	C29—C30—C31—C35	−0.6 (11)
P1—C1—C2—C3	−172.0 (4)	C35—C31—C32—C33	0.2 (10)
C1—C2—C3—C4	0.5 (9)	C30—C31—C32—C33	178.1 (7)
C2—C3—C4—C5	−0.7 (11)	C31—C32—C33—C34	0.1 (10)
C3—C4—C5—C6	1.1 (11)	C35—N3—C34—C33	−2.1 (8)
C2—C1—C6—C5	1.0 (8)	Cu1—N3—C34—C33	−171.7 (4)
P1—C1—C6—C5	172.3 (5)	C32—C33—C34—N3	1.0 (10)
C4—C5—C6—C1	−1.2 (10)	C34—N3—C35—C31	2.3 (7)
$N1^{i}$—P1—C7—C12	−137.2 (4)	Cu1—N3—C35—C31	173.6 (4)
C1—P1—C7—C12	117.0 (4)	C34—N3—C35—C36	−177.3 (4)
Cu1—P1—C7—C12	0.3 (4)	Cu1—N3—C35—C36	−6.0 (5)
$N1^{i}$—P1—C7—C8	44.6 (5)	C32—C31—C35—N3	−1.4 (8)
C1—P1—C7—C8	−61.1 (4)	C30—C31—C35—N3	−179.5 (6)
Cu1—P1—C7—C8	−177.8 (4)	C32—C31—C35—C36	178.2 (5)
C12—C7—C8—C9	1.5 (8)	C30—C31—C35—C36	0.2 (9)
P1—C7—C8—C9	179.6 (5)	C25—N2—C36—C28	−1.1 (7)
C7—C8—C9—C10	−0.4 (10)	Cu1—N2—C36—C28	−174.8 (4)
C8—C9—C10—C11	−0.7 (11)	C25—N2—C36—C35	176.8 (4)
C9—C10—C11—C12	0.6 (10)	Cu1—N2—C36—C35	3.0 (5)
C8—C7—C12—C11	−1.5 (8)	C27—C28—C36—N2	−0.8 (8)
P1—C7—C12—C11	−179.7 (4)	C29—C28—C36—N2	177.5 (5)
C10—C11—C12—C7	0.5 (9)	C27—C28—C36—C35	−178.7 (5)
C19—P2—N1—$P1^{i}$	122.7 (3)	C29—C28—C36—C35	−0.3 (8)

C13—P2—N1—P1^{i}	−132.0 (3)	N3—C35—C36—N2	2.0 (7)
Cu1—P2—N1—P1^{i}	−11.6 (3)	C31—C35—C36—N2	−177.7 (5)
N1—P2—C13—C14	33.5 (4)	N3—C35—C36—C28	179.9 (5)
C19—P2—C13—C14	142.2 (4)	C31—C35—C36—C28	0.3 (7)

Symmetry codes: (i) −*x*, *y*, −*z*+1/2.

Fig. 1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