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Bis[μ-bis(diphenylphosphino)methane-κ^2P:P']bis[(2,2′-bipyridine-κ^2N,N')-copper(I)] bis(tetrafluoridoborate) diethyl ether disolvate

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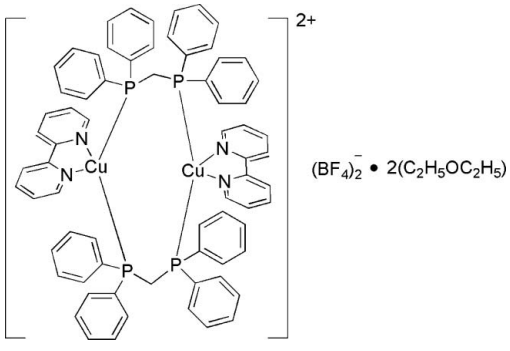
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.008 Å; disorder in solvent or counterion; R factor = 0.045; wR factor = 0.132; data-to-parameter ratio = 12.4.

The dinuclear cation of the title complex, $[Cu_2(C_{25}H_{22}P_2)_2(C_{10}H_8N_2)_2](BF_4)_2{\cdot}2C_4H_{10}O$, lies on a centre of inversion. Each Cu^I atom is coordinated by 2,2′-bipyridine (bpy) and bis(diphenylphosphino)methane (dppm) ligands, and has a distorted tetrahedral coordination geometry. The distance between the two Cu^I atoms separated by two dppm bridging ligands is 4.671 (3) Å. The solvent molecule and anion are each disordered over two positions; the site occupancy factor ratios are *ca* 0.56:0.44 and 0.6:0.4, respectively

Related literature

For related literature, see: Che *et al.* (2000); Harvey *et al.* (1997); Ho & Bau (1983); King *et al.* (1989); Pan *et al.* (2006); Perreault *et al.* (1992); Pyykkö & Mendizabal (1998); Ryu *et al.* (1993).



Experimental

Crystal data

$[Cu_2(C_{25}H_{22}P_2)_2(C_{10}H_8N_2)_2](BF_4)_2{\cdot}2C_4H_{10}O$
M_r = 1530.09
Monoclinic, $P2_1/n$
a = 14.942 (5) Å
b = 13.432 (4) Å
c = 19.734 (6) Å
β = 108.970 (6)°
V = 3746 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 294 (2) K
0.22 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.857, T_{max} = 0.895
19160 measured reflections
6602 independent reflections
4337 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.132
S = 1.04
6602 reflections
534 parameters
60 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.080 (3)	Cu1—P2^i	2.2268 (12)
Cu1—N2	2.109 (3)	Cu1—P1	2.2720 (12)
N1—Cu1—N2	78.56 (14)	P2^i—Cu1—P1	133.33 (4)

Symmetry code: (i) $-x+2, -y+1, -z$.

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: *XP* (Sheldrick, 1998); software used to prepare material for publication: *SHELXL97* and *XP*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2248).

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supplementary materials

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Bis[μ-bis(diphenylphosphino)methane-κ^2P:P']bis[(2,2'-bipyridine-κ^2N,N')copper(I)] bis(tetrafluoridoborate) diethyl ether disolvate

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Comment

d^{10} polynuclear copper complexes generally exhibit rich luminescence and recently have attracted much attention on both a theoretical and a spectroscopic level (Pan *et al.*, 2006; Pyykkö & Mendizabal, 1998; Ryu *et al.*, 1993). A series of luminescent dinuclear d^{10} complexes with bridging phosphane ligands have been studied (Harvey *et al.*, 1997; King *et al.*, 1989; Perreault *et al.*, 1992; Che *et al.*, 2000). Here, we report crystal structure of $[Cu_2(dppm)_2(bpy)_2](BF_4)_2{\cdot}2C_4H_{10}O$, (I).

The Cu atom in (I) (Fig. 1) has a distorted tetrahedral coordination geometry involving two N atoms of 2,2'-bipyridine ligand and two P atoms of two (diphenylphosphino)methane ligand. The Cu—N bond lengths are 2.080 (3) and 2.109 (3) Å, while the Cu—P bonds are 2.272 (1) and 2.227 (1)Å [$2-x$, $1-y$, $-z$](Table 1). The two Cu^I ions in (I) are doubly bridged by two (diphenylphosphino)methane ligands. There are no Cu—Cu bonds, as the measured distance ($r_{Cu\cdots Cu}$ = 4.471 (3) Å) is greater than the sum of the van der Waals radii (r_{vdW}(Cu) = 1.40 Å).

Experimental

A 10 ml me thanolic solution of 2,2'-bipyridine (0.078 g, 0.5 mmol, *i.e.* large excess) was added to a 20 mL me thanolic suspension of $[Cu_3(dppm)_3(OH)](BF_4)_2$ (0.0767 g, 0.05 mmol) (Ho & Bau, 1983) under N_2 atmosphere. The mixture was stirred for 2 days. The filtrate was kept in diethyl ether atmosphere for two weeks, yellow crystals suitable for X-ray diffraction were formed.

Refinement

All hydrogen atoms were generated geometrically (C—H bond lengths fixed at 0.93 Å), assigned appropriated isotropic thermal parameters, U_{iso}(H) = 1.2U_{eq}(C). The $(BF_4)^-$ anions are disordered, F—B distances were restrained to 1.36 (1) Å. The ethyl ether molecules are disordered over two sites, the C···O and C···C distances were restrained to ensure a reasonable geometry.

Figures

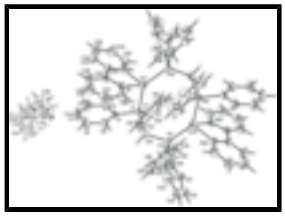


Fig. 1. Molecular structure of the title compound showing the atom-numbering scheme and displacement ellipsoids drawn at the 40% probability level. The symmetry code for the unlabelled atoms is ($2-x$, $1-y$, $-z$). Free $(BF_4)^-$ anions are not shown.

Bis[μ-bis(diphenylphosphino)methane-κ^{2}P:P'] bis[(2,2'-bipyridine-κ^{2}N,N')copper(I)] bis(tetrafluoridoborate) diethyl ether disolvate

Crystal data

$[Cu_2(C_{25}H_{22}P_2)_2(C_{10}H_8N_2)_2](BF_4)_2{\cdot}2C_4H_{10}O$	F_{000} = 1584
M_r = 1530.09	D_x = 1.357 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2605 reflections
a = 14.942 (5) Å	θ = 3.0–26.4º
b = 13.432 (4) Å	μ = 0.72 mm^{-1}
c = 19.734 (6) Å	T = 294 (2) K
β = 108.970 (6)º	Block, yellow
V = 3746 (2) Å^3	0.22 × 0.18 × 0.16 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	6602 independent reflections
Radiation source: fine-focus sealed tube	4337 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −17→17
T_{min} = 0.857, T_{max} = 0.895	k = −15→15
19160 measured reflections	l = −23→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.132	$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 2.5517P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.002
6602 reflections	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
534 parameters	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
60 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	0.89350 (3)	0.40826 (4)	0.03928 (2)	0.04066 (16)	
P1	1.03081 (7)	0.45536 (8)	0.12368 (5)	0.0379 (2)	
P2	1.14667 (7)	0.62233 (7)	0.07772 (5)	0.0375 (2)	
N1	0.7958 (2)	0.4649 (3)	0.08405 (17)	0.0475 (8)	
N2	0.8587 (2)	0.2798 (3)	0.08685 (16)	0.0490 (8)	
C1	1.0103 (3)	0.4376 (3)	0.20948 (19)	0.0435 (10)	
C2	1.0196 (3)	0.3430 (4)	0.2392 (2)	0.0608 (12)	
H2	1.0435	0.2915	0.2186	0.073*	
C3	0.9941 (4)	0.3247 (5)	0.2986 (3)	0.0835 (17)	
H3	1.0008	0.2610	0.3180	0.100*	
C4	0.9592 (5)	0.3989 (6)	0.3295 (3)	0.102 (2)	
H4	0.9422	0.3861	0.3700	0.122*	
C5	0.9491 (4)	0.4928 (5)	0.3008 (3)	0.0912 (18)	
H5	0.9249	0.5435	0.3218	0.109*	
C6	0.9749 (3)	0.5131 (4)	0.2402 (2)	0.0611 (12)	
H6	0.9681	0.5769	0.2209	0.073*	
C7	1.1341 (3)	0.3783 (3)	0.1327 (2)	0.0433 (9)	
C8	1.1349 (3)	0.3209 (3)	0.0746 (2)	0.0602 (12)	
H8	1.0836	0.3226	0.0325	0.072*	
C9	1.2120 (4)	0.2610 (4)	0.0791 (3)	0.0836 (16)	
H9	1.2126	0.2226	0.0400	0.100*	
C10	1.2877 (4)	0.2588 (4)	0.1416 (4)	0.0833 (16)	
H10	1.3396	0.2186	0.1446	0.100*	
C11	1.2874 (3)	0.3146 (4)	0.1988 (3)	0.0683 (14)	
H11	1.3391	0.3126	0.2407	0.082*	
C12	1.2114 (3)	0.3739 (3)	0.1953 (2)	0.0522 (11)	
H12	1.2115	0.4115	0.2349	0.063*	
C13	1.0725 (3)	0.5853 (3)	0.13178 (19)	0.0419 (9)	
H13A	1.0174	0.6285	0.1191	0.050*	
H13B	1.1079	0.5978	0.1817	0.050*	
C14	1.2651 (3)	0.5858 (3)	0.1340 (2)	0.0412 (9)	
C15	1.3211 (3)	0.5318 (4)	0.1053 (2)	0.0602 (12)	
H15	1.2986	0.5141	0.0572	0.072*	

C16	1.4115 (3)	0.5026 (4)	0.1473 (3)	0.0801 (16)	
H16	1.4490	0.4651	0.1275	0.096*	
C17	1.4449 (4)	0.5295 (4)	0.2179 (3)	0.0793 (16)	
H17	1.5051	0.5100	0.2461	0.095*	
C18	1.3902 (3)	0.5849 (4)	0.2470 (3)	0.0691 (14)	
H18	1.4137	0.6037	0.2949	0.083*	
C19	1.3001 (3)	0.6131 (3)	0.2056 (2)	0.0569 (11)	
H19	1.2628	0.6504	0.2258	0.068*	
C20	1.1524 (3)	0.7576 (3)	0.08989 (19)	0.0441 (10)	
C21	1.2357 (3)	0.8070 (3)	0.0957 (2)	0.0610 (12)	
H21	1.2891	0.7704	0.0972	0.073*	
C22	1.2411 (4)	0.9089 (4)	0.0993 (3)	0.0800 (16)	
H22	1.2980	0.9410	0.1039	0.096*	
C23	1.1627 (6)	0.9626 (4)	0.0960 (3)	0.099 (2)	
H23	1.1659	1.0317	0.0978	0.118*	
C24	1.0790 (5)	0.9161 (4)	0.0902 (3)	0.0911 (18)	
H24	1.0258	0.9535	0.0882	0.109*	
C25	1.0738 (4)	0.8137 (3)	0.0875 (3)	0.0640 (13)	
H25	1.0170	0.7822	0.0840	0.077*	
C26	0.7694 (3)	0.5600 (4)	0.0828 (2)	0.0627 (12)	
H26	0.7902	0.6048	0.0552	0.075*	
C27	0.7126 (4)	0.5950 (5)	0.1205 (3)	0.0807 (16)	
H27	0.6944	0.6615	0.1180	0.097*	
C28	0.6842 (4)	0.5284 (6)	0.1613 (3)	0.094 (2)	
H28	0.6459	0.5495	0.1874	0.113*	
C29	0.7113 (4)	0.4309 (5)	0.1644 (3)	0.0818 (17)	
H29	0.6925	0.3859	0.1930	0.098*	
C30	0.7671 (3)	0.4002 (4)	0.1244 (2)	0.0553 (12)	
C31	0.7986 (3)	0.2970 (4)	0.1233 (2)	0.0541 (11)	
C32	0.7680 (4)	0.2190 (5)	0.1572 (3)	0.0801 (16)	
H32	0.7270	0.2310	0.1831	0.096*	
C33	0.7994 (4)	0.1252 (5)	0.1518 (3)	0.0911 (19)	
H33	0.7784	0.0724	0.1732	0.109*	
C34	0.8606 (4)	0.1078 (4)	0.1155 (3)	0.0785 (16)	
H34	0.8828	0.0439	0.1122	0.094*	
C35	0.8889 (3)	0.1871 (3)	0.0839 (2)	0.0601 (12)	
H35	0.9312	0.1757	0.0590	0.072*	
B1	0.3873 (4)	0.7013 (4)	0.6889 (4)	0.104 (3)	
F1	0.4849 (4)	0.7197 (6)	0.7232 (5)	0.147 (4)	0.610 (11)
F2	0.3676 (7)	0.7312 (8)	0.6190 (4)	0.122 (3)	0.610 (11)
F3	0.3700 (6)	0.6049 (4)	0.6941 (4)	0.112 (3)	0.610 (11)
F4	0.3431 (5)	0.7569 (5)	0.7258 (3)	0.105 (3)	0.610 (11)
F1'	0.3974 (9)	0.7667 (8)	0.6416 (7)	0.097 (4)	0.390 (11)
F2'	0.2924 (7)	0.6907 (12)	0.6820 (9)	0.178 (7)	0.390 (11)
F3'	0.4112 (11)	0.6097 (7)	0.6678 (8)	0.145 (6)	0.390 (11)
F4'	0.4378 (13)	0.7177 (14)	0.7567 (6)	0.250 (11)	0.390 (11)
O1	0.9395 (6)	0.3004 (6)	0.4884 (4)	0.111 (4)	0.565 (13)
C36	0.8268 (11)	0.4325 (12)	0.4737 (10)	0.154 (7)	0.565 (13)
H36A	0.8128	0.4911	0.4963	0.231*	0.565 (13)

H36B	0.7763	0.3853	0.4663	0.231*	0.565 (13)
H36C	0.8334	0.4501	0.4284	0.231*	0.565 (13)
C37	0.9196 (10)	0.3860 (10)	0.5220 (8)	0.132 (6)	0.565 (13)
H37A	0.9709	0.4336	0.5302	0.158*	0.565 (13)
H37B	0.9136	0.3684	0.5680	0.158*	0.565 (13)
C38	1.0271 (10)	0.2522 (11)	0.5241 (11)	0.174 (9)	0.565 (13)
H38A	1.0383	0.2524	0.5753	0.208*	0.565 (13)
H38B	1.0783	0.2884	0.5151	0.208*	0.565 (13)
C39	1.0260 (11)	0.1472 (10)	0.4984 (10)	0.140 (7)	0.565 (13)
H39A	1.0853	0.1158	0.5234	0.210*	0.565 (13)
H39B	1.0166	0.1472	0.4479	0.210*	0.565 (13)
H39C	0.9755	0.1113	0.5075	0.210*	0.565 (13)
O1'	0.9797 (12)	0.3255 (13)	0.5339 (14)	0.282 (14)	0.435 (13)
C36'	0.878 (2)	0.4681 (16)	0.486 (2)	0.26 (2)	0.435 (13)
H36D	0.8131	0.4894	0.4724	0.388*	0.435 (13)
H36E	0.9017	0.4773	0.4472	0.388*	0.435 (13)
H36F	0.9149	0.5066	0.5268	0.388*	0.435 (13)
C37'	0.8839 (11)	0.3579 (14)	0.5071 (14)	0.132 (9)	0.435 (13)
H37C	0.8539	0.3476	0.5433	0.159*	0.435 (13)
H37D	0.8501	0.3185	0.4654	0.159*	0.435 (13)
C38'	0.9885 (14)	0.2185 (13)	0.5302 (11)	0.136 (9)	0.435 (13)
H38C	0.9265	0.1892	0.5082	0.163*	0.435 (13)
H38D	1.0148	0.1916	0.5782	0.163*	0.435 (13)
C39'	1.0519 (12)	0.1928 (14)	0.4870 (8)	0.095 (6)	0.435 (13)
H39D	1.0608	0.1220	0.4874	0.142*	0.435 (13)
H39E	1.1120	0.2250	0.5075	0.142*	0.435 (13)
H39F	1.0232	0.2151	0.4385	0.142*	0.435 (13)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0417 (3)	0.0494 (3)	0.0327 (3)	−0.0030 (2)	0.0147 (2)	0.0003 (2)
P1	0.0407 (5)	0.0450 (6)	0.0298 (5)	−0.0031 (4)	0.0139 (4)	0.0015 (4)
P2	0.0400 (5)	0.0418 (6)	0.0323 (5)	−0.0020 (4)	0.0139 (4)	0.0004 (4)
N1	0.0436 (18)	0.059 (2)	0.0419 (19)	−0.0036 (17)	0.0164 (16)	−0.0069 (16)
N2	0.054 (2)	0.056 (2)	0.0365 (18)	−0.0080 (17)	0.0140 (16)	0.0053 (16)
C1	0.042 (2)	0.062 (3)	0.0276 (19)	−0.0058 (19)	0.0123 (17)	0.0022 (18)
C2	0.065 (3)	0.077 (3)	0.042 (2)	−0.006 (2)	0.019 (2)	0.017 (2)
C3	0.095 (4)	0.102 (5)	0.056 (3)	−0.007 (3)	0.029 (3)	0.028 (3)
C4	0.117 (5)	0.149 (7)	0.057 (3)	−0.011 (5)	0.052 (4)	0.027 (4)
C5	0.101 (4)	0.130 (6)	0.060 (3)	0.003 (4)	0.049 (3)	−0.013 (4)
C6	0.066 (3)	0.079 (3)	0.044 (2)	0.000 (2)	0.026 (2)	0.000 (2)
C7	0.047 (2)	0.042 (2)	0.045 (2)	−0.0052 (18)	0.0205 (19)	0.0032 (18)
C8	0.061 (3)	0.064 (3)	0.057 (3)	0.006 (2)	0.021 (2)	−0.005 (2)
C9	0.093 (4)	0.072 (4)	0.095 (4)	0.019 (3)	0.043 (4)	−0.014 (3)
C10	0.071 (4)	0.071 (4)	0.117 (5)	0.026 (3)	0.042 (4)	0.019 (3)
C11	0.056 (3)	0.076 (4)	0.070 (3)	0.010 (3)	0.016 (3)	0.028 (3)
C12	0.049 (2)	0.061 (3)	0.046 (2)	0.000 (2)	0.013 (2)	0.013 (2)

C13	0.049 (2)	0.045 (2)	0.037 (2)	−0.0013 (18)	0.0205 (18)	−0.0009 (17)
C14	0.041 (2)	0.043 (2)	0.039 (2)	−0.0022 (18)	0.0124 (17)	0.0020 (18)
C15	0.046 (2)	0.077 (3)	0.053 (3)	0.002 (2)	0.010 (2)	−0.001 (2)
C16	0.052 (3)	0.099 (4)	0.085 (4)	0.015 (3)	0.016 (3)	0.001 (3)
C17	0.050 (3)	0.088 (4)	0.080 (4)	−0.002 (3)	−0.006 (3)	0.016 (3)
C18	0.064 (3)	0.075 (3)	0.049 (3)	−0.013 (3)	−0.008 (2)	0.010 (2)
C19	0.064 (3)	0.057 (3)	0.046 (2)	−0.008 (2)	0.012 (2)	−0.005 (2)
C20	0.060 (3)	0.043 (2)	0.033 (2)	−0.004 (2)	0.0193 (19)	−0.0005 (17)
C21	0.069 (3)	0.053 (3)	0.059 (3)	−0.016 (2)	0.018 (2)	0.006 (2)
C22	0.102 (4)	0.058 (3)	0.082 (4)	−0.030 (3)	0.031 (3)	−0.001 (3)
C23	0.168 (7)	0.046 (3)	0.101 (5)	−0.016 (4)	0.070 (5)	−0.001 (3)
C24	0.131 (5)	0.052 (3)	0.113 (5)	0.017 (3)	0.072 (4)	−0.001 (3)
C25	0.086 (3)	0.047 (3)	0.074 (3)	0.002 (2)	0.046 (3)	−0.004 (2)
C26	0.052 (3)	0.074 (4)	0.060 (3)	−0.003 (2)	0.015 (2)	−0.018 (2)
C27	0.064 (3)	0.092 (4)	0.090 (4)	0.004 (3)	0.029 (3)	−0.035 (3)
C28	0.063 (3)	0.139 (6)	0.094 (4)	−0.004 (4)	0.042 (3)	−0.046 (4)
C29	0.061 (3)	0.124 (5)	0.073 (3)	−0.019 (3)	0.040 (3)	−0.017 (3)
C30	0.040 (2)	0.089 (4)	0.039 (2)	−0.015 (2)	0.0163 (19)	−0.009 (2)
C31	0.046 (2)	0.076 (3)	0.040 (2)	−0.016 (2)	0.014 (2)	0.006 (2)
C32	0.068 (3)	0.107 (5)	0.071 (3)	−0.015 (3)	0.031 (3)	0.020 (3)
C33	0.089 (4)	0.090 (5)	0.091 (4)	−0.023 (4)	0.023 (4)	0.035 (4)
C34	0.090 (4)	0.063 (3)	0.072 (3)	0.000 (3)	0.013 (3)	0.025 (3)
C35	0.068 (3)	0.060 (3)	0.048 (3)	−0.001 (2)	0.012 (2)	0.012 (2)
B1	0.094 (6)	0.087 (6)	0.145 (8)	0.034 (5)	0.057 (6)	0.046 (6)
F1	0.103 (5)	0.167 (6)	0.176 (7)	−0.011 (4)	0.051 (5)	−0.010 (5)
F2	0.131 (7)	0.137 (7)	0.113 (5)	0.028 (5)	0.057 (5)	0.022 (5)
F3	0.136 (6)	0.061 (4)	0.147 (6)	−0.006 (3)	0.055 (4)	0.009 (3)
F4	0.133 (6)	0.105 (5)	0.108 (5)	0.040 (4)	0.080 (4)	0.024 (3)
F1'	0.097 (7)	0.072 (6)	0.142 (9)	−0.001 (5)	0.067 (6)	0.023 (6)
F2'	0.161 (9)	0.189 (11)	0.207 (11)	−0.017 (8)	0.093 (8)	0.043 (8)
F3'	0.169 (9)	0.090 (7)	0.180 (10)	0.013 (6)	0.063 (7)	0.009 (6)
F4'	0.261 (14)	0.261 (14)	0.235 (13)	−0.019 (10)	0.092 (9)	−0.018 (9)
O1	0.116 (6)	0.120 (7)	0.077 (5)	0.026 (5)	0.003 (4)	0.013 (4)
C36	0.161 (10)	0.152 (10)	0.162 (10)	0.022 (8)	0.070 (8)	−0.010 (8)
C37	0.140 (10)	0.135 (10)	0.108 (9)	−0.039 (8)	0.024 (8)	0.009 (8)
C38	0.168 (12)	0.172 (12)	0.168 (11)	0.004 (9)	0.036 (9)	0.006 (9)
C39	0.128 (10)	0.150 (10)	0.133 (10)	0.013 (8)	0.030 (7)	0.011 (8)
O1'	0.281 (16)	0.279 (16)	0.283 (17)	0.025 (10)	0.088 (10)	−0.028 (10)
C36'	0.25 (2)	0.27 (2)	0.25 (2)	0.008 (10)	0.092 (12)	−0.009 (10)
C37'	0.127 (12)	0.173 (13)	0.112 (11)	−0.034 (9)	0.060 (9)	−0.001 (9)
C38'	0.139 (11)	0.124 (12)	0.133 (11)	−0.022 (9)	0.030 (9)	0.014 (8)
C39'	0.099 (9)	0.087 (9)	0.084 (8)	0.015 (7)	0.009 (7)	0.017 (7)

Geometric parameters (Å, °)

Cu1—N1	2.080 (3)	C23—H23	0.9300
Cu1—N2	2.109 (3)	C24—C25	1.377 (7)
Cu1—P2^{i}	2.2268 (12)	C24—H24	0.9300
Cu1—P1	2.2720 (12)	C25—H25	0.9300

P1—C7	1.819 (4)	C26—C27	1.380 (7)
P1—C1	1.831 (4)	C26—H26	0.9300
P1—C13	1.843 (4)	C27—C28	1.361 (8)
P2—C14	1.824 (4)	C27—H27	0.9300
P2—C20	1.831 (4)	C28—C29	1.366 (8)
P2—C13	1.839 (4)	C28—H28	0.9300
P2—Cu1^{i}	2.2267 (12)	C29—C30	1.385 (6)
N1—C26	1.335 (6)	C29—H29	0.9300
N1—C30	1.340 (5)	C30—C31	1.467 (6)
N2—C35	1.331 (5)	C31—C32	1.398 (6)
N2—C31	1.340 (5)	C32—C33	1.361 (8)
C1—C6	1.372 (6)	C32—H32	0.9300
C1—C2	1.387 (6)	C33—C34	1.353 (8)
C2—C3	1.367 (6)	C33—H33	0.9300
C2—H2	0.9300	C34—C35	1.370 (6)
C3—C4	1.357 (8)	C34—H34	0.9300
C3—H3	0.9300	C35—H35	0.9300
C4—C5	1.371 (8)	B1—F4'	1.324 (9)
C4—H4	0.9300	B1—F1'	1.325 (9)
C5—C6	1.397 (6)	B1—F3	1.331 (7)
C5—H5	0.9300	B1—F4	1.356 (7)
C6—H6	0.9300	B1—F2	1.374 (8)
C7—C8	1.385 (6)	B1—F3'	1.383 (9)
C7—C12	1.391 (5)	B1—F2'	1.388 (9)
C8—C9	1.383 (6)	B1—F1	1.416 (7)
C8—H8	0.9300	O1—C37	1.408 (9)
C9—C10	1.377 (7)	O1—C38	1.425 (9)
C9—H9	0.9300	C36—C37	1.537 (9)
C10—C11	1.357 (7)	C36—H36A	0.9600
C10—H10	0.9300	C36—H36B	0.9600
C11—C12	1.370 (6)	C36—H36C	0.9600
C11—H11	0.9300	C37—H37A	0.9700
C12—H12	0.9300	C37—H37B	0.9700
C13—H13A	0.9700	C38—C39	1.497 (10)
C13—H13B	0.9700	C38—H38A	0.9700
C14—C15	1.361 (6)	C38—H38B	0.9700
C14—C19	1.388 (5)	C39—H39A	0.9600
C15—C16	1.392 (6)	C39—H39B	0.9600
C15—H15	0.9300	C39—H39C	0.9600
C16—C17	1.366 (7)	O1'—C37'	1.424 (10)
C16—H16	0.9300	O1'—C38'	1.446 (10)
C17—C18	1.361 (7)	C36'—C37'	1.530 (10)
C17—H17	0.9300	C36'—H36D	0.9600
C18—C19	1.382 (6)	C36'—H36E	0.9600
C18—H18	0.9300	C36'—H36F	0.9600
C19—H19	0.9300	C37'—H37C	0.9700
C20—C21	1.382 (6)	C37'—H37D	0.9700
C20—C25	1.384 (6)	C38'—C39'	1.507 (10)
C21—C22	1.372 (7)	C38'—H38C	0.9700

C21—H21	0.9300	C38'—H38D	0.9700
C22—C23	1.360 (8)	C39'—H39D	0.9600
C22—H22	0.9300	C39'—H39E	0.9600
C23—C24	1.369 (8)	C39'—H39F	0.9600
N1—Cu1—N2	78.56 (14)	C28—C27—C26	117.3 (6)
N1—Cu1—P2^{i}	121.20 (9)	C28—C27—H27	121.3
N2—Cu1—P2^{i}	106.75 (9)	C26—C27—H27	121.3
N1—Cu1—P1	100.25 (9)	C27—C28—C29	120.9 (5)
N2—Cu1—P1	101.31 (9)	C27—C28—H28	119.6
P2^{i}—Cu1—P1	133.33 (4)	C29—C28—H28	119.6
C7—P1—C1	103.12 (18)	C28—C29—C30	118.9 (6)
C7—P1—C13	106.19 (17)	C28—C29—H29	120.5
C1—P1—C13	101.34 (18)	C30—C29—H29	120.5
C7—P1—Cu1	116.65 (13)	N1—C30—C29	121.0 (5)
C1—P1—Cu1	105.00 (12)	N1—C30—C31	115.9 (4)
C13—P1—Cu1	121.76 (13)	C29—C30—C31	123.1 (5)
C14—P2—C20	101.10 (18)	N2—C31—C32	120.5 (5)
C14—P2—C13	102.87 (18)	N2—C31—C30	116.5 (4)
C20—P2—C13	101.71 (17)	C32—C31—C30	123.0 (4)
C14—P2—Cu1^{i}	117.56 (13)	C33—C32—C31	118.8 (5)
C20—P2—Cu1^{i}	107.72 (12)	C33—C32—H32	120.6
C13—P2—Cu1^{i}	122.78 (13)	C31—C32—H32	120.6
C26—N1—C30	118.8 (4)	C34—C33—C32	120.8 (5)
C26—N1—Cu1	125.9 (3)	C34—C33—H33	119.6
C30—N1—Cu1	114.8 (3)	C32—C33—H33	119.6
C35—N2—C31	118.7 (4)	C33—C34—C35	117.9 (5)
C35—N2—Cu1	127.5 (3)	C33—C34—H34	121.0
C31—N2—Cu1	113.7 (3)	C35—C34—H34	121.0
C6—C1—C2	119.3 (4)	N2—C35—C34	123.2 (5)
C6—C1—P1	121.1 (3)	N2—C35—H35	118.4
C2—C1—P1	119.1 (3)	C34—C35—H35	118.4
C3—C2—C1	120.6 (5)	F4'—B1—F1'	116.4 (9)
C3—C2—H2	119.7	F4'—B1—F3	98.3 (10)
C1—C2—H2	119.7	F1'—B1—F3	140.2 (8)
C4—C3—C2	120.5 (5)	F4'—B1—F4	65.3 (9)
C4—C3—H3	119.8	F1'—B1—F4	101.6 (7)
C2—C3—H3	119.8	F3—B1—F4	110.7 (6)
C3—C4—C5	119.8 (5)	F4'—B1—F2	146.4 (10)
C3—C4—H4	120.1	F1'—B1—F2	30.1 (6)
C5—C4—H4	120.1	F3—B1—F2	112.2 (7)
C4—C5—C6	120.6 (6)	F4—B1—F2	113.3 (6)
C4—C5—H5	119.7	F4'—B1—F3'	109.5 (9)
C6—C5—H5	119.7	F1'—B1—F3'	106.2 (8)
C1—C6—C5	119.2 (5)	F3—B1—F3'	39.9 (6)
C1—C6—H6	120.4	F4—B1—F3'	150.5 (8)
C5—C6—H6	120.4	F2—B1—F3'	87.1 (8)
C8—C7—C12	118.9 (4)	F4'—B1—F2'	110.1 (9)

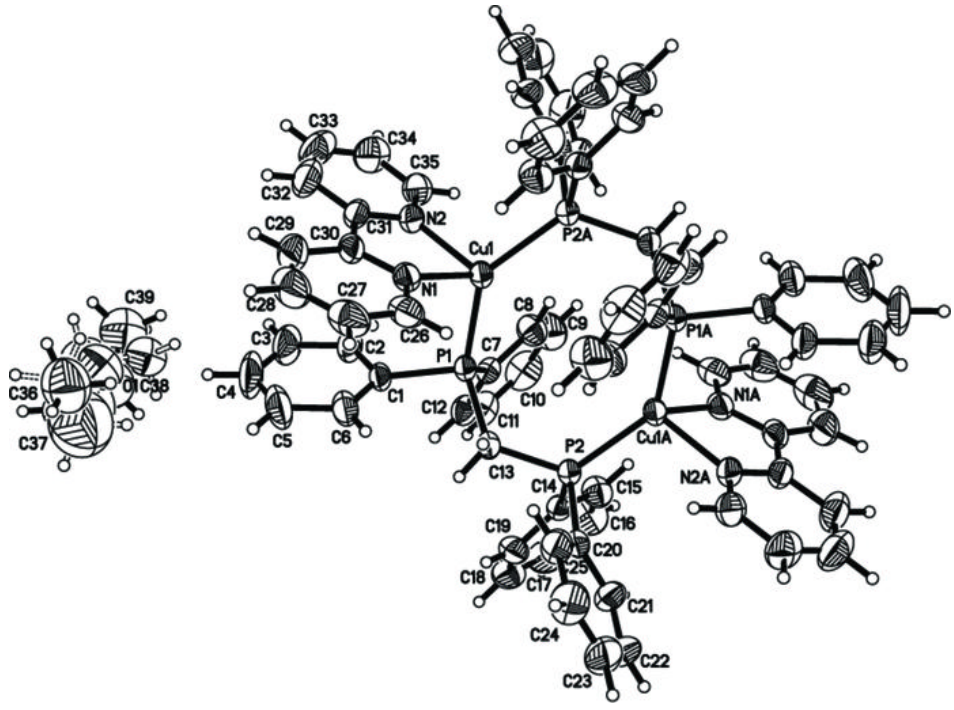
C8—C7—P1	118.1 (3)	F1'—B1—F2'	110.2 (8)
C12—C7—P1	122.9 (3)	F3—B1—F2'	71.9 (7)
C9—C8—C7	120.1 (5)	F4—B1—F2'	56.5 (7)
C9—C8—H8	119.9	F2—B1—F2'	93.0 (8)
C7—C8—H8	119.9	F3'—B1—F2'	103.5 (8)
C10—C9—C8	119.6 (5)	F4'—B1—F1	47.8 (8)
C10—C9—H9	120.2	F1'—B1—F1	83.5 (7)
C8—C9—H9	120.2	F3—B1—F1	109.2 (6)
C11—C10—C9	120.6 (5)	F4—B1—F1	104.6 (6)
C11—C10—H10	119.7	F2—B1—F1	106.3 (7)
C9—C10—H10	119.7	F3'—B1—F1	88.5 (7)
C10—C11—C12	120.4 (5)	F2'—B1—F1	157.8 (9)
C10—C11—H11	119.8	C37—O1—C38	116.0 (8)
C12—C11—H11	119.8	C37—C36—H36A	109.5
C11—C12—C7	120.3 (4)	C37—C36—H36B	109.5
C11—C12—H12	119.8	H36A—C36—H36B	109.5
C7—C12—H12	119.8	C37—C36—H36C	109.5
P2—C13—P1	117.1 (2)	H36A—C36—H36C	109.5
P2—C13—H13A	108.0	H36B—C36—H36C	109.5
P1—C13—H13A	108.0	O1—C37—C36	109.0 (9)
P2—C13—H13B	108.0	O1—C37—H37A	109.9
P1—C13—H13B	108.0	C36—C37—H37A	109.9
H13A—C13—H13B	107.3	O1—C37—H37B	109.9
C15—C14—C19	119.0 (4)	C36—C37—H37B	109.9
C15—C14—P2	119.7 (3)	H37A—C37—H37B	108.3
C19—C14—P2	121.3 (3)	O1—C38—C39	110.7 (9)
C14—C15—C16	120.7 (4)	O1—C38—H38A	109.5
C14—C15—H15	119.6	C39—C38—H38A	109.5
C16—C15—H15	119.6	O1—C38—H38B	109.5
C17—C16—C15	119.6 (5)	C39—C38—H38B	109.5
C17—C16—H16	120.2	H38A—C38—H38B	108.1
C15—C16—H16	120.2	C38—C39—H39A	109.5
C18—C17—C16	120.3 (5)	C38—C39—H39B	109.5
C18—C17—H17	119.8	H39A—C39—H39B	109.5
C16—C17—H17	119.8	C38—C39—H39C	109.5
C17—C18—C19	120.2 (5)	H39A—C39—H39C	109.5
C17—C18—H18	119.9	H39B—C39—H39C	109.5
C19—C18—H18	119.9	C37'—O1'—C38'	112.4 (11)
C18—C19—C14	120.1 (5)	C37'—C36'—H36D	109.5
C18—C19—H19	119.9	C37'—C36'—H36E	109.5
C14—C19—H19	119.9	H36D—C36'—H36E	109.5
C21—C20—C25	118.2 (4)	C37'—C36'—H36F	109.5
C21—C20—P2	119.3 (3)	H36D—C36'—H36F	109.5
C25—C20—P2	122.3 (3)	H36E—C36'—H36F	109.5
C22—C21—C20	121.4 (5)	O1'—C37'—C36'	111.1 (11)
C22—C21—H21	119.3	O1'—C37'—H37C	109.4
C20—C21—H21	119.3	C36'—C37'—H37C	109.4
C23—C22—C21	119.3 (5)	O1'—C37'—H37D	109.4
C23—C22—H22	120.3	C36'—C37'—H37D	109.4

C21—C22—H22	120.3	H37C—C37'—H37D	108.0
C22—C23—C24	120.8 (5)	O1'—C38'—C39'	109.8 (10)
C22—C23—H23	119.6	O1'—C38'—H38C	109.7
C24—C23—H23	119.6	C39'—C38'—H38C	109.7
C23—C24—C25	119.8 (6)	O1'—C38'—H38D	109.7
C23—C24—H24	120.1	C39'—C38'—H38D	109.7
C25—C24—H24	120.1	H38C—C38'—H38D	108.2
C24—C25—C20	120.4 (5)	C38'—C39'—H39D	109.5
C24—C25—H25	119.8	C38'—C39'—H39E	109.5
C20—C25—H25	119.8	H39D—C39'—H39E	109.5
N1—C26—C27	123.1 (5)	C38'—C39'—H39F	109.5
N1—C26—H26	118.5	H39D—C39'—H39F	109.5
C27—C26—H26	118.5	H39E—C39'—H39F	109.5
N1—Cu1—P1—C7	152.08 (17)	Cu1^{i}—P2—C14—C15	−7.4 (4)
N2—Cu1—P1—C7	71.83 (17)	C20—P2—C14—C19	55.0 (4)
P2^{i}—Cu1—P1—C7	−54.52 (15)	C13—P2—C14—C19	−49.9 (4)
N1—Cu1—P1—C1	38.66 (18)	Cu1^{i}—P2—C14—C19	171.9 (3)
N2—Cu1—P1—C1	−41.59 (18)	C19—C14—C15—C16	1.1 (7)
P2^{i}—Cu1—P1—C1	−167.94 (15)	P2—C14—C15—C16	−179.7 (4)
N1—Cu1—P1—C13	−75.26 (17)	C14—C15—C16—C17	−0.7 (8)
N2—Cu1—P1—C13	−155.50 (17)	C15—C16—C17—C18	−0.3 (8)
P2^{i}—Cu1—P1—C13	78.15 (15)	C16—C17—C18—C19	0.9 (8)
N2—Cu1—N1—C26	177.6 (3)	C17—C18—C19—C14	−0.5 (7)
P2^{i}—Cu1—N1—C26	−79.6 (3)	C15—C14—C19—C18	−0.5 (6)
P1—Cu1—N1—C26	78.0 (3)	P2—C14—C19—C18	−179.7 (3)
N2—Cu1—N1—C30	5.9 (3)	C14—P2—C20—C21	36.8 (4)
P2^{i}—Cu1—N1—C30	108.7 (3)	C13—P2—C20—C21	142.6 (3)
P1—Cu1—N1—C30	−93.7 (3)	Cu1^{i}—P2—C20—C21	−87.1 (3)
N1—Cu1—N2—C35	176.5 (4)	C14—P2—C20—C25	−148.7 (3)
P2^{i}—Cu1—N2—C35	57.1 (3)	C13—P2—C20—C25	−42.9 (4)
P1—Cu1—N2—C35	−85.2 (3)	Cu1^{i}—P2—C20—C25	87.4 (3)
N1—Cu1—N2—C31	−3.0 (3)	C25—C20—C21—C22	0.2 (6)
P2^{i}—Cu1—N2—C31	−122.4 (2)	P2—C20—C21—C22	174.9 (4)
P1—Cu1—N2—C31	95.3 (3)	C20—C21—C22—C23	−1.0 (8)
C7—P1—C1—C6	146.7 (3)	C21—C22—C23—C24	0.9 (9)
C13—P1—C1—C6	36.9 (4)	C22—C23—C24—C25	−0.1 (10)
Cu1—P1—C1—C6	−90.7 (3)	C23—C24—C25—C20	−0.6 (8)
C7—P1—C1—C2	−41.4 (4)	C21—C20—C25—C24	0.6 (7)
C13—P1—C1—C2	−151.2 (3)	P2—C20—C25—C24	−173.9 (4)
Cu1—P1—C1—C2	81.3 (3)	C30—N1—C26—C27	−0.9 (6)
C6—C1—C2—C3	−0.1 (6)	Cu1—N1—C26—C27	−172.3 (3)
P1—C1—C2—C3	−172.2 (4)	N1—C26—C27—C28	1.0 (7)
C1—C2—C3—C4	0.0 (8)	C26—C27—C28—C29	0.0 (8)
C2—C3—C4—C5	0.2 (9)	C27—C28—C29—C30	−1.0 (8)
C3—C4—C5—C6	−0.3 (10)	C26—N1—C30—C29	−0.2 (6)
C2—C1—C6—C5	0.1 (6)	Cu1—N1—C30—C29	172.1 (3)

P1—C1—C6—C5	172.0 (4)	C26—N1—C30—C31	179.9 (3)
C4—C5—C6—C1	0.1 (8)	Cu1—N1—C30—C31	−7.8 (4)
C1—P1—C7—C8	137.7 (3)	C28—C29—C30—N1	1.1 (7)
C13—P1—C7—C8	−116.2 (3)	C28—C29—C30—C31	−179.0 (4)
Cu1—P1—C7—C8	23.2 (4)	C35—N2—C31—C32	−0.2 (6)
C1—P1—C7—C12	−41.8 (4)	Cu1—N2—C31—C32	179.3 (3)
C13—P1—C7—C12	64.4 (4)	C35—N2—C31—C30	−179.6 (4)
Cu1—P1—C7—C12	−156.3 (3)	Cu1—N2—C31—C30	−0.1 (4)
C12—C7—C8—C9	−0.5 (7)	N1—C30—C31—N2	5.2 (5)
P1—C7—C8—C9	−179.9 (4)	C29—C30—C31—N2	−174.7 (4)
C7—C8—C9—C10	0.1 (8)	N1—C30—C31—C32	−174.1 (4)
C8—C9—C10—C11	0.0 (8)	C29—C30—C31—C32	6.0 (6)
C9—C10—C11—C12	0.2 (8)	N2—C31—C32—C33	−0.9 (7)
C10—C11—C12—C7	−0.6 (7)	C30—C31—C32—C33	178.4 (5)
C8—C7—C12—C11	0.7 (6)	C31—C32—C33—C34	1.4 (8)
P1—C7—C12—C11	−179.8 (3)	C32—C33—C34—C35	−0.9 (8)
C14—P2—C13—P1	−85.4 (2)	C31—N2—C35—C34	0.8 (6)
C20—P2—C13—P1	170.2 (2)	Cu1—N2—C35—C34	−178.6 (3)
$Cu1^{i}$—P2—C13—P1	50.0 (3)	C33—C34—C35—N2	−0.3 (7)
C7—P1—C13—P2	48.3 (3)	C38—O1—C37—C36	175.7 (16)
C1—P1—C13—P2	155.7 (2)	C37—O1—C38—C39	160.8 (17)
Cu1—P1—C13—P2	−88.6 (2)	C38'—O1'—C37'—C36'	−160 (2)
C20—P2—C14—C15	−124.2 (4)	C37'—O1'—C38'—C39'	123 (2)
C13—P2—C14—C15	130.9 (3)		

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

Fig. 1


C33
C34
C35
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P1A
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C23