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(*μ-trans*-1,2-Di-4-pyridylethylene-κ^2N:N')bis[(bipyridine-κ^2N,N')-(triphenylphosphine-κP)copper(I)] bis(tetrafluoroborate)

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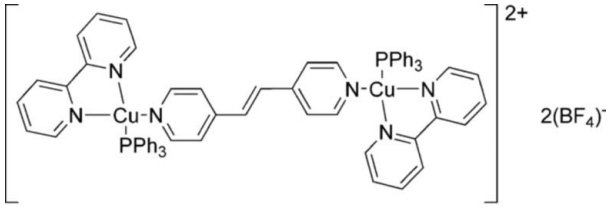
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; disorder in solvent or counterion; R factor = 0.056; wR factor = 0.151; data-to-parameter ratio = 18.8.

In the centrosymmetric dinuclear cation of the title complex, $[Cu_2(C_{10}H_8N_2)_2(C_{12}H_{10}N_2)(C_{18}H_{15}P)_2](BF_4)_2$, each Cu atom is coordinated by two N atoms from a 2,2-bipyridine ligand and a P atom from a triphenylphosphine ligand, and the two N_2PCu^+ fragments are bridged by a *trans*-1,2-di-4-pyridylethylene ligand, resulting in a distorted tetrahedral coordination geometry. Two F atoms are disordered over two sites each, with almost equal occupancies.

Related literature

For related literature, see: Chen *et al.* (2007); Horváth (1994); Kubas *et al.* (1990); McMillin & McNett (1998); Scaltrito *et al.* (2000); Wang *et al.* (2007).



Experimental

Crystal data

$[Cu_2(C_{10}H_8N_2)_2(C_{12}H_{10}N_2)(C_{18}H_{15}P)_2](BF_4)_2$
M_r = 1319.83
Monoclinic, $P2_1/c$
a = 9.9800 (17) Å
b = 15.420 (3) Å
c = 20.461 (4) Å
β = 97.021 (3)°
V = 3125.1 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 298 (2) K
0.43 × 0.33 × 0.28 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.724, T_{max} = 0.807
18965 measured reflections
7853 independent reflections
5153 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.151
S = 1.02
7853 reflections
417 parameters
24 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	2.045 (2)	Cu1—N1	2.054 (2)
Cu1—N2	2.049 (2)	Cu1—P1	2.1877 (9)
N3—Cu1—N2	108.80 (10)	N3—Cu1—P1	105.30 (7)
N3—Cu1—N1	111.53 (10)	N2—Cu1—P1	131.18 (7)
N2—Cu1—N1	80.03 (10)	N1—Cu1—P1	117.94 (7)

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: BX2080).

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supplementary materials

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(*μ*-*trans*-1,2-Di-4-pyridylethylene-κ^2N:*N*')bis[(bipyridine-κ^2N,*N*')(triphenylphosphine-κP)copper(I)] bis(tetrafluoroborate)

J.-S. Chen, P.-H. Liu and W.-F. Fu

Comment

It is well documented in the literature that copper(I) complexes with diimine ligands exhibit low energy metal-to-ligand charge-transfer (MLCT) transition (Horváth *et al.*, 1994; McMillin *et al.*, 1998; Scaltrito *et al.*, 2000). Specially, dinuclear polypyridine copper(I) complexes with unexpected stablity diplay potential applicance in photocatalysts and multi-electron storage systems. Electron transfer between two copper(I) centers is influenced by the acceptor and donor properties of the coordination sites, as well as the length and rigidity of the spacers. Previously, we reported two copper(I) complexes with 4,4'-bipyridine ligand as a bridge (Chen *et al.*, 2007; Wang *et al.*, 2007). We report here the title complex, (I).

The structure of the *trans*-$[Cu_2(C_{12}H_{10}N_2)\ (C_{10}H_8N_2)_2(C_{18}H_{15}P)_2]^{2+}$ cation is shown in Fig. 1, and selected bond lengths and angles are dipicted in Table 1. The cation is centrosymmetric with the center of symmetry at the mid-point of the C=C bond. Each Cu atom has a distorted tetrahedral geometry. The mean Cu—N distance of 2.049 (2) Å and Cu—P bond length of 2.1877 (9) Å are consistent with those in the case of $[Cu_2(2,2'\text{-bipyridine})_2(PPh_3)_2\ (4,4'\text{-bipyridine})]^{2+}$(PPh3 = triphenylphosphine). All bond angles are similar with its analogues, also (Chen *et al.*, 2007; Wang *et al.*, 2007).

Experimental

Triphenylphosphine, 2,2'-bipyridine and *trans*-1,2-di-4-pyridylethylene were obtained commercially. $[Cu(CH_3CN)_4]BF_4$ was prepared according to a published method (Kubas *et al.*, 1990). Solvents were distilled using standard techniques and saturated with dinitrogen before use. All reactions were performed under a nitrogen atmosphere.

Trans-1,2-di-4-pyridylethylene (18.2 mg, 0.10 mmol) and $[Cu(CH_3CN)_4]BF_4$ (63.0 mg, 0.20 mmol) in CH_2Cl_2 (30 ml) was stirred at room temperature for 2 h, then 2,2'-bipyridine (21.2 mg, 0.20 mmol) was added to above red solution. And after another 4 h, triphenylphosphine (52.4 mg, 0.2 mmol) in CH_2Cl_2 (20 ml) was added dropwise. Recrystallization by slow diffusion of diethyl ether into the resulting solution gave orange crystals suitable for X-ray diffraction (yield 84.5 mg, 64%).

Refinement

All H atoms were placed in calculated positions, The H atoms were then constrained to an ideal geometry with C—H distances of 0.93 Å, $U_{iso}(H) = 1.2U_{eq}(C)$. The fluorine atoms F3 and F4 were disordered over two sites, with site occupancy factors being refined to 0.53 (2) and 0.47 (2).

Figures

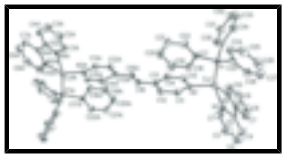


Fig. 1. The structure of the cation of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted. [symmetry code: (A) −*x* + 1, −*y*, −*z* + 1.]

(μ-*trans*-1,2-Di-4-pyridylethylene-κ^2*N*:*N*')bis[(bipyridine- κ^2*N*,*N*')(triphenylphosphine-κ*P*)copper(I)] bis(tetrafluoroborate)

Crystal data

$[Cu_2(C_{10}H_8N_2)_2(C_{12}H_{10}N_2)(C_{18}H_{15}P)_2](BF_4)_2$	F_{000} = 1352
M_r = 1319.83	D_x = 1.403 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4281 reflections
a = 9.9800 (17) Å	θ = 2.4–23.9º
b = 15.420 (3) Å	μ = 0.80 mm^{-1}
c = 20.461 (4) Å	*T* = 298 (2) K
β = 97.021 (3)º	Block, orange
V = 3125.1 (9) Å^3	0.43 × 0.33 × 0.28 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	7853 independent reflections
Radiation source: fine-focus sealed tube	5153 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 298(2) K	θ_{max} = 28.5º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	*h* = −12→11
T_{min} = 0.724, T_{max} = 0.807	*k* = −20→19
18965 measured reflections	*l* = −24→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.056	H-atom parameters constrained
$wR(F^2)$ = 0.151	$w = 1/[\sigma^2(F_o^2) + (0.08P)^2 + 0.3449P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$

7853 reflections	$\Delta\rho_{max}$ = 0.58 e Å^{-3}
417 parameters	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
24 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	0.42023 (3)	0.38370 (2)	0.344472 (16)	0.04103 (13)	
B1	0.9491 (4)	0.2631 (3)	0.4471 (2)	0.0644 (11)	
F1	1.0554 (3)	0.2971 (3)	0.48247 (17)	0.1462 (14)	
F2	0.8749 (4)	0.3173 (3)	0.4106 (3)	0.204 (2)	
F3	0.8605 (10)	0.2406 (11)	0.4895 (5)	0.111 (3)	0.53 (2)
F4	1.0069 (8)	0.1932 (6)	0.4234 (10)	0.120 (4)	0.53 (2)
F3'	0.8805 (14)	0.1996 (11)	0.4747 (8)	0.116 (4)	0.47 (2)
F4'	0.9873 (12)	0.2275 (13)	0.3889 (7)	0.121 (5)	0.47 (2)
N1	0.2699 (2)	0.46424 (17)	0.36860 (12)	0.0478 (6)	
N2	0.5345 (2)	0.47842 (16)	0.39456 (11)	0.0447 (6)	
N3	0.4329 (2)	0.27321 (15)	0.40019 (12)	0.0441 (6)	
P1	0.41005 (8)	0.33931 (5)	0.24243 (4)	0.04054 (19)	
C1	0.1367 (3)	0.4520 (3)	0.35548 (18)	0.0652 (9)	
H1	0.1056	0.3998	0.3366	0.078*	
C2	0.0443 (4)	0.5131 (4)	0.3686 (2)	0.0876 (13)	
H2	−0.0477	0.5029	0.3584	0.105*	
C3	0.0895 (5)	0.5886 (4)	0.3969 (3)	0.1018 (16)	
H3	0.0285	0.6309	0.4068	0.122*	
C4	0.2254 (5)	0.6024 (3)	0.4110 (2)	0.0830 (13)	
H4	0.2575	0.6543	0.4302	0.100*	
C5	0.3149 (3)	0.5387 (2)	0.39656 (15)	0.0491 (7)	
C6	0.4622 (3)	0.5462 (2)	0.41245 (14)	0.0492 (7)	
C7	0.5263 (5)	0.6166 (2)	0.4450 (2)	0.0747 (11)	
H7	0.4757	0.6637	0.4562	0.090*	
C8	0.6619 (5)	0.6170 (3)	0.4604 (2)	0.0888 (15)	
H8	0.7048	0.6646	0.4816	0.107*	
C9	0.7351 (4)	0.5474 (3)	0.44471 (19)	0.0795 (13)	

H9	0.8281	0.5457	0.4564	0.095*
C10	0.6687 (3)	0.4794 (3)	0.41107 (17)	0.0623 (9)
H10	0.7190	0.4323	0.3994	0.075*
C11	0.3221 (3)	0.2292 (2)	0.40972 (16)	0.0519 (8)
H11	0.2387	0.2545	0.3964	0.062*
C12	0.3244 (3)	0.1487 (2)	0.43810 (17)	0.0550 (8)
H12	0.2437	0.1211	0.4435	0.066*
C13	0.4454 (3)	0.10855 (19)	0.45863 (15)	0.0474 (7)
C14	0.5616 (3)	0.1536 (2)	0.44819 (15)	0.0514 (8)
H14	0.6462	0.1291	0.4603	0.062*
C15	0.5508 (3)	0.2342 (2)	0.41999 (15)	0.0492 (7)
H15	0.6299	0.2636	0.4142	0.059*
C16	0.4468 (3)	0.0232 (2)	0.48979 (16)	0.0530 (8)
H16	0.3635	−0.0006	0.4957	0.064*
C17	0.3409 (3)	0.22928 (19)	0.23978 (14)	0.0460 (7)
C18	0.2070 (4)	0.2191 (2)	0.24903 (19)	0.0646 (9)
H18	0.1519	0.2678	0.2486	0.077*
C19	0.1535 (4)	0.1386 (3)	0.2589 (2)	0.0800 (12)
H19	0.0632	0.1329	0.2653	0.096*
C20	0.2350 (5)	0.0670 (3)	0.2593 (2)	0.0811 (12)
H20	0.2001	0.0124	0.2666	0.097*
C21	0.3662 (4)	0.0750 (2)	0.2490 (2)	0.0769 (11)
H21	0.4200	0.0258	0.2483	0.092*
C22	0.4205 (4)	0.1564 (2)	0.23954 (18)	0.0606 (9)
H22	0.5107	0.1616	0.2330	0.073*
C23	0.2975 (3)	0.3979 (2)	0.18074 (15)	0.0475 (7)
C24	0.2294 (4)	0.3593 (3)	0.12521 (16)	0.0617 (9)
H24	0.2436	0.3010	0.1168	0.074*
C25	0.1402 (4)	0.4072 (4)	0.08217 (19)	0.0792 (12)
H25	0.0936	0.3806	0.0454	0.095*
C26	0.1208 (4)	0.4925 (4)	0.0935 (2)	0.0875 (14)
H26	0.0620	0.5245	0.0640	0.105*
C27	0.1871 (4)	0.5319 (3)	0.1479 (2)	0.0807 (12)
H27	0.1732	0.5905	0.1554	0.097*
C28	0.2744 (3)	0.4847 (2)	0.19161 (17)	0.0600 (9)
H28	0.3183	0.5116	0.2289	0.072*
C29	0.5715 (3)	0.33021 (18)	0.20944 (14)	0.0445 (7)
C30	0.6839 (3)	0.3112 (2)	0.25418 (17)	0.0606 (9)
H30	0.6738	0.3029	0.2983	0.073*
C31	0.8103 (4)	0.3045 (3)	0.2338 (2)	0.0727 (11)
H31	0.8844	0.2904	0.2641	0.087*
C32	0.8271 (4)	0.3185 (3)	0.1696 (2)	0.0765 (11)
H32	0.9124	0.3149	0.1559	0.092*
C33	0.7172 (4)	0.3377 (3)	0.1256 (2)	0.0833 (13)
H33	0.7280	0.3466	0.0816	0.100*
C34	0.5904 (4)	0.3441 (3)	0.14528 (17)	0.0631 (9)
H34	0.5169	0.3580	0.1146	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0438 (2)	0.0354 (2)	0.0437 (2)	0.00140 (14)	0.00421 (15)	−0.00142 (15)
B1	0.042 (2)	0.061 (3)	0.088 (3)	0.0003 (19)	0.001 (2)	−0.008 (2)
F1	0.0811 (19)	0.203 (4)	0.153 (3)	−0.052 (2)	0.0074 (18)	−0.076 (3)
F2	0.131 (3)	0.188 (4)	0.287 (6)	0.042 (3)	−0.001 (3)	0.116 (4)
F3	0.085 (4)	0.148 (8)	0.108 (5)	−0.037 (5)	0.037 (3)	−0.014 (5)
F4	0.102 (4)	0.099 (5)	0.158 (9)	0.021 (4)	0.012 (5)	−0.022 (5)
F3'	0.101 (6)	0.120 (7)	0.123 (7)	−0.036 (5)	0.000 (5)	0.027 (6)
F4'	0.111 (6)	0.152 (9)	0.097 (6)	−0.023 (5)	0.009 (4)	−0.037 (6)
N1	0.0456 (14)	0.0488 (15)	0.0494 (15)	0.0084 (11)	0.0072 (11)	−0.0006 (12)
N2	0.0445 (14)	0.0452 (14)	0.0441 (13)	−0.0061 (11)	0.0038 (11)	−0.0007 (11)
N3	0.0481 (14)	0.0412 (13)	0.0424 (13)	−0.0004 (11)	0.0037 (11)	0.0065 (11)
P1	0.0428 (4)	0.0375 (4)	0.0406 (4)	0.0047 (3)	0.0022 (3)	−0.0004 (3)
C1	0.049 (2)	0.074 (2)	0.072 (2)	0.0068 (17)	0.0040 (17)	−0.0035 (19)
C2	0.052 (2)	0.104 (4)	0.108 (3)	0.023 (2)	0.015 (2)	−0.002 (3)
C3	0.086 (3)	0.088 (3)	0.136 (4)	0.044 (3)	0.033 (3)	−0.001 (3)
C4	0.089 (3)	0.058 (2)	0.107 (3)	0.018 (2)	0.030 (3)	−0.008 (2)
C5	0.062 (2)	0.0404 (16)	0.0470 (17)	0.0069 (14)	0.0159 (15)	0.0042 (13)
C6	0.066 (2)	0.0432 (17)	0.0399 (16)	−0.0055 (15)	0.0138 (14)	−0.0008 (13)
C7	0.094 (3)	0.062 (2)	0.071 (3)	−0.018 (2)	0.022 (2)	−0.024 (2)
C8	0.106 (4)	0.097 (4)	0.066 (3)	−0.049 (3)	0.018 (2)	−0.033 (2)
C9	0.062 (2)	0.114 (4)	0.062 (2)	−0.036 (2)	0.0053 (19)	−0.013 (2)
C10	0.053 (2)	0.072 (2)	0.062 (2)	−0.0132 (17)	0.0058 (16)	−0.0056 (18)
C11	0.0486 (18)	0.0519 (19)	0.0562 (19)	0.0079 (14)	0.0105 (14)	0.0100 (15)
C12	0.0480 (18)	0.0500 (18)	0.068 (2)	−0.0027 (15)	0.0107 (15)	0.0139 (16)
C13	0.0574 (19)	0.0422 (17)	0.0428 (16)	0.0011 (14)	0.0073 (14)	0.0035 (13)
C14	0.0490 (18)	0.0522 (18)	0.0522 (18)	0.0082 (15)	0.0024 (14)	0.0124 (15)
C15	0.0482 (18)	0.0495 (18)	0.0486 (17)	−0.0053 (14)	0.0008 (14)	0.0083 (14)
C16	0.0541 (19)	0.0506 (19)	0.0547 (18)	0.0001 (14)	0.0085 (15)	0.0102 (15)
C17	0.0538 (18)	0.0405 (16)	0.0426 (16)	−0.0011 (13)	0.0016 (13)	−0.0049 (13)
C18	0.055 (2)	0.049 (2)	0.091 (3)	−0.0012 (16)	0.0105 (18)	−0.0096 (19)
C19	0.070 (3)	0.066 (3)	0.104 (3)	−0.023 (2)	0.013 (2)	−0.011 (2)
C20	0.107 (4)	0.046 (2)	0.088 (3)	−0.023 (2)	0.003 (2)	−0.006 (2)
C21	0.087 (3)	0.0392 (19)	0.102 (3)	0.0015 (19)	0.004 (2)	−0.008 (2)
C22	0.064 (2)	0.0415 (18)	0.076 (2)	0.0038 (16)	0.0073 (18)	−0.0062 (17)
C23	0.0440 (17)	0.0535 (19)	0.0450 (16)	0.0063 (13)	0.0050 (13)	0.0041 (14)
C24	0.059 (2)	0.073 (2)	0.0508 (19)	0.0030 (18)	−0.0007 (16)	−0.0007 (17)
C25	0.063 (2)	0.118 (4)	0.052 (2)	0.000 (2)	−0.0101 (18)	0.011 (2)
C26	0.067 (3)	0.116 (4)	0.076 (3)	0.021 (3)	−0.004 (2)	0.037 (3)
C27	0.083 (3)	0.073 (3)	0.084 (3)	0.027 (2)	0.003 (2)	0.022 (2)
C28	0.060 (2)	0.056 (2)	0.063 (2)	0.0106 (16)	0.0005 (16)	0.0099 (17)
C29	0.0479 (17)	0.0405 (16)	0.0460 (17)	0.0027 (13)	0.0092 (13)	−0.0012 (13)
C30	0.054 (2)	0.077 (2)	0.0510 (19)	0.0099 (18)	0.0080 (15)	0.0054 (17)
C31	0.049 (2)	0.094 (3)	0.074 (3)	0.0117 (19)	0.0036 (18)	−0.001 (2)
C32	0.058 (2)	0.088 (3)	0.089 (3)	0.008 (2)	0.031 (2)	0.006 (2)

C33	0.078 (3)	0.110 (4)	0.066 (3)	0.014 (3)	0.029 (2)	0.016 (2)
C34	0.063 (2)	0.076 (3)	0.052 (2)	0.0132 (18)	0.0105 (16)	0.0103 (17)

Geometric parameters (Å, °)

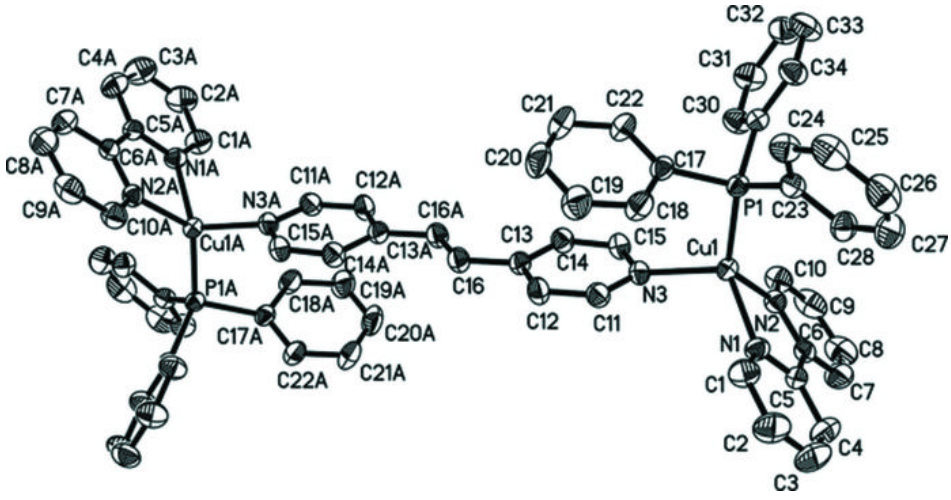
Cu1—N3	2.045 (2)	C13—C14	1.391 (4)
Cu1—N2	2.049 (2)	C13—C16	1.462 (4)
Cu1—N1	2.054 (2)	C14—C15	1.369 (4)
Cu1—P1	2.1877 (9)	C14—H14	0.9300
B1—F2	1.292 (5)	C15—H15	0.9300
B1—F1	1.318 (5)	C16—C16^{i}	1.305 (6)
B1—F4	1.340 (8)	C16—H16	0.9300
B1—F3'	1.356 (11)	C17—C22	1.377 (4)
B1—F3	1.358 (10)	C17—C18	1.381 (5)
B1—F4'	1.405 (9)	C18—C19	1.376 (5)
N1—C5	1.336 (4)	C18—H18	0.9300
N1—C1	1.337 (4)	C19—C20	1.372 (6)
N2—C10	1.341 (4)	C19—H19	0.9300
N2—C6	1.346 (4)	C20—C21	1.356 (6)
N3—C11	1.332 (4)	C20—H20	0.9300
N3—C15	1.339 (4)	C21—C22	1.391 (5)
P1—C23	1.824 (3)	C21—H21	0.9300
P1—C29	1.827 (3)	C22—H22	0.9300
P1—C17	1.830 (3)	C23—C28	1.380 (4)
C1—C2	1.368 (5)	C23—C24	1.385 (5)
C1—H1	0.9300	C24—C25	1.386 (5)
C2—C3	1.353 (7)	C24—H24	0.9300
C2—H2	0.9300	C25—C26	1.353 (6)
C3—C4	1.369 (7)	C25—H25	0.9300
C3—H3	0.9300	C26—C27	1.366 (6)
C4—C5	1.383 (5)	C26—H26	0.9300
C4—H4	0.9300	C27—C28	1.378 (5)
C5—C6	1.471 (5)	C27—H27	0.9300
C6—C7	1.388 (5)	C28—H28	0.9300
C7—C8	1.352 (6)	C29—C34	1.366 (4)
C7—H7	0.9300	C29—C30	1.390 (4)
C8—C9	1.358 (6)	C30—C31	1.380 (5)
C8—H8	0.9300	C30—H30	0.9300
C9—C10	1.379 (5)	C31—C32	1.362 (5)
C9—H9	0.9300	C31—H31	0.9300
C10—H10	0.9300	C32—C33	1.365 (6)
C11—C12	1.369 (4)	C32—H32	0.9300
C11—H11	0.9300	C33—C34	1.378 (5)
C12—C13	1.376 (4)	C33—H33	0.9300
C12—H12	0.9300	C34—H34	0.9300
N3—Cu1—N2	108.80 (10)	C11—C12—C13	120.4 (3)
N3—Cu1—N1	111.53 (10)	C11—C12—H12	119.8
N2—Cu1—N1	80.03 (10)	C13—C12—H12	119.8
N3—Cu1—P1	105.30 (7)	C12—C13—C14	116.4 (3)

N2—Cu1—P1	131.18 (7)	C12—C13—C16	120.0 (3)
N1—Cu1—P1	117.94 (7)	C14—C13—C16	123.5 (3)
F2—B1—F1	115.2 (5)	C15—C14—C13	119.6 (3)
F2—B1—F4	123.7 (9)	C15—C14—H14	120.2
F1—B1—F4	99.5 (6)	C13—C14—H14	120.2
F2—B1—F3'	115.1 (7)	N3—C15—C14	123.8 (3)
F1—B1—F3'	118.1 (7)	N3—C15—H15	118.1
F4—B1—F3'	80.3 (7)	C14—C15—H15	118.1
F2—B1—F3	99.3 (7)	C16^{i}—C16—C13	126.6 (4)
F1—B1—F3	107.1 (6)	C16^{i}—C16—H16	116.7
F4—B1—F3	111.6 (6)	C13—C16—H16	116.7
F3'—B1—F3	31.6 (6)	C22—C17—C18	118.5 (3)
F2—B1—F4'	87.7 (10)	C22—C17—P1	122.8 (3)
F1—B1—F4'	109.7 (5)	C18—C17—P1	118.0 (2)
F4—B1—F4'	37.5 (4)	C19—C18—C17	121.5 (4)
F3'—B1—F4'	105.9 (7)	C19—C18—H18	119.3
F3—B1—F4'	135.0 (6)	C17—C18—H18	119.3
C5—N1—C1	118.7 (3)	C20—C19—C18	119.1 (4)
C5—N1—Cu1	114.0 (2)	C20—C19—H19	120.5
C1—N1—Cu1	127.1 (2)	C18—C19—H19	120.5
C10—N2—C6	118.4 (3)	C21—C20—C19	120.6 (4)
C10—N2—Cu1	127.7 (2)	C21—C20—H20	119.7
C6—N2—Cu1	113.9 (2)	C19—C20—H20	119.7
C11—N3—C15	116.2 (3)	C20—C21—C22	120.2 (4)
C11—N3—Cu1	120.7 (2)	C20—C21—H21	119.9
C15—N3—Cu1	122.3 (2)	C22—C21—H21	119.9
C23—P1—C29	106.18 (14)	C17—C22—C21	120.1 (3)
C23—P1—C17	103.95 (14)	C17—C22—H22	119.9
C29—P1—C17	105.34 (14)	C21—C22—H22	119.9
C23—P1—Cu1	117.28 (10)	C28—C23—C24	118.3 (3)
C29—P1—Cu1	115.88 (10)	C28—C23—P1	118.0 (2)
C17—P1—Cu1	106.96 (10)	C24—C23—P1	123.6 (3)
N1—C1—C2	122.7 (4)	C23—C24—C25	120.3 (4)
N1—C1—H1	118.6	C23—C24—H24	119.9
C2—C1—H1	118.6	C25—C24—H24	119.9
C3—C2—C1	118.7 (4)	C26—C25—C24	120.2 (4)
C3—C2—H2	120.7	C26—C25—H25	119.9
C1—C2—H2	120.7	C24—C25—H25	119.9
C2—C3—C4	119.6 (4)	C25—C26—C27	120.4 (4)
C2—C3—H3	120.2	C25—C26—H26	119.8
C4—C3—H3	120.2	C27—C26—H26	119.8
C3—C4—C5	119.6 (4)	C26—C27—C28	119.9 (4)
C3—C4—H4	120.2	C26—C27—H27	120.0
C5—C4—H4	120.2	C28—C27—H27	120.0
N1—C5—C4	120.7 (3)	C27—C28—C23	120.8 (4)
N1—C5—C6	115.8 (3)	C27—C28—H28	119.6
C4—C5—C6	123.4 (3)	C23—C28—H28	119.6
N2—C6—C7	120.4 (3)	C34—C29—C30	118.1 (3)

N2—C6—C5	115.7 (3)	C34—C29—P1	125.1 (2)
C7—C6—C5	123.8 (3)	C30—C29—P1	116.8 (2)
C8—C7—C6	120.3 (4)	C31—C30—C29	120.8 (3)
C8—C7—H7	119.8	C31—C30—H30	119.6
C6—C7—H7	119.8	C29—C30—H30	119.6
C7—C8—C9	119.6 (4)	C32—C31—C30	120.3 (3)
C7—C8—H8	120.2	C32—C31—H31	119.9
C9—C8—H8	120.2	C30—C31—H31	119.9
C8—C9—C10	118.6 (4)	C31—C32—C33	119.2 (4)
C8—C9—H9	120.7	C31—C32—H32	120.4
C10—C9—H9	120.7	C33—C32—H32	120.4
N2—C10—C9	122.5 (4)	C32—C33—C34	121.0 (4)
N2—C10—H10	118.7	C32—C33—H33	119.5
C9—C10—H10	118.7	C34—C33—H33	119.5
N3—C11—C12	123.6 (3)	C29—C34—C33	120.7 (3)
N3—C11—H11	118.2	C29—C34—H34	119.7
C12—C11—H11	118.2	C33—C34—H34	119.7

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

Fig. 1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