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Poly[di- μ_3 -chlorido-di- μ_2 -chlorido- $\{\mu_4$ - N,N,N',N' -tetrakis[(diphenylphosphanyl)methyl]benzene-1,4-diamine- $\kappa^4P:P':P'':P'''$ }]tetracopper(II)]

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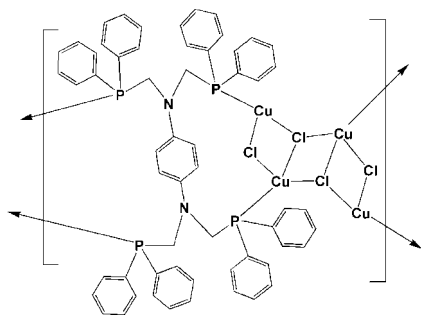
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.009$ Å; R factor = 0.054; wR factor = 0.143; data-to-parameter ratio = 16.4.

In the title complex, $[Cu_4Cl_4(C_{58}H_{52}N_2P_4)]_n$, four Cu^{II} atoms are held together *via* two doubly bridging and two triply bridging chlorides, forming a stair-like Cu_4Cl_4 core having crystallographically imposed inversion symmetry, while the benzene-1,4-diamine ligand (with a crystallographic inversion center at the centroid) acts in a tetradentate coordination mode, bridging two adjacent Cu_4Cl_4 cores, resulting in a chain along the a -axis direction. One Cu atom has a distorted tetrahedral geometry, coordinated by one P atom, one μ_2 -Cl and two μ_3 -Cl atoms, while the second Cu atom adopts a trigonal geometry, coordinated by one P atom, one μ_2 -Cl and one μ_3 -Cl atoms.

Related literature

For the structures and properties of Cu^I complexes containing polyphosphine ligands, see: Li *et al.* (2009); Kohl *et al.* (2006); Wang *et al.* (2008); Hou *et al.* (2011); Ni *et al.* (2011). For the synthesis of $Cu(I)$ complexes with diphosphine ligands, see: Saravanabharathi *et al.* (2002); Sivasankar *et al.* (2004).



Experimental

Crystal data

$[Cu_4Cl_4(C_{58}H_{52}N_2P_4)]_n$
 $M_r = 1296.86$
 Monoclinic, $P2_1/c$
 $a = 10.298$ (7) Å
 $b = 17.649$ (12) Å
 $c = 18.009$ (9) Å
 $\beta = 123.94$ (3)°

$V = 2715$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.90$ mm⁻¹
 $T = 296$ K
 $0.20 \times 0.15 \times 0.13$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 1998)
 $T_{min} = 0.852$, $T_{max} = 1.000$

15819 measured reflections
 5333 independent reflections
 3089 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.085$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$
 $wR(F^2) = 0.143$
 $S = 0.94$
 5333 reflections

325 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.70$ e Å⁻³
 $\Delta\rho_{min} = -0.62$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cu1—P1	2.1998 (19)	Cu2—P2 ⁱⁱ	2.188 (2)
Cu1—Cl2	2.3975 (19)	Cu2—Cl2	2.3062 (18)
Cu1—Cl1	2.4140 (17)	Cu2—Cl1	2.3255 (18)
Cu1—Cl1 ⁱ	2.565 (2)		

Symmetry codes: (i) $-x - 1, -y, -z + 1$; (ii) $-x, -y, -z + 1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: ZQ2150).

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supporting information

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Poly[di- μ_3 -chlorido-di- μ_2 -chlorido- $\{\mu_4$ - N,N,N',N' -tetrakis[(diphenylphosphanyl)methyl]benzene-1,4-diamine- $\kappa^4 P:P':P'':P'''$ }]tetracopper(II)]

Jia-Qin Liu, Yan Zhang, Ya-Jing Lü and Zhen-Jü Jiang

S1. Comment

Recently, Cu^I complexes containing multiphosphine ligands have received much attention so far due to their special structures, novel reactivity, as well as catalytic and luminescent properties (Kohl *et al.*, 2006; Wang *et al.*, 2008; Hou *et al.*, 2011; Ni *et al.*, 2011). However, synthesis of Cu^I complexes with tetraphosphine ligands have been virtually not explored, though a great number of Cu(I) complexes with diphosphines were reported (Saravanabharathi *et al.*, 2002; Sivasankar *et al.*, 2004; Li *et al.*, 2009). Herein, we report the synthesis and crystal structure of a new Cu^I complex with the tetrakis[(diphenylphosphanyl)methyl]benzene-1,4-diamine ligand (dpppda), the title complex [Cu₄Cl₄(dpppda)]_n.

The asymmetric unit of the title complex, [Cu₂Cl₂(C₂₉H₂₆NP₂)]_n, contains two copper ions, two chlorine atoms and one half of the N,N,N',N' -tetrakis[(diphenylphosphanyl)methyl]benzene-1,4-diamine ligand (dpppda). Four copper atoms are held together *via* two doubly bridging and two triply-bridging chlorides to form a stair-like Cu₄Cl₄ core having a crystallographically imposed centrosymmetry, while the N,N,N',N' -tetrakis[(diphenylphosphanyl)methyl]benzene-1,4-diamine ligand (with a crystallographic inversion center at the midpoint of the central phenyl ring) acts as a tetradentate coordination mode to bridge two adjacent Cu₄Cl₄ cores resulting in a one-dimensional chain. The structure of the title complex is analogous to the reported complex [Cu₄L₄(dpppda)] (Li *et al.*, 2009). Cu1 has a distorted tetrahedral geometry, coordinated by one P atom, one μ_2 -Cl and two μ_3 -Cl atoms, while Cu2 adopts a trigonal geometry, coordinated by one P atom, one μ_2 -Cl and one μ_3 -Cl atoms. The mean Cu—Cl and Cu—P bond distances are 2.40 (1) and 2.19 (2) Å, respectively.

S2. Experimental

CuCl (0.0198 g, 0.2 mmol) was added with stirring to a solution of N,N,N',N' -tetrakis[(diphenylphosphanyl)methyl]benzene-1,4-diamine (0.0900 g, 0.10 mmol) in DMF (5 ml), and the resulting solution was allowed to stir for 1 h at room temperature. Slow diffusion of diethyl ether into the solution give colourless block crystals suitable for X-ray analysis after three days.

S3. Refinement

All hydrogen atoms were generated geometrically with C—H distances of 0.93 Å (aromatic H atoms) and 0.97 Å (methylene H atoms) and refined with a riding model with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

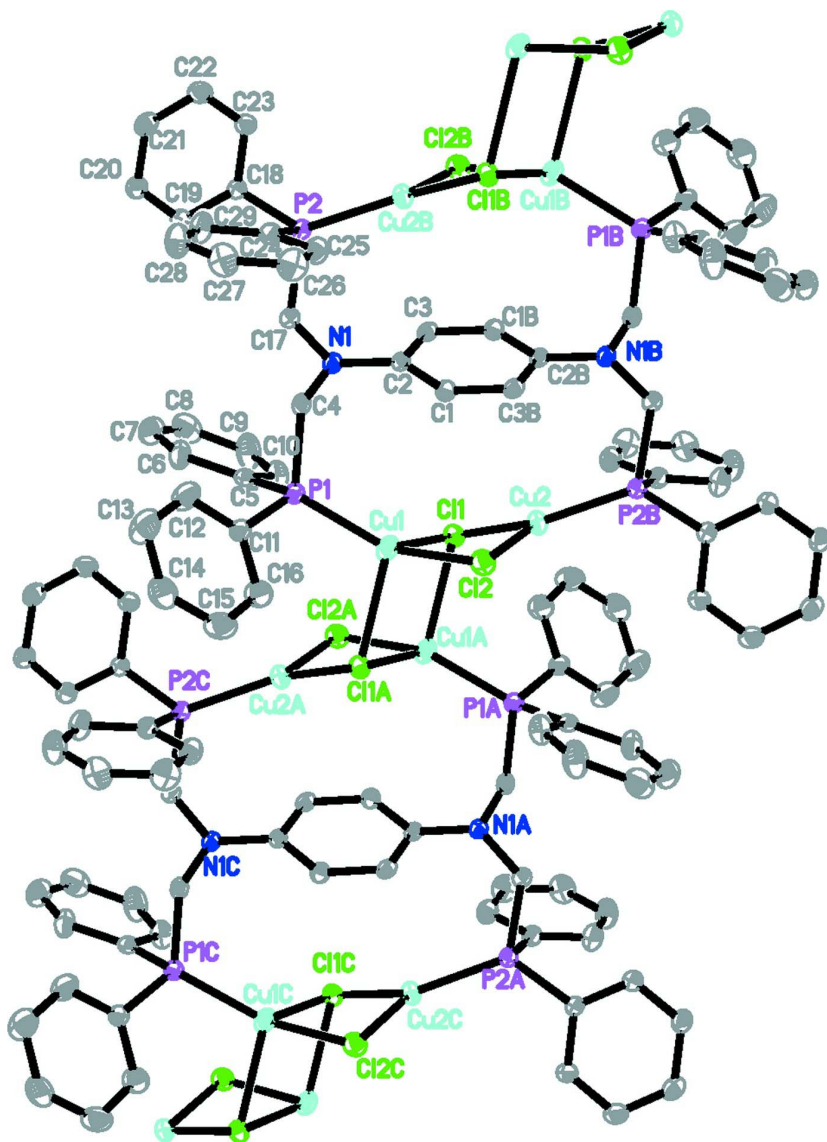


Figure 1

The structure of the title compound with displacement ellipsoids drawn at the 20% probability level. Hydrogen atoms are omitted for clarity. [symmetry code: (A) $1-x, -y, 1-z$; (B) $-x, -y, 1-z$; (C) $-1+x, y, z$.]

Poly[di- μ_3 -chlorido-di- μ_2 -chlorido- $\{\mu_4$ - N,N,N',N' - tetrakis[(diphenylphosphanyl)methyl]benzene-1,4-diamine- $\kappa^4P:P':P'':P'''$ }]tetracopper(II)]

Crystal data

$[\text{Cu}_4\text{Cl}_4(\text{C}_{58}\text{H}_{52}\text{N}_2\text{P}_4)]$

$M_r = 1296.86$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 10.298\ (7)\ \text{\AA}$

$b = 17.649\ (12)\ \text{\AA}$

$c = 18.009\ (9)\ \text{\AA}$

$\beta = 123.94\ (3)^\circ$

$V = 2715\ (3)\ \text{\AA}^3$

$Z = 2$

$F(000) = 1316$

$D_x = 1.586\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5682 reflections

$\theta = 2.8\text{--}26.3^\circ$

$\mu = 1.90\ \text{mm}^{-1}$

$T = 296$ K $0.20 \times 0.15 \times 0.13$ mm
 Block, colourless

Data collection

Bruker SMART CCD area-detector diffractometer	15819 measured reflections 5333 independent reflections
Radiation source: fine-focus sealed tube	3089 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\text{int}} = 0.085$
ω scans	$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 1.8^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$h = -12 \rightarrow 9$ $k = -19 \rightarrow 21$ $l = -21 \rightarrow 22$
$T_{\text{min}} = 0.852$, $T_{\text{max}} = 1.000$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H-atom parameters constrained
$wR(F^2) = 0.143$	$w = 1/[\sigma^2(F_o^2) + (0.P)^2]$
$S = 0.94$	where $P = (F_o^2 + 2F_c^2)/3$
5333 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
325 parameters	$\Delta\rho_{\text{max}} = 0.70 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.62 \text{ e } \text{\AA}^{-3}$
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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	-0.45394 (8)	0.04466 (4)	0.43168 (4)	0.0540 (2)
Cu2	-0.15464 (7)	0.07255 (4)	0.62081 (4)	0.0487 (2)
Cl1	-0.30501 (14)	-0.03659 (7)	0.56069 (8)	0.0417 (3)
Cl2	-0.32846 (15)	0.15805 (7)	0.51454 (9)	0.0526 (4)
P1	-0.52339 (15)	0.01608 (8)	0.29527 (8)	0.0402 (3)
P2	-0.07631 (15)	-0.08176 (7)	0.25371 (8)	0.0367 (3)
N1	-0.2438 (4)	-0.0268 (2)	0.3202 (2)	0.0397 (10)
C1	-0.1055 (6)	0.0562 (3)	0.4500 (3)	0.0370 (12)
H1A	-0.1767	0.0948	0.4172	0.044*
C2	-0.1233 (5)	-0.0133 (3)	0.4094 (3)	0.0336 (11)
C3	-0.0155 (6)	-0.0698 (3)	0.4619 (3)	0.0364 (11)
H3A	-0.0251	-0.1175	0.4372	0.044*
C4	-0.3712 (5)	0.0258 (3)	0.2699 (3)	0.0393 (12)
H4A	-0.4193	0.0173	0.2064	0.047*

H4B	-0.3304	0.0771	0.2835	0.047*
C5	-0.5742 (6)	-0.0830 (3)	0.2617 (3)	0.0430 (13)
C6	-0.6482 (7)	-0.1100 (4)	0.1736 (4)	0.0658 (18)
H6A	-0.6962	-0.0752	0.1269	0.079*
C7	-0.6531 (8)	-0.1842 (4)	0.1535 (5)	0.077 (2)
H7A	-0.7037	-0.1999	0.0943	0.092*
C8	-0.5818 (8)	-0.2361 (4)	0.2222 (5)	0.087 (2)
H8A	-0.5802	-0.2870	0.2094	0.104*
C9	-0.5123 (8)	-0.2134 (4)	0.3103 (4)	0.088 (2)
H9A	-0.4684	-0.2490	0.3562	0.105*
C10	-0.5089 (7)	-0.1380 (3)	0.3292 (4)	0.0647 (17)
H10A	-0.4619	-0.1230	0.3884	0.078*
C11	-0.6787 (6)	0.0772 (3)	0.2085 (3)	0.0481 (14)
C12	-0.7157 (8)	0.0836 (4)	0.1220 (4)	0.078 (2)
H12A	-0.6607	0.0545	0.1053	0.094*
C13	-0.8307 (9)	0.1312 (4)	0.0603 (4)	0.099 (3)
H13A	-0.8583	0.1319	0.0015	0.118*
C14	-0.9051 (8)	0.1783 (4)	0.0868 (5)	0.086 (2)
H14A	-0.9836	0.2108	0.0454	0.103*
C15	-0.8645 (7)	0.1776 (4)	0.1730 (5)	0.0743 (19)
H15A	-0.9118	0.2110	0.1910	0.089*
C16	-0.7513 (7)	0.1263 (3)	0.2341 (4)	0.0647 (17)
H16A	-0.7245	0.1253	0.2927	0.078*
C17	-0.2353 (5)	-0.0931 (3)	0.2727 (3)	0.0402 (12)
H17A	-0.3346	-0.0990	0.2156	0.048*
H17B	-0.2165	-0.1385	0.3077	0.048*
C18	-0.1096 (5)	-0.1626 (2)	0.1820 (3)	0.0352 (11)
C19	-0.2520 (6)	-0.1996 (3)	0.1284 (3)	0.0516 (14)
H19A	-0.3385	-0.1823	0.1271	0.062*
C20	-0.2680 (7)	-0.2612 (3)	0.0773 (4)	0.0551 (15)
H20A	-0.3647	-0.2849	0.0418	0.066*
C21	-0.1420 (7)	-0.2879 (3)	0.0785 (4)	0.0525 (14)
H21A	-0.1526	-0.3296	0.0441	0.063*
C22	-0.0008 (7)	-0.2525 (3)	0.1307 (4)	0.0548 (15)
H22A	0.0849	-0.2699	0.1312	0.066*
C23	0.0160 (6)	-0.1911 (3)	0.1827 (3)	0.0453 (13)
H23A	0.1138	-0.1685	0.2190	0.054*
C24	-0.1553 (6)	0.0012 (3)	0.1797 (3)	0.0430 (13)
C25	-0.1172 (7)	0.0719 (3)	0.2188 (4)	0.0545 (15)
H25A	-0.0423	0.0769	0.2798	0.065*
C26	-0.1918 (8)	0.1364 (3)	0.1661 (5)	0.0701 (19)
H26A	-0.1672	0.1840	0.1928	0.084*
C27	-0.2981 (8)	0.1301 (4)	0.0776 (4)	0.0710 (19)
H27A	-0.3477	0.1732	0.0435	0.085*
C28	-0.3334 (8)	0.0610 (4)	0.0378 (4)	0.0714 (19)
H28A	-0.4057	0.0570	-0.0237	0.086*
C29	-0.2629 (7)	-0.0035 (3)	0.0880 (4)	0.0607 (17)
H29A	-0.2878	-0.0505	0.0599	0.073*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0651 (5)	0.0619 (5)	0.0341 (4)	0.0056 (3)	0.0270 (4)	0.0001 (3)
Cu2	0.0389 (4)	0.0554 (4)	0.0406 (4)	-0.0038 (3)	0.0154 (3)	-0.0054 (3)
Cl1	0.0392 (7)	0.0407 (7)	0.0396 (7)	-0.0005 (5)	0.0187 (6)	0.0031 (5)
Cl2	0.0503 (8)	0.0430 (8)	0.0577 (9)	0.0049 (6)	0.0259 (7)	0.0008 (6)
P1	0.0376 (8)	0.0506 (9)	0.0318 (7)	0.0042 (6)	0.0190 (6)	0.0011 (6)
P2	0.0355 (7)	0.0419 (8)	0.0322 (7)	-0.0021 (6)	0.0185 (6)	-0.0041 (6)
N1	0.038 (2)	0.043 (2)	0.035 (2)	0.0018 (19)	0.018 (2)	-0.0083 (18)
C1	0.040 (3)	0.038 (3)	0.032 (3)	0.001 (2)	0.020 (2)	0.004 (2)
C2	0.035 (3)	0.039 (3)	0.029 (2)	-0.002 (2)	0.019 (2)	-0.001 (2)
C3	0.046 (3)	0.031 (3)	0.040 (3)	-0.006 (2)	0.030 (3)	-0.006 (2)
C4	0.041 (3)	0.048 (3)	0.026 (2)	-0.002 (2)	0.017 (2)	0.001 (2)
C5	0.035 (3)	0.055 (3)	0.047 (3)	-0.004 (2)	0.027 (3)	-0.008 (3)
C6	0.066 (4)	0.079 (5)	0.044 (3)	-0.022 (3)	0.026 (3)	-0.010 (3)
C7	0.083 (5)	0.070 (5)	0.087 (5)	-0.034 (4)	0.053 (4)	-0.037 (4)
C8	0.068 (5)	0.058 (4)	0.119 (7)	-0.011 (4)	0.044 (5)	-0.022 (5)
C9	0.088 (5)	0.063 (5)	0.066 (5)	0.000 (4)	0.014 (4)	0.005 (4)
C10	0.064 (4)	0.058 (4)	0.054 (4)	-0.006 (3)	0.021 (3)	0.000 (3)
C11	0.044 (3)	0.064 (4)	0.034 (3)	0.010 (3)	0.021 (3)	0.003 (2)
C12	0.093 (5)	0.090 (5)	0.047 (4)	0.045 (4)	0.037 (4)	0.017 (3)
C13	0.123 (7)	0.107 (6)	0.053 (4)	0.055 (5)	0.041 (5)	0.022 (4)
C14	0.065 (5)	0.106 (6)	0.064 (5)	0.027 (4)	0.021 (4)	0.022 (4)
C15	0.075 (5)	0.072 (5)	0.083 (5)	0.027 (4)	0.048 (4)	0.016 (4)
C16	0.064 (4)	0.070 (4)	0.057 (4)	0.018 (3)	0.032 (3)	0.015 (3)
C17	0.040 (3)	0.047 (3)	0.036 (3)	-0.001 (2)	0.023 (2)	-0.002 (2)
C18	0.038 (3)	0.034 (3)	0.034 (3)	0.000 (2)	0.020 (2)	-0.001 (2)
C19	0.043 (3)	0.058 (4)	0.053 (3)	-0.005 (3)	0.026 (3)	-0.017 (3)
C20	0.052 (4)	0.061 (4)	0.056 (4)	-0.018 (3)	0.033 (3)	-0.022 (3)
C21	0.068 (4)	0.043 (3)	0.056 (4)	-0.006 (3)	0.040 (3)	-0.011 (3)
C22	0.052 (4)	0.053 (4)	0.065 (4)	0.005 (3)	0.036 (3)	-0.007 (3)
C23	0.040 (3)	0.048 (3)	0.050 (3)	0.000 (2)	0.027 (3)	-0.007 (2)
C24	0.043 (3)	0.046 (3)	0.041 (3)	-0.004 (2)	0.025 (3)	-0.004 (2)
C25	0.062 (4)	0.048 (3)	0.053 (3)	-0.011 (3)	0.032 (3)	-0.009 (3)
C26	0.090 (5)	0.035 (3)	0.085 (5)	-0.005 (3)	0.048 (4)	-0.002 (3)
C27	0.077 (5)	0.056 (4)	0.068 (4)	0.006 (3)	0.033 (4)	0.021 (3)
C28	0.077 (5)	0.067 (5)	0.046 (4)	0.000 (3)	0.020 (3)	0.008 (3)
C29	0.074 (4)	0.048 (4)	0.046 (3)	-0.003 (3)	0.025 (3)	-0.004 (3)

Geometric parameters (\AA , $^\circ$)

Cu1—P1	2.1998 (19)	C10—H10A	0.9300
Cu1—Cl2	2.3975 (19)	C11—C16	1.381 (7)
Cu1—Cl1	2.4140 (17)	C11—C12	1.386 (8)
Cu1—Cl1 ⁱ	2.565 (2)	C12—C13	1.369 (8)
Cu2—P2 ⁱⁱ	2.188 (2)	C12—H12A	0.9300
Cu2—Cl2	2.3062 (18)	C13—C14	1.382 (9)

Cu2—C11	2.3255 (18)	C13—H13A	0.9300
C11—Cu1 ⁱ	2.565 (2)	C14—C15	1.364 (9)
P1—C5	1.828 (5)	C14—H14A	0.9300
P1—C11	1.837 (5)	C15—C16	1.399 (7)
P1—C4	1.869 (5)	C15—H15A	0.9300
P2—C18	1.824 (5)	C16—H16A	0.9300
P2—C24	1.836 (5)	C17—H17A	0.9700
P2—C17	1.861 (5)	C17—H17B	0.9700
P2—Cu2 ⁱⁱ	2.188 (2)	C18—C23	1.381 (7)
N1—C2	1.397 (5)	C18—C19	1.389 (6)
N1—C4	1.442 (6)	C19—C20	1.374 (7)
N1—C17	1.479 (6)	C19—H19A	0.9300
C1—C3 ⁱⁱ	1.386 (6)	C20—C21	1.368 (8)
C1—C2	1.387 (6)	C20—H20A	0.9300
C1—H1A	0.9300	C21—C22	1.364 (7)
C2—C3	1.396 (6)	C21—H21A	0.9300
C3—C1 ⁱⁱ	1.386 (6)	C22—C23	1.378 (7)
C3—H3A	0.9300	C22—H22A	0.9300
C4—H4A	0.9700	C23—H23A	0.9300
C4—H4B	0.9700	C24—C25	1.378 (7)
C5—C10	1.400 (7)	C24—C29	1.386 (7)
C5—C6	1.405 (7)	C25—C26	1.404 (7)
C6—C7	1.352 (8)	C25—H25A	0.9300
C6—H6A	0.9300	C26—C27	1.342 (8)
C7—C8	1.377 (9)	C26—H26A	0.9300
C7—H7A	0.9300	C27—C28	1.358 (8)
C8—C9	1.387 (9)	C27—H27A	0.9300
C8—H8A	0.9300	C28—C29	1.380 (7)
C9—C10	1.368 (8)	C28—H28A	0.9300
C9—H9A	0.9300	C29—H29A	0.9300
P1—Cu1—C12	127.78 (6)	C16—C11—C12	117.7 (5)
P1—Cu1—C11	125.05 (7)	C16—C11—P1	117.4 (4)
C12—Cu1—C11	93.71 (7)	C12—C11—P1	124.5 (4)
P1—Cu1—C11 ⁱ	109.03 (6)	C13—C12—C11	122.2 (6)
C12—Cu1—C11 ⁱ	102.38 (6)	C13—C12—H12A	118.9
C11—Cu1—C11 ⁱ	91.68 (6)	C11—C12—H12A	118.9
P2 ⁱⁱ —Cu2—C12	134.50 (6)	C12—C13—C14	118.9 (7)
P2 ⁱⁱ —Cu2—C11	126.84 (6)	C12—C13—H13A	120.5
C12—Cu2—C11	98.57 (7)	C14—C13—H13A	120.5
Cu2—C11—Cu1	81.73 (6)	C15—C14—C13	120.7 (6)
Cu2—C11—Cu1 ⁱ	115.71 (6)	C15—C14—H14A	119.6
Cu1—C11—Cu1 ⁱ	88.32 (6)	C13—C14—H14A	119.6
Cu2—C12—Cu1	82.49 (7)	C14—C15—C16	119.5 (6)
C5—P1—C11	109.2 (2)	C14—C15—H15A	120.2
C5—P1—C4	97.5 (2)	C16—C15—H15A	120.2
C11—P1—C4	100.9 (2)	C11—C16—C15	120.8 (6)
C5—P1—Cu1	116.30 (18)	C11—C16—H16A	119.6

C11—P1—Cu1	113.65 (18)	C15—C16—H16A	119.6
C4—P1—Cu1	117.26 (16)	N1—C17—P2	111.4 (3)
C18—P2—C24	106.1 (2)	N1—C17—H17A	109.4
C18—P2—C17	102.1 (2)	P2—C17—H17A	109.4
C24—P2—C17	98.1 (2)	N1—C17—H17B	109.4
C18—P2—Cu2 ⁱⁱ	117.10 (16)	P2—C17—H17B	109.4
C24—P2—Cu2 ⁱⁱ	118.43 (17)	H17A—C17—H17B	108.0
C17—P2—Cu2 ⁱⁱ	112.24 (17)	C23—C18—C19	117.1 (4)
C2—N1—C4	121.7 (4)	C23—C18—P2	118.3 (4)
C2—N1—C17	119.9 (4)	C19—C18—P2	124.6 (4)
C4—N1—C17	118.2 (4)	C20—C19—C18	121.5 (5)
C3 ⁱⁱ —C1—C2	121.7 (4)	C20—C19—H19A	119.2
C3 ⁱⁱ —C1—H1A	119.1	C18—C19—H19A	119.2
C2—C1—H1A	119.1	C21—C20—C19	120.2 (5)
C1—C2—C3	117.0 (4)	C21—C20—H20A	119.9
C1—C2—N1	121.9 (4)	C19—C20—H20A	119.9
C3—C2—N1	121.1 (4)	C22—C21—C20	119.3 (5)
C1 ⁱⁱ —C3—C2	121.2 (4)	C22—C21—H21A	120.3
C1 ⁱⁱ —C3—H3A	119.4	C20—C21—H21A	120.3
C2—C3—H3A	119.4	C21—C22—C23	120.6 (5)
N1—C4—P1	112.3 (3)	C21—C22—H22A	119.7
N1—C4—H4A	109.1	C23—C22—H22A	119.7
P1—C4—H4A	109.1	C22—C23—C18	121.2 (5)
N1—C4—H4B	109.1	C22—C23—H23A	119.4
P1—C4—H4B	109.1	C18—C23—H23A	119.4
H4A—C4—H4B	107.9	C25—C24—C29	118.2 (5)
C10—C5—C6	116.0 (5)	C25—C24—P2	117.9 (4)
C10—C5—P1	117.8 (4)	C29—C24—P2	123.6 (4)
C6—C5—P1	125.0 (4)	C24—C25—C26	119.8 (5)
C7—C6—C5	123.2 (6)	C24—C25—H25A	120.1
C7—C6—H6A	118.4	C26—C25—H25A	120.1
C5—C6—H6A	118.4	C27—C26—C25	120.8 (5)
C6—C7—C8	118.8 (6)	C27—C26—H26A	119.6
C6—C7—H7A	120.6	C25—C26—H26A	119.6
C8—C7—H7A	120.6	C26—C27—C28	120.1 (6)
C7—C8—C9	120.8 (6)	C26—C27—H27A	120.0
C7—C8—H8A	119.6	C28—C27—H27A	120.0
C9—C8—H8A	119.6	C27—C28—C29	120.5 (6)
C10—C9—C8	119.4 (6)	C27—C28—H28A	119.8
C10—C9—H9A	120.3	C29—C28—H28A	119.8
C8—C9—H9A	120.3	C28—C29—C24	120.6 (5)
C9—C10—C5	121.7 (6)	C28—C29—H29A	119.7
C9—C10—H10A	119.1	C24—C29—H29A	119.7
C5—C10—H10A	119.1		

Symmetry codes: (i) $-x-1, -y, -z+1$; (ii) $-x, -y, -z+1$.